

# Generative Models in Finance

## Week 1: The Mathematics of Large Language Models

Cristopher Salvi  
Imperial College London

Spring 2026

# Overview

## 1 Statistical Language Modelling

# Overview

- 1 Statistical Language Modelling
- 2 Neural Networks as Function Approximators

# Overview

- 1 Statistical Language Modelling
- 2 Neural Networks as Function Approximators
- 3 Recurrent Neural Networks

# Overview

- ① Statistical Language Modelling
- ② Neural Networks as Function Approximators
- ③ Recurrent Neural Networks
- ④ The Transformer Architecture

# Overview

- ① Statistical Language Modelling
- ② Neural Networks as Function Approximators
- ③ Recurrent Neural Networks
- ④ The Transformer Architecture
- ⑤ Scaling Laws

[Reference:](#) M. R. Douglas, *Large Language Models*, arXiv:2307.05782, 2023.

# Part 1: Statistical Language Modelling

**Goal:** Build a mathematical framework for the problem of modelling natural language with probability distributions.

- What is language modelling?

# Part 1: Statistical Language Modelling

**Goal:** Build a mathematical framework for the problem of modelling natural language with probability distributions.

- What is language modelling?
- The chain rule decomposition



# Part 1: Statistical Language Modelling

**Goal:** Build a mathematical framework for the problem of modelling natural language with probability distributions.

- What is language modelling?
- The chain rule decomposition
- Tokenisation strategies

# Part 1: Statistical Language Modelling

**Goal:** Build a mathematical framework for the problem of modelling natural language with probability distributions.

- What is language modelling?
- The chain rule decomposition
- Tokenisation strategies
- $N$ -gram models and their limitations

# Part 1: Statistical Language Modelling

**Goal:** Build a mathematical framework for the problem of modelling natural language with probability distributions.

- What is language modelling?
- The chain rule decomposition
- Tokenisation strategies
- $N$ -gram models and their limitations
- Evaluation via perplexity

# Part 1: Statistical Language Modelling

**Goal:** Build a mathematical framework for the problem of modelling natural language with probability distributions.

- What is language modelling?
- The chain rule decomposition
- Tokenisation strategies
- $N$ -gram models and their limitations
- Evaluation via perplexity
- Neural language models

# What is Language Modelling?

- A **language model** is a probability distribution over sequences of tokens (words, characters, or subwords)

# What is Language Modelling?

- A **language model** is a probability distribution over sequences of tokens (words, characters, or subwords)
- Given a **vocabulary**  $\mathcal{V} = \{v_1, v_2, \dots, v_{|\mathcal{V}|}\}$  (a finite set of tokens), a language model assigns a probability to every finite sequence  $(x_1, x_2, \dots, x_T) \in \mathcal{V}^T$

# What is Language Modelling?

- A **language model** is a probability distribution over sequences of tokens (words, characters, or subwords)
- Given a **vocabulary**  $\mathcal{V} = \{v_1, v_2, \dots, v_{|\mathcal{V}|}\}$  (a finite set of tokens), a language model assigns a probability to every finite sequence  $(x_1, x_2, \dots, x_T) \in \mathcal{V}^T$
- **Core tasks:**
  - ▶ *Estimation:* Given a sequence  $(x_1, \dots, x_T)$ , compute  $P(x_1, \dots, x_T)$
  - ▶ *Generation:* Sample new sequences from the learned distribution
  - ▶ *Next-token prediction:* Compute  $P(x_{t+1} \mid x_1, \dots, x_t)$

# What is Language Modelling?

- A **language model** is a probability distribution over sequences of tokens (words, characters, or subwords)
- Given a **vocabulary**  $\mathcal{V} = \{v_1, v_2, \dots, v_{|\mathcal{V}|}\}$  (a finite set of tokens), a language model assigns a probability to every finite sequence  $(x_1, x_2, \dots, x_T) \in \mathcal{V}^T$
- **Core tasks:**
  - ▶ *Estimation:* Given a sequence  $(x_1, \dots, x_T)$ , compute  $P(x_1, \dots, x_T)$
  - ▶ *Generation:* Sample new sequences from the learned distribution
  - ▶ *Next-token prediction:* Compute  $P(x_{t+1} \mid x_1, \dots, x_t)$
- Modern LLMs (GPT, LLaMA, Claude, etc.) are fundamentally **autoregressive language models**: they are trained to predict the next token given all preceding tokens



# The Chain Rule Decomposition

- By the [chain rule of probability](#), any joint distribution over a sequence can be factored as:

$$P(x_1, x_2, \dots, x_T) = \prod_{t=1}^T P(x_t \mid x_1, x_2, \dots, x_{t-1}) \quad (1.1)$$

# The Chain Rule Decomposition

- By the [chain rule of probability](#), any joint distribution over a sequence can be factored as:

$$P(x_1, x_2, \dots, x_T) = \prod_{t=1}^T P(x_t \mid x_1, x_2, \dots, x_{t-1}) \quad (1.1)$$

- This is an *exact* identity — no modelling assumptions have been made

# The Chain Rule Decomposition

- By the [chain rule of probability](#), any joint distribution over a sequence can be factored as:

$$P(x_1, x_2, \dots, x_T) = \prod_{t=1}^T P(x_t \mid x_1, x_2, \dots, x_{t-1}) \quad (1.1)$$

- This is an *exact* identity — no modelling assumptions have been made
- The entire language modelling problem thus reduces to modelling the [conditional distributions](#)

$$P(x_t \mid x_1, \dots, x_{t-1}) \quad \text{for each } t = 1, \dots, T$$

# The Chain Rule Decomposition

- By the [chain rule of probability](#), any joint distribution over a sequence can be factored as:

$$P(x_1, x_2, \dots, x_T) = \prod_{t=1}^T P(x_t \mid x_1, x_2, \dots, x_{t-1}) \quad (1.1)$$

- This is an *exact* identity — no modelling assumptions have been made
- The entire language modelling problem thus reduces to modelling the [conditional distributions](#)

$$P(x_t \mid x_1, \dots, x_{t-1}) \quad \text{for each } t = 1, \dots, T$$

- Convention:  $P(x_1 \mid x_0) := P(x_1)$  where  $x_0$  is a special start-of-sequence token

# The Chain Rule Decomposition

- By the **chain rule of probability**, any joint distribution over a sequence can be factored as:

$$P(x_1, x_2, \dots, x_T) = \prod_{t=1}^T P(x_t \mid x_1, x_2, \dots, x_{t-1}) \quad (1.1)$$

- This is an *exact* identity — no modelling assumptions have been made
- The entire language modelling problem thus reduces to modelling the **conditional distributions**

$$P(x_t \mid x_1, \dots, x_{t-1}) \quad \text{for each } t = 1, \dots, T$$

- Convention:  $P(x_1 \mid x_0) := P(x_1)$  where  $x_0$  is a special start-of-sequence token
- Key challenge:** The context  $(x_1, \dots, x_{t-1})$  can be arbitrarily long, making direct estimation intractable for large  $t$

# Tokenisation

- Before modelling, raw text must be converted into a sequence of elements from a fixed vocabulary  $\mathcal{V}$ . This process is called **tokenisation**

# Tokenisation

- Before modelling, raw text must be converted into a sequence of elements from a fixed vocabulary  $\mathcal{V}$ . This process is called **tokenisation**
- **Word-level tokenisation**: Each token is a word
  - ▶ Vocabulary can be very large ( $|\mathcal{V}| > 100,000$ )
  - ▶ Cannot handle out-of-vocabulary (OOV) words

# Tokenisation

- Before modelling, raw text must be converted into a sequence of elements from a fixed vocabulary  $\mathcal{V}$ . This process is called **tokenisation**
- **Word-level tokenisation:** Each token is a word
  - ▶ Vocabulary can be very large ( $|\mathcal{V}| > 100,000$ )
  - ▶ Cannot handle out-of-vocabulary (OOV) words
- **Character-level tokenisation:** Each token is a single character
  - ▶ Very small vocabulary ( $|\mathcal{V}| \approx 256$  for ASCII)
  - ▶ Sequences become very long, making modelling harder



# Tokenisation

- Before modelling, raw text must be converted into a sequence of elements from a fixed vocabulary  $\mathcal{V}$ . This process is called **tokenisation**
- **Word-level tokenisation**: Each token is a word
  - ▶ Vocabulary can be very large ( $|\mathcal{V}| > 100,000$ )
  - ▶ Cannot handle out-of-vocabulary (OOV) words
- **Character-level tokenisation**: Each token is a single character
  - ▶ Very small vocabulary ( $|\mathcal{V}| \approx 256$  for ASCII)
  - ▶ Sequences become very long, making modelling harder
- **Byte Pair Encoding (BPE)** (Sennrich et al., 2016): A data-driven subword method
  - 1 Start with character-level vocabulary
  - 2 Iteratively merge the most frequent pair of adjacent tokens into a new token
  - 3 Repeat until desired vocabulary size is reached

# Tokenisation

- Before modelling, raw text must be converted into a sequence of elements from a fixed vocabulary  $\mathcal{V}$ . This process is called **tokenisation**
- **Word-level tokenisation**: Each token is a word
  - ▶ Vocabulary can be very large ( $|\mathcal{V}| > 100,000$ )
  - ▶ Cannot handle out-of-vocabulary (OOV) words
- **Character-level tokenisation**: Each token is a single character
  - ▶ Very small vocabulary ( $|\mathcal{V}| \approx 256$  for ASCII)
  - ▶ Sequences become very long, making modelling harder
- **Byte Pair Encoding (BPE)** (Sennrich et al., 2016): A data-driven subword method
  - 1 Start with character-level vocabulary
  - 2 Iteratively merge the most frequent pair of adjacent tokens into a new token
  - 3 Repeat until desired vocabulary size is reached
- BPE provides a practical compromise:  $|\mathcal{V}| \approx 30,000\text{--}100,000$ , handles rare words via subword decomposition, and is used by most modern LLMs (GPT uses a variant with  $|\mathcal{V}| \approx 50,000$ )

# N-gram Language Models

- **Idea:** Approximate the conditional distribution by truncating the context to the most recent  $n - 1$  tokens (a **Markov assumption** of order  $n - 1$ ):

$$P(x_t \mid x_1, \dots, x_{t-1}) \approx P(x_t \mid x_{t-n+1}, \dots, x_{t-1}) \quad (1.2)$$

# N-gram Language Models

- **Idea:** Approximate the conditional distribution by truncating the context to the most recent  $n - 1$  tokens (a **Markov assumption** of order  $n - 1$ ):

$$P(x_t \mid x_1, \dots, x_{t-1}) \approx P(x_t \mid x_{t-n+1}, \dots, x_{t-1}) \quad (1.2)$$

- These conditional probabilities are estimated by **counting** from a training corpus:

$$\hat{P}(x_t \mid x_{t-n+1}, \dots, x_{t-1}) = \frac{\text{count}(x_{t-n+1}, \dots, x_t)}{\text{count}(x_{t-n+1}, \dots, x_{t-1})} \quad (1.3)$$

# N-gram Language Models

- **Idea:** Approximate the conditional distribution by truncating the context to the most recent  $n - 1$  tokens (a **Markov assumption** of order  $n - 1$ ):

$$P(x_t \mid x_1, \dots, x_{t-1}) \approx P(x_t \mid x_{t-n+1}, \dots, x_{t-1}) \quad (1.2)$$

- These conditional probabilities are estimated by **counting** from a training corpus:

$$\hat{P}(x_t \mid x_{t-n+1}, \dots, x_{t-1}) = \frac{\text{count}(x_{t-n+1}, \dots, x_t)}{\text{count}(x_{t-n+1}, \dots, x_{t-1})} \quad (1.3)$$

- **Curse of dimensionality:** The number of possible  $n$ -grams is  $|\mathcal{V}|^n$ 
  - ▶ For  $|\mathcal{V}| = 50,000$  and  $n = 5$ : there are  $50,000^5 \approx 3.1 \times 10^{23}$  possible 5-grams
  - ▶ Most  $n$ -grams will never appear in any finite corpus

# N-gram Language Models

- **Idea:** Approximate the conditional distribution by truncating the context to the most recent  $n - 1$  tokens (a **Markov assumption** of order  $n - 1$ ):

$$P(x_t \mid x_1, \dots, x_{t-1}) \approx P(x_t \mid x_{t-n+1}, \dots, x_{t-1}) \quad (1.2)$$

- These conditional probabilities are estimated by **counting** from a training corpus:

$$\hat{P}(x_t \mid x_{t-n+1}, \dots, x_{t-1}) = \frac{\text{count}(x_{t-n+1}, \dots, x_t)}{\text{count}(x_{t-n+1}, \dots, x_{t-1})} \quad (1.3)$$

- **Curse of dimensionality:** The number of possible  $n$ -grams is  $|\mathcal{V}|^n$ 
  - ▶ For  $|\mathcal{V}| = 50,000$  and  $n = 5$ : there are  $50,000^5 \approx 3.1 \times 10^{23}$  possible 5-grams
  - ▶ Most  $n$ -grams will never appear in any finite corpus
- In practice,  $n$ -gram models are limited to small  $n$  (typically  $n \leq 5$ ) and require **smoothing techniques** (e.g. Laplace smoothing, Kneser-Ney) to handle unseen  $n$ -grams

# N-gram Language Models

- **Idea:** Approximate the conditional distribution by truncating the context to the most recent  $n - 1$  tokens (a **Markov assumption** of order  $n - 1$ ):

$$P(x_t \mid x_1, \dots, x_{t-1}) \approx P(x_t \mid x_{t-n+1}, \dots, x_{t-1}) \quad (1.2)$$

- These conditional probabilities are estimated by **counting** from a training corpus:

$$\hat{P}(x_t \mid x_{t-n+1}, \dots, x_{t-1}) = \frac{\text{count}(x_{t-n+1}, \dots, x_t)}{\text{count}(x_{t-n+1}, \dots, x_{t-1})} \quad (1.3)$$

- **Curse of dimensionality:** The number of possible  $n$ -grams is  $|\mathcal{V}|^n$ 
  - ▶ For  $|\mathcal{V}| = 50,000$  and  $n = 5$ : there are  $50,000^5 \approx 3.1 \times 10^{23}$  possible 5-grams
  - ▶ Most  $n$ -grams will never appear in any finite corpus
- In practice,  $n$ -gram models are limited to small  $n$  (typically  $n \leq 5$ ) and require **smoothing techniques** (e.g. Laplace smoothing, Kneser-Ney) to handle unseen  $n$ -grams
- **Fundamental limitation:**  $N$ -gram models cannot capture long-range dependencies in language

# Evaluation: Cross-Entropy and Perplexity

- Let  $P$  be the true (unknown) distribution over sequences and  $Q$  be our model. The **cross-entropy** of  $Q$  relative to  $P$  is:

$$H(P, Q) = -\mathbb{E}_{X \sim P}[\log_2 Q(X)] = -\sum_x P(x) \log_2 Q(x) \quad (1.4)$$



# Evaluation: Cross-Entropy and Perplexity

- Let  $P$  be the true (unknown) distribution over sequences and  $Q$  be our model. The **cross-entropy** of  $Q$  relative to  $P$  is:

$$H(P, Q) = -\mathbb{E}_{X \sim P}[\log_2 Q(X)] = -\sum_x P(x) \log_2 Q(x) \quad (1.4)$$

- For a test corpus  $(x_1, \dots, x_T)$ , the per-token cross-entropy is estimated as:

$$\hat{H}(P, Q) = -\frac{1}{T} \sum_{t=1}^T \log_2 Q(x_t \mid x_1, \dots, x_{t-1}) \quad (1.5)$$

# Evaluation: Cross-Entropy and Perplexity

- Let  $P$  be the true (unknown) distribution over sequences and  $Q$  be our model. The **cross-entropy** of  $Q$  relative to  $P$  is:

$$H(P, Q) = -\mathbb{E}_{X \sim P}[\log_2 Q(X)] = -\sum_x P(x) \log_2 Q(x) \quad (1.4)$$

- For a test corpus  $(x_1, \dots, x_T)$ , the per-token cross-entropy is estimated as:

$$\hat{H}(P, Q) = -\frac{1}{T} \sum_{t=1}^T \log_2 Q(x_t \mid x_1, \dots, x_{t-1}) \quad (1.5)$$

- The **perplexity** is defined as:

$$\text{PP}(Q) = 2^{\hat{H}(P, Q)} = \left( \prod_{t=1}^T Q(x_t \mid x_1, \dots, x_{t-1}) \right)^{-1/T} \quad (1.6)$$

# Evaluation: Cross-Entropy and Perplexity

- Let  $P$  be the true (unknown) distribution over sequences and  $Q$  be our model. The **cross-entropy** of  $Q$  relative to  $P$  is:

$$H(P, Q) = -\mathbb{E}_{X \sim P}[\log_2 Q(X)] = -\sum_x P(x) \log_2 Q(x) \quad (1.4)$$

- For a test corpus  $(x_1, \dots, x_T)$ , the per-token cross-entropy is estimated as:

$$\hat{H}(P, Q) = -\frac{1}{T} \sum_{t=1}^T \log_2 Q(x_t \mid x_1, \dots, x_{t-1}) \quad (1.5)$$

- The **perplexity** is defined as:

$$\text{PP}(Q) = 2^{\hat{H}(P, Q)} = \left( \prod_{t=1}^T Q(x_t \mid x_1, \dots, x_{t-1}) \right)^{-1/T} \quad (1.6)$$

- Interpretation:** Perplexity is the (geometric) average number of equally likely tokens the model considers at each step. Lower perplexity = better model

# Evaluation: Cross-Entropy and Perplexity

- Let  $P$  be the true (unknown) distribution over sequences and  $Q$  be our model. The **cross-entropy** of  $Q$  relative to  $P$  is:

$$H(P, Q) = -\mathbb{E}_{X \sim P}[\log_2 Q(X)] = -\sum_x P(x) \log_2 Q(x) \quad (1.4)$$

- For a test corpus  $(x_1, \dots, x_T)$ , the per-token cross-entropy is estimated as:

$$\hat{H}(P, Q) = -\frac{1}{T} \sum_{t=1}^T \log_2 Q(x_t \mid x_1, \dots, x_{t-1}) \quad (1.5)$$

- The **perplexity** is defined as:

$$\text{PP}(Q) = 2^{\hat{H}(P, Q)} = \left( \prod_{t=1}^T Q(x_t \mid x_1, \dots, x_{t-1}) \right)^{-1/T} \quad (1.6)$$

- Interpretation:** Perplexity is the (geometric) average number of equally likely tokens the model considers at each step. Lower perplexity = better model
- A perfect model has  $\text{PP} = 1$ ; a uniform random model over  $\mathcal{V}$  has  $\text{PP} = |\mathcal{V}|$

# Neural Language Models

- **Key idea:** Replace the counting-based estimation (1.3) with a neural network  $P_\theta$  parameterised by  $\theta$ :

$$P_\theta(x_t \mid x_1, \dots, x_{t-1}) = \text{softmax}(f_\theta(x_1, \dots, x_{t-1}))_{x_t}$$

where  $f_\theta : \mathcal{V}^* \rightarrow \mathbb{R}^{|\mathcal{V}|}$  maps a context to a vector of **logits**

# Neural Language Models

- **Key idea:** Replace the counting-based estimation (1.3) with a neural network  $P_\theta$  parameterised by  $\theta$ :

$$P_\theta(x_t \mid x_1, \dots, x_{t-1}) = \text{softmax}(f_\theta(x_1, \dots, x_{t-1}))_{x_t}$$

where  $f_\theta : \mathcal{V}^* \rightarrow \mathbb{R}^{|\mathcal{V}|}$  maps a context to a vector of **logits**

- The **softmax** function converts logits  $z \in \mathbb{R}^{|\mathcal{V}|}$  to a probability distribution:

$$\text{softmax}(z)_i = \frac{e^{z_i}}{\sum_{j=1}^{|\mathcal{V}|} e^{z_j}}, \quad i = 1, \dots, |\mathcal{V}| \quad (1.7)$$

# Neural Language Models

- **Key idea:** Replace the counting-based estimation (1.3) with a neural network  $P_\theta$  parameterised by  $\theta$ :

$$P_\theta(x_t \mid x_1, \dots, x_{t-1}) = \text{softmax}(f_\theta(x_1, \dots, x_{t-1}))_{x_t}$$

where  $f_\theta : \mathcal{V}^* \rightarrow \mathbb{R}^{|\mathcal{V}|}$  maps a context to a vector of **logits**

- The **softmax** function converts logits  $z \in \mathbb{R}^{|\mathcal{V}|}$  to a probability distribution:

$$\text{softmax}(z)_i = \frac{e^{z_i}}{\sum_{j=1}^{|\mathcal{V}|} e^{z_j}}, \quad i = 1, \dots, |\mathcal{V}| \quad (1.7)$$

- The model is trained by minimising the **cross-entropy loss** over a training corpus:

$$\mathcal{L}(\theta) = -\frac{1}{N} \sum_{t=1}^N \log P_\theta(x_t \mid x_1, \dots, x_{t-1}) \quad (1.8)$$

# Neural Language Models

- **Key idea:** Replace the counting-based estimation (1.3) with a neural network  $P_\theta$  parameterised by  $\theta$ :

$$P_\theta(x_t \mid x_1, \dots, x_{t-1}) = \text{softmax}(f_\theta(x_1, \dots, x_{t-1}))_{x_t}$$

where  $f_\theta : \mathcal{V}^* \rightarrow \mathbb{R}^{|\mathcal{V}|}$  maps a context to a vector of **logits**

- The **softmax** function converts logits  $z \in \mathbb{R}^{|\mathcal{V}|}$  to a probability distribution:

$$\text{softmax}(z)_i = \frac{e^{z_i}}{\sum_{j=1}^{|\mathcal{V}|} e^{z_j}}, \quad i = 1, \dots, |\mathcal{V}| \quad (1.7)$$

- The model is trained by minimising the **cross-entropy loss** over a training corpus:

$$\mathcal{L}(\theta) = -\frac{1}{N} \sum_{t=1}^N \log P_\theta(x_t \mid x_1, \dots, x_{t-1}) \quad (1.8)$$

- **Advantages over  $n$ -grams:**

- ▶ Continuous representations allow generalisation to unseen contexts
- ▶ No fixed context window limitation (depending on architecture)
- ▶ The network  $f_\theta$  can be an RNN, Transformer, or other architecture



## Part 2: Neural Networks as Function Approximators

**Goal:** Review the mathematical foundations of feedforward neural networks and their approximation-theoretic properties.

- Feedforward architecture

## Part 2: Neural Networks as Function Approximators

**Goal:** Review the mathematical foundations of feedforward neural networks and their approximation-theoretic properties.

- Feedforward architecture
- Activation functions

## Part 2: Neural Networks as Function Approximators

**Goal:** Review the mathematical foundations of feedforward neural networks and their approximation-theoretic properties.

- Feedforward architecture
- Activation functions
- Universal Approximation Theorem

## Part 2: Neural Networks as Function Approximators

**Goal:** Review the mathematical foundations of feedforward neural networks and their approximation-theoretic properties.

- Feedforward architecture
- Activation functions
- Universal Approximation Theorem
- Depth efficiency

## Part 2: Neural Networks as Function Approximators

**Goal:** Review the mathematical foundations of feedforward neural networks and their approximation-theoretic properties.

- Feedforward architecture
- Activation functions
- Universal Approximation Theorem
- Depth efficiency
- SGD and backpropagation

## Part 2: Neural Networks as Function Approximators

**Goal:** Review the mathematical foundations of feedforward neural networks and their approximation-theoretic properties.

- Feedforward architecture
- Activation functions
- Universal Approximation Theorem
- Depth efficiency
- SGD and backpropagation
- Generalisation and double descent

# Feedforward Neural Networks

## Definition 1.1 (Feedforward Neural Network)

A *feedforward neural network* (FNN) with  $L$  layers is a function  $f : \mathbb{R}^{d_0} \rightarrow \mathbb{R}^{d_L}$  defined as:

$$f(\mathbf{x}) = W_L \sigma(W_{L-1} \sigma(\cdots \sigma(W_1 \mathbf{x} + \mathbf{b}_1) \cdots) + \mathbf{b}_{L-1}) + \mathbf{b}_L \quad (1.9)$$

where:

- $W_\ell \in \mathbb{R}^{d_\ell \times d_{\ell-1}}$  are *weight matrices*,  $\mathbf{b}_\ell \in \mathbb{R}^{d_\ell}$  are *bias vectors*
- $\sigma : \mathbb{R} \rightarrow \mathbb{R}$  is a nonlinear *activation function* applied element-wise
- $d_0$  is the input dimension,  $d_L$  is the output dimension
- $d_1, \dots, d_{L-1}$  are the *hidden layer widths*

# Feedforward Neural Networks

## Definition 1.1 (Feedforward Neural Network)

A *feedforward neural network* (FNN) with  $L$  layers is a function  $f : \mathbb{R}^{d_0} \rightarrow \mathbb{R}^{d_L}$  defined as:

$$f(\mathbf{x}) = W_L \sigma(W_{L-1} \sigma(\cdots \sigma(W_1 \mathbf{x} + \mathbf{b}_1) \cdots) + \mathbf{b}_{L-1}) + \mathbf{b}_L \quad (1.9)$$

where:

- $W_\ell \in \mathbb{R}^{d_\ell \times d_{\ell-1}}$  are *weight matrices*,  $\mathbf{b}_\ell \in \mathbb{R}^{d_\ell}$  are *bias vectors*
  - $\sigma : \mathbb{R} \rightarrow \mathbb{R}$  is a nonlinear *activation function* applied element-wise
  - $d_0$  is the input dimension,  $d_L$  is the output dimension
  - $d_1, \dots, d_{L-1}$  are the *hidden layer widths*
- 
- The parameters  $\theta = \{(W_\ell, \mathbf{b}_\ell)\}_{\ell=1}^L$  are learned from data
  - **Depth** = number of layers  $L$ ; **Width** =  $\max_\ell d_\ell$
  - Total number of parameters:  $\sum_{\ell=1}^L (d_\ell \cdot d_{\ell-1} + d_\ell)$



# Activation Functions

- Without nonlinear activations, a composition of affine maps is just another affine map — the network would have no more expressive power than linear regression

# Activation Functions

- Without nonlinear activations, a composition of affine maps is just another affine map — the network would have no more expressive power than linear regression
- Common choices of activation function  $\sigma$ :

# Activation Functions

- Without nonlinear activations, a composition of affine maps is just another affine map — the network would have no more expressive power than linear regression
- Common choices of activation function  $\sigma$ :
  - ▶ Sigmoid:  $\sigma(z) = \frac{1}{1 + e^{-z}} \in (0, 1)$
  - ▶ Hyperbolic tangent:  $\sigma(z) = \tanh(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}} \in (-1, 1)$
  - ▶ ReLU (Rectified Linear Unit):  $\sigma(z) = \max(0, z)$

# Activation Functions

- Without nonlinear activations, a composition of affine maps is just another affine map — the network would have no more expressive power than linear regression
- Common choices of activation function  $\sigma$ :
  - ▶ Sigmoid:  $\sigma(z) = \frac{1}{1 + e^{-z}} \in (0, 1)$
  - ▶ Hyperbolic tangent:  $\sigma(z) = \tanh(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}} \in (-1, 1)$
  - ▶ ReLU (Rectified Linear Unit):  $\sigma(z) = \max(0, z)$
- ReLU is the most widely used in practice due to:
  - ▶ Computational efficiency (no exponentials)
  - ▶ Mitigates the vanishing gradient problem (gradient is 1 for  $z > 0$ )

# Activation Functions

- **Without nonlinear activations**, a composition of affine maps is just another affine map — the network would have no more expressive power than linear regression
- Common choices of activation function  $\sigma$ :
  - ▶ **Sigmoid**:  $\sigma(z) = \frac{1}{1 + e^{-z}} \in (0, 1)$
  - ▶ **Hyperbolic tangent**:  $\sigma(z) = \tanh(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}} \in (-1, 1)$
  - ▶ **ReLU** (Rectified Linear Unit):  $\sigma(z) = \max(0, z)$
- **ReLU** is the most widely used in practice due to:
  - ▶ Computational efficiency (no exponentials)
  - ▶ Mitigates the vanishing gradient problem (gradient is 1 for  $z > 0$ )
- **Variants**: Leaky ReLU ( $\max(\alpha z, z)$  for small  $\alpha > 0$ ), GELU, SiLU/Swish ( $z \cdot \sigma(z)$ ) — used in modern Transformers

# Universal Approximation Theorem

## Theorem 1.2 (Universal Approximation — Cybenko 1989, Hornik 1991)

Let  $\sigma : \mathbb{R} \rightarrow \mathbb{R}$  be a continuous, non-constant, bounded activation function (e.g. sigmoid). Let  $K \subset \mathbb{R}^d$  be compact and let  $f \in C(K, \mathbb{R})$ . Then for every  $\varepsilon > 0$ , there exist  $N \in \mathbb{N}$ , weights  $W \in \mathbb{R}^{N \times d}$ ,  $\mathbf{v} \in \mathbb{R}^N$ , and biases  $\mathbf{b} \in \mathbb{R}^N$  such that

$$\sup_{\mathbf{x} \in K} \left| f(\mathbf{x}) - \sum_{i=1}^N v_i \sigma(\mathbf{w}_i^\top \mathbf{x} + b_i) \right| < \varepsilon \quad (1.10)$$

where  $\mathbf{w}_i^\top$  is the  $i$ -th row of  $W$ .

# Universal Approximation Theorem

## Theorem 1.2 (Universal Approximation — Cybenko 1989, Hornik 1991)

Let  $\sigma : \mathbb{R} \rightarrow \mathbb{R}$  be a continuous, non-constant, bounded activation function (e.g. sigmoid). Let  $K \subset \mathbb{R}^d$  be compact and let  $f \in C(K, \mathbb{R})$ . Then for every  $\varepsilon > 0$ , there exist  $N \in \mathbb{N}$ , weights  $W \in \mathbb{R}^{N \times d}$ ,  $\mathbf{v} \in \mathbb{R}^N$ , and biases  $\mathbf{b} \in \mathbb{R}^N$  such that

$$\sup_{\mathbf{x} \in K} \left| f(\mathbf{x}) - \sum_{i=1}^N v_i \sigma(\mathbf{w}_i^\top \mathbf{x} + b_i) \right| < \varepsilon \quad (1.10)$$

where  $\mathbf{w}_i^\top$  is the  $i$ -th row of  $W$ .

- A **single hidden layer** network with  $N$  sufficiently large neurons can approximate any continuous function on a compact set to arbitrary accuracy

# Universal Approximation Theorem

## Theorem 1.2 (Universal Approximation — Cybenko 1989, Hornik 1991)

Let  $\sigma : \mathbb{R} \rightarrow \mathbb{R}$  be a continuous, non-constant, bounded activation function (e.g. sigmoid). Let  $K \subset \mathbb{R}^d$  be compact and let  $f \in C(K, \mathbb{R})$ . Then for every  $\varepsilon > 0$ , there exist  $N \in \mathbb{N}$ , weights  $W \in \mathbb{R}^{N \times d}$ ,  $\mathbf{v} \in \mathbb{R}^N$ , and biases  $\mathbf{b} \in \mathbb{R}^N$  such that

$$\sup_{\mathbf{x} \in K} \left| f(\mathbf{x}) - \sum_{i=1}^N v_i \sigma(\mathbf{w}_i^\top \mathbf{x} + b_i) \right| < \varepsilon \quad (1.10)$$

where  $\mathbf{w}_i^\top$  is the  $i$ -th row of  $W$ .

- A **single hidden layer** network with  $N$  sufficiently large neurons can approximate any continuous function on a compact set to arbitrary accuracy
- **Caveat:** The theorem is an *existence* result — it says nothing about:
  - ▶ How large  $N$  needs to be (it may be exponentially large in  $d$ )
  - ▶ Whether gradient-based training will find the approximating parameters



# Depth Efficiency

- The Universal Approximation Theorem concerns *shallow* (single hidden layer) networks. A natural question: **does depth help?**

# Depth Efficiency

- The Universal Approximation Theorem concerns *shallow* (single hidden layer) networks. A natural question: **does depth help?**
- **Answer: Yes.** Deep networks can be **exponentially more parameter-efficient** than shallow ones for certain function classes

# Depth Efficiency

- The Universal Approximation Theorem concerns *shallow* (single hidden layer) networks. A natural question: **does depth help?**
- **Answer: Yes.** Deep networks can be **exponentially more parameter-efficient** than shallow ones for certain function classes
- Informally, there exist functions computable by a network of depth  $L$  with polynomial width, but any network of depth  $L - 1$  computing the same function requires exponential width

# Depth Efficiency

- The Universal Approximation Theorem concerns *shallow* (single hidden layer) networks. A natural question: **does depth help?**
- **Answer: Yes.** Deep networks can be **exponentially more parameter-efficient** than shallow ones for certain function classes
- Informally, there exist functions computable by a network of depth  $L$  with polynomial width, but any network of depth  $L - 1$  computing the same function requires exponential width
- **Intuition:** Deep networks compose features hierarchically
  - ▶ Layer 1: detect simple patterns (edges, basic motifs)
  - ▶ Layer 2: combine simple patterns into intermediate features
  - ▶ Layer  $L$ : combine all into complex, high-level representations

# Depth Efficiency

- The Universal Approximation Theorem concerns *shallow* (single hidden layer) networks. A natural question: **does depth help?**
- **Answer: Yes.** Deep networks can be **exponentially more parameter-efficient** than shallow ones for certain function classes
- Informally, there exist functions computable by a network of depth  $L$  with polynomial width, but any network of depth  $L - 1$  computing the same function requires exponential width
- **Intuition:** Deep networks compose features hierarchically
  - ▶ Layer 1: detect simple patterns (edges, basic motifs)
  - ▶ Layer 2: combine simple patterns into intermediate features
  - ▶ Layer  $L$ : combine all into complex, high-level representations
- This provides a theoretical justification for why modern architectures (including Transformers) use many layers rather than a single wide layer

# Depth Efficiency

- The Universal Approximation Theorem concerns *shallow* (single hidden layer) networks. A natural question: **does depth help?**
- **Answer: Yes.** Deep networks can be **exponentially more parameter-efficient** than shallow ones for certain function classes
- Informally, there exist functions computable by a network of depth  $L$  with polynomial width, but any network of depth  $L - 1$  computing the same function requires exponential width
- **Intuition:** Deep networks compose features hierarchically
  - ▶ Layer 1: detect simple patterns (edges, basic motifs)
  - ▶ Layer 2: combine simple patterns into intermediate features
  - ▶ Layer  $L$ : combine all into complex, high-level representations
- This provides a theoretical justification for why modern architectures (including Transformers) use many layers rather than a single wide layer
- **Telgarsky (2016):** For ReLU networks, there exist functions representable with  $O(L)$  parameters at depth  $L$  that require  $\Omega(2^{L/2})$  parameters at depth  $O(1)$

# Stochastic Gradient Descent and Backpropagation

- Given a loss function  $\mathcal{L}(\theta)$  (e.g. cross-entropy (1.8)), we seek  $\theta^* = \arg \min_{\theta} \mathcal{L}(\theta)$

# Stochastic Gradient Descent and Backpropagation

- Given a loss function  $\mathcal{L}(\theta)$  (e.g. cross-entropy (1.8)), we seek  $\theta^* = \arg \min_{\theta} \mathcal{L}(\theta)$
- Gradient descent (GD):

$$\theta_{k+1} = \theta_k - \eta \nabla_{\theta} \mathcal{L}(\theta_k)$$

where  $\eta > 0$  is the learning rate



# Stochastic Gradient Descent and Backpropagation

- Given a loss function  $\mathcal{L}(\theta)$  (e.g. cross-entropy (1.8)), we seek  $\theta^* = \arg \min_{\theta} \mathcal{L}(\theta)$
- **Gradient descent (GD):**

$$\theta_{k+1} = \theta_k - \eta \nabla_{\theta} \mathcal{L}(\theta_k)$$

where  $\eta > 0$  is the **learning rate**

- **Stochastic gradient descent (SGD):** Replace full gradient with an estimate from a random mini-batch  $\mathcal{B} \subset \{1, \dots, N\}$ :

$$\theta_{k+1} = \theta_k - \eta \cdot \frac{1}{|\mathcal{B}|} \sum_{i \in \mathcal{B}} \nabla_{\theta} \ell_i(\theta_k)$$

# Stochastic Gradient Descent and Backpropagation

- Given a loss function  $\mathcal{L}(\theta)$  (e.g. cross-entropy (1.8)), we seek  $\theta^* = \arg \min_{\theta} \mathcal{L}(\theta)$
- Gradient descent (GD):

$$\theta_{k+1} = \theta_k - \eta \nabla_{\theta} \mathcal{L}(\theta_k)$$

where  $\eta > 0$  is the **learning rate**

- Stochastic gradient descent (SGD)**: Replace full gradient with an estimate from a random mini-batch  $\mathcal{B} \subset \{1, \dots, N\}$ :

$$\theta_{k+1} = \theta_k - \eta \cdot \frac{1}{|\mathcal{B}|} \sum_{i \in \mathcal{B}} \nabla_{\theta} \ell_i(\theta_k)$$

- Backpropagation** (Rumelhart et al., 1986): An efficient algorithm to compute  $\nabla_{\theta} \mathcal{L}$  by applying the **chain rule** layer by layer, from output to input

# Stochastic Gradient Descent and Backpropagation

- Given a loss function  $\mathcal{L}(\theta)$  (e.g. cross-entropy (1.8)), we seek  $\theta^* = \arg \min_{\theta} \mathcal{L}(\theta)$
- Gradient descent (GD):

$$\theta_{k+1} = \theta_k - \eta \nabla_{\theta} \mathcal{L}(\theta_k)$$

where  $\eta > 0$  is the **learning rate**

- Stochastic gradient descent (SGD)**: Replace full gradient with an estimate from a random mini-batch  $\mathcal{B} \subset \{1, \dots, N\}$ :

$$\theta_{k+1} = \theta_k - \eta \cdot \frac{1}{|\mathcal{B}|} \sum_{i \in \mathcal{B}} \nabla_{\theta} \ell_i(\theta_k)$$

- Backpropagation** (Rumelhart et al., 1986): An efficient algorithm to compute  $\nabla_{\theta} \mathcal{L}$  by applying the **chain rule** layer by layer, from output to input
- Computational cost of backpropagation:  $O(|\theta|)$  per sample — the same order as a single forward pass

# Stochastic Gradient Descent and Backpropagation

- Given a loss function  $\mathcal{L}(\theta)$  (e.g. cross-entropy (1.8)), we seek  $\theta^* = \arg \min_{\theta} \mathcal{L}(\theta)$
- Gradient descent (GD):

$$\theta_{k+1} = \theta_k - \eta \nabla_{\theta} \mathcal{L}(\theta_k)$$

where  $\eta > 0$  is the **learning rate**

- Stochastic gradient descent (SGD)**: Replace full gradient with an estimate from a random mini-batch  $\mathcal{B} \subset \{1, \dots, N\}$ :

$$\theta_{k+1} = \theta_k - \eta \cdot \frac{1}{|\mathcal{B}|} \sum_{i \in \mathcal{B}} \nabla_{\theta} \ell_i(\theta_k)$$

- Backpropagation** (Rumelhart et al., 1986): An efficient algorithm to compute  $\nabla_{\theta} \mathcal{L}$  by applying the **chain rule** layer by layer, from output to input
- Computational cost of backpropagation:  $O(|\theta|)$  per sample — the same order as a single forward pass
- Modern optimisers**: Adam (Kingma & Ba, 2015) and variants, which adaptively scale learning rates per parameter

# Generalisation and the Double Descent Phenomenon

- **Classical statistical learning theory:** Test error  $\approx$  training error + complexity penalty. Overfitting occurs when the model is “too complex” relative to the training data

# Generalisation and the Double Descent Phenomenon

- **Classical statistical learning theory:** Test error  $\approx$  training error + complexity penalty. Overfitting occurs when the model is “too complex” relative to the training data
- **Puzzle:** Modern neural networks are heavily *overparameterised* (more parameters than training examples), yet they generalise well in practice

# Generalisation and the Double Descent Phenomenon

- **Classical statistical learning theory:** Test error  $\approx$  training error + complexity penalty. Overfitting occurs when the model is “too complex” relative to the training data
- **Puzzle:** Modern neural networks are heavily *overparameterised* (more parameters than training examples), yet they generalise well in practice
- **Double descent** (Belkin et al., 2019): As model complexity grows, test error follows a U-shaped curve (classical regime), but then *decreases again* beyond the interpolation threshold

# Generalisation and the Double Descent Phenomenon

- **Classical statistical learning theory:** Test error  $\approx$  training error + complexity penalty. Overfitting occurs when the model is “too complex” relative to the training data
- **Puzzle:** Modern neural networks are heavily *overparameterised* (more parameters than training examples), yet they generalise well in practice
- **Double descent** (Belkin et al., 2019): As model complexity grows, test error follows a U-shaped curve (classical regime), but then *decreases again* beyond the interpolation threshold
  - 1 **Underparameterised regime:** Classical bias-variance tradeoff applies
  - 2 **Interpolation threshold:** Model just barely fits training data — worst generalisation
  - 3 **Overparameterised regime:** Among all interpolating solutions, SGD finds one with *low complexity* (implicit regularisation), leading to good generalisation



# Generalisation and the Double Descent Phenomenon

- **Classical statistical learning theory:** Test error  $\approx$  training error + complexity penalty. Overfitting occurs when the model is “too complex” relative to the training data
- **Puzzle:** Modern neural networks are heavily *overparameterised* (more parameters than training examples), yet they generalise well in practice
- **Double descent** (Belkin et al., 2019): As model complexity grows, test error follows a U-shaped curve (classical regime), but then *decreases again* beyond the interpolation threshold
  - 1 **Underparameterised regime:** Classical bias-variance tradeoff applies
  - 2 **Interpolation threshold:** Model just barely fits training data — worst generalisation
  - 3 **Overparameterised regime:** Among all interpolating solutions, SGD finds one with *low complexity* (implicit regularisation), leading to good generalisation
- **Implications for LLMs:** Modern LLMs have billions of parameters (far exceeding training examples in many senses), yet they generalise remarkably well — this is consistent with the overparameterised regime of double descent

# Part 3: Recurrent Neural Networks

**Goal:** Introduce sequential architectures for language modelling and analyse their limitations.

- RNN architecture

# Part 3: Recurrent Neural Networks

**Goal:** Introduce sequential architectures for language modelling and analyse their limitations.

- RNN architecture
- Backpropagation through time

# Part 3: Recurrent Neural Networks

**Goal:** Introduce sequential architectures for language modelling and analyse their limitations.

- RNN architecture
- Backpropagation through time
- Vanishing and exploding gradients

## Part 3: Recurrent Neural Networks

**Goal:** Introduce sequential architectures for language modelling and analyse their limitations.

- RNN architecture
- Backpropagation through time
- Vanishing and exploding gradients
- Long Short-Term Memory (LSTM)

# Recurrent Neural Network (RNN) Architecture

## Definition 1.3 (Elman RNN)

A *recurrent neural network* processes a sequence  $(\mathbf{x}_1, \dots, \mathbf{x}_T)$  with  $\mathbf{x}_t \in \mathbb{R}^d$  via the recurrence:

$$\mathbf{h}_t = \sigma(W_h \mathbf{h}_{t-1} + W_x \mathbf{x}_t + \mathbf{b}_h) \quad (1.11)$$

$$\mathbf{y}_t = W_y \mathbf{h}_t + \mathbf{b}_y \quad (1.12)$$

where:

- $\mathbf{h}_t \in \mathbb{R}^{d_h}$  is the *hidden state* at time  $t$ , with  $\mathbf{h}_0 = \mathbf{0}$
- $W_h \in \mathbb{R}^{d_h \times d_h}$ ,  $W_x \in \mathbb{R}^{d_h \times d}$ ,  $W_y \in \mathbb{R}^{d_y \times d_h}$  are weight matrices
- $\sigma$  is an element-wise activation (typically  $\tanh$ )

# Recurrent Neural Network (RNN) Architecture

## Definition 1.3 (Elman RNN)

A *recurrent neural network* processes a sequence  $(\mathbf{x}_1, \dots, \mathbf{x}_T)$  with  $\mathbf{x}_t \in \mathbb{R}^d$  via the recurrence:

$$\mathbf{h}_t = \sigma(W_h \mathbf{h}_{t-1} + W_x \mathbf{x}_t + \mathbf{b}_h) \quad (1.11)$$

$$\mathbf{y}_t = W_y \mathbf{h}_t + \mathbf{b}_y \quad (1.12)$$

where:

- $\mathbf{h}_t \in \mathbb{R}^{d_h}$  is the *hidden state* at time  $t$ , with  $\mathbf{h}_0 = \mathbf{0}$
- $W_h \in \mathbb{R}^{d_h \times d_h}$ ,  $W_x \in \mathbb{R}^{d_h \times d}$ ,  $W_y \in \mathbb{R}^{d_y \times d_h}$  are weight matrices
- $\sigma$  is an element-wise activation (typically  $\tanh$ )
- The same parameters  $(W_h, W_x, W_y, \mathbf{b}_h, \mathbf{b}_y)$  are *shared across all time steps*

# Recurrent Neural Network (RNN) Architecture

## Definition 1.3 (Elman RNN)

A *recurrent neural network* processes a sequence  $(\mathbf{x}_1, \dots, \mathbf{x}_T)$  with  $\mathbf{x}_t \in \mathbb{R}^d$  via the recurrence:

$$\mathbf{h}_t = \sigma(W_h \mathbf{h}_{t-1} + W_x \mathbf{x}_t + \mathbf{b}_h) \quad (1.11)$$

$$\mathbf{y}_t = W_y \mathbf{h}_t + \mathbf{b}_y \quad (1.12)$$

where:

- $\mathbf{h}_t \in \mathbb{R}^{d_h}$  is the *hidden state* at time  $t$ , with  $\mathbf{h}_0 = \mathbf{0}$
- $W_h \in \mathbb{R}^{d_h \times d_h}$ ,  $W_x \in \mathbb{R}^{d_h \times d}$ ,  $W_y \in \mathbb{R}^{d_y \times d_h}$  are weight matrices
- $\sigma$  is an element-wise activation (typically  $\tanh$ )
- The same parameters ( $W_h, W_x, W_y, \mathbf{b}_h, \mathbf{b}_y$ ) are *shared across all time steps*
- The hidden state  $\mathbf{h}_t$  serves as a compressed summary of all past inputs  $(\mathbf{x}_1, \dots, \mathbf{x}_t)$  — a form of memory



# Recurrent Neural Network (RNN) Architecture

## Definition 1.3 (Elman RNN)

A *recurrent neural network* processes a sequence  $(\mathbf{x}_1, \dots, \mathbf{x}_T)$  with  $\mathbf{x}_t \in \mathbb{R}^d$  via the recurrence:

$$\mathbf{h}_t = \sigma(W_h \mathbf{h}_{t-1} + W_x \mathbf{x}_t + \mathbf{b}_h) \quad (1.11)$$

$$\mathbf{y}_t = W_y \mathbf{h}_t + \mathbf{b}_y \quad (1.12)$$

where:

- $\mathbf{h}_t \in \mathbb{R}^{d_h}$  is the *hidden state* at time  $t$ , with  $\mathbf{h}_0 = \mathbf{0}$
- $W_h \in \mathbb{R}^{d_h \times d_h}$ ,  $W_x \in \mathbb{R}^{d_h \times d}$ ,  $W_y \in \mathbb{R}^{d_y \times d_h}$  are weight matrices
- $\sigma$  is an element-wise activation (typically  $\tanh$ )
- The same parameters ( $W_h, W_x, W_y, \mathbf{b}_h, \mathbf{b}_y$ ) are *shared across all time steps*
- The hidden state  $\mathbf{h}_t$  serves as a compressed summary of all past inputs  $(\mathbf{x}_1, \dots, \mathbf{x}_t)$  — a form of memory
- For language modelling:  $\mathbf{y}_t$  produces logits, and  $\text{softmax}(\mathbf{y}_t)$  gives  $P_\theta(\mathbf{x}_{t+1} \mid \mathbf{x}_1, \dots, \mathbf{x}_t)$

# Backpropagation Through Time (BPTT)

- To train an RNN, we “unroll” the recurrence over  $T$  time steps and apply backpropagation to the resulting computational graph

# Backpropagation Through Time (BPTT)

- To train an RNN, we “unroll” the recurrence over  $T$  time steps and apply backpropagation to the resulting computational graph
- The loss for a sequence of length  $T$  is:

$$\mathcal{L} = \sum_{t=1}^T \ell_t(\mathbf{y}_t)$$

# Backpropagation Through Time (BPTT)

- To train an RNN, we “unroll” the recurrence over  $T$  time steps and apply backpropagation to the resulting computational graph
- The loss for a sequence of length  $T$  is:

$$\mathcal{L} = \sum_{t=1}^T \ell_t(\mathbf{y}_t)$$

- The gradient with respect to  $W_h$  involves a sum over time steps, each requiring a product of Jacobians:

$$\frac{\partial \mathcal{L}}{\partial W_h} = \sum_{t=1}^T \frac{\partial \ell_t}{\partial \mathbf{y}_t} \frac{\partial \mathbf{y}_t}{\partial \mathbf{h}_t} \left( \sum_{k=1}^t \prod_{j=k+1}^t \frac{\partial \mathbf{h}_j}{\partial \mathbf{h}_{j-1}} \cdot \frac{\partial \mathbf{h}_k}{\partial W_h} \right) \quad (1.13)$$

# Backpropagation Through Time (BPTT)

- To train an RNN, we “unroll” the recurrence over  $T$  time steps and apply backpropagation to the resulting computational graph
- The loss for a sequence of length  $T$  is:

$$\mathcal{L} = \sum_{t=1}^T \ell_t(\mathbf{y}_t)$$

- The gradient with respect to  $W_h$  involves a sum over time steps, each requiring a product of Jacobians:

$$\frac{\partial \mathcal{L}}{\partial W_h} = \sum_{t=1}^T \frac{\partial \ell_t}{\partial \mathbf{y}_t} \frac{\partial \mathbf{y}_t}{\partial \mathbf{h}_t} \left( \sum_{k=1}^t \prod_{j=k+1}^t \frac{\partial \mathbf{h}_j}{\partial \mathbf{h}_{j-1}} \cdot \frac{\partial \mathbf{h}_k}{\partial W_h} \right) \quad (1.13)$$

- The **key quantity** is the Jacobian product:

$$\prod_{j=k+1}^t \frac{\partial \mathbf{h}_j}{\partial \mathbf{h}_{j-1}} = \prod_{j=k+1}^t \text{diag}(\sigma'(\mathbf{z}_j)) \cdot W_h \quad (1.14)$$

where  $\mathbf{z}_j = W_h \mathbf{h}_{j-1} + W_x \mathbf{x}_j + \mathbf{b}_h$

# Vanishing and Exploding Gradients

- The Jacobian product (1.14) involves  $t - k$  matrix multiplications. As this product length grows:

# Vanishing and Exploding Gradients

- The Jacobian product (1.14) involves  $t - k$  matrix multiplications. As this product length grows:

- ▶ If  $\|W_h\|$  is “small”:  $\left\| \prod_{j=k+1}^t \frac{\partial \mathbf{h}_j}{\partial \mathbf{h}_{j-1}} \right\| \rightarrow 0$  exponentially fast  
 $\Rightarrow$  **vanishing gradients**
- ▶ If  $\|W_h\|$  is “large”:  $\left\| \prod_{j=k+1}^t \frac{\partial \mathbf{h}_j}{\partial \mathbf{h}_{j-1}} \right\| \rightarrow \infty$  exponentially fast  
 $\Rightarrow$  **exploding gradients**

# Vanishing and Exploding Gradients

- The Jacobian product (1.14) involves  $t - k$  matrix multiplications. As this product length grows:
  - ▶ If  $\|W_h\|$  is “small”:  $\left\| \prod_{j=k+1}^t \frac{\partial \mathbf{h}_j}{\partial \mathbf{h}_{j-1}} \right\| \rightarrow 0$  exponentially fast  
 $\Rightarrow$  **vanishing gradients**
  - ▶ If  $\|W_h\|$  is “large”:  $\left\| \prod_{j=k+1}^t \frac{\partial \mathbf{h}_j}{\partial \mathbf{h}_{j-1}} \right\| \rightarrow \infty$  exponentially fast  
 $\Rightarrow$  **exploding gradients**
- More precisely (Bengio et al., 1994): if  $\lambda_1$  is the largest singular value of  $W_h$  and  $\gamma = \max_z |\sigma'(z)|$ , then:

$$\left\| \prod_{j=k+1}^t \frac{\partial \mathbf{h}_j}{\partial \mathbf{h}_{j-1}} \right\| \leq (\gamma \cdot \lambda_1)^{t-k}$$



# Vanishing and Exploding Gradients

- The Jacobian product (1.14) involves  $t - k$  matrix multiplications. As this product length grows:
  - ▶ If  $\|W_h\|$  is “small”:  $\left\| \prod_{j=k+1}^t \frac{\partial \mathbf{h}_j}{\partial \mathbf{h}_{j-1}} \right\| \rightarrow 0$  exponentially fast  
 $\Rightarrow$  **vanishing gradients**
  - ▶ If  $\|W_h\|$  is “large”:  $\left\| \prod_{j=k+1}^t \frac{\partial \mathbf{h}_j}{\partial \mathbf{h}_{j-1}} \right\| \rightarrow \infty$  exponentially fast  
 $\Rightarrow$  **exploding gradients**
- More precisely (Bengio et al., 1994): if  $\lambda_1$  is the largest singular value of  $W_h$  and  $\gamma = \max_z |\sigma'(z)|$ , then:

$$\left\| \prod_{j=k+1}^t \frac{\partial \mathbf{h}_j}{\partial \mathbf{h}_{j-1}} \right\| \leq (\gamma \cdot \lambda_1)^{t-k}$$

- **Consequence:** Vanilla RNNs struggle to learn **long-range dependencies** — the gradient signal from distant time steps is lost

# Vanishing and Exploding Gradients

- The Jacobian product (1.14) involves  $t - k$  matrix multiplications. As this product length grows:

- ▶ If  $\|W_h\|$  is “small”:  $\left\| \prod_{j=k+1}^t \frac{\partial \mathbf{h}_j}{\partial \mathbf{h}_{j-1}} \right\| \rightarrow 0$  exponentially fast

⇒ **vanishing gradients**

- ▶ If  $\|W_h\|$  is “large”:  $\left\| \prod_{j=k+1}^t \frac{\partial \mathbf{h}_j}{\partial \mathbf{h}_{j-1}} \right\| \rightarrow \infty$  exponentially fast

⇒ **exploding gradients**

- More precisely (Bengio et al., 1994): if  $\lambda_1$  is the largest singular value of  $W_h$  and  $\gamma = \max_z |\sigma'(z)|$ , then:

$$\left\| \prod_{j=k+1}^t \frac{\partial \mathbf{h}_j}{\partial \mathbf{h}_{j-1}} \right\| \leq (\gamma \cdot \lambda_1)^{t-k}$$

- **Consequence:** Vanilla RNNs struggle to learn **long-range dependencies** — the gradient signal from distant time steps is lost
- **Exploding gradients** can be mitigated by *gradient clipping*:  $\mathbf{g} \leftarrow \mathbf{g} \cdot \min \left( 1, \frac{c}{\|\mathbf{g}\|} \right)$  for some threshold  $c > 0$

# Vanishing and Exploding Gradients

- The Jacobian product (1.14) involves  $t - k$  matrix multiplications. As this product length grows:

- ▶ If  $\|W_h\|$  is “small”:  $\left\| \prod_{j=k+1}^t \frac{\partial \mathbf{h}_j}{\partial \mathbf{h}_{j-1}} \right\| \rightarrow 0$  exponentially fast

⇒ **vanishing gradients**

- ▶ If  $\|W_h\|$  is “large”:  $\left\| \prod_{j=k+1}^t \frac{\partial \mathbf{h}_j}{\partial \mathbf{h}_{j-1}} \right\| \rightarrow \infty$  exponentially fast

⇒ **exploding gradients**

- More precisely (Bengio et al., 1994): if  $\lambda_1$  is the largest singular value of  $W_h$  and  $\gamma = \max_z |\sigma'(z)|$ , then:

$$\left\| \prod_{j=k+1}^t \frac{\partial \mathbf{h}_j}{\partial \mathbf{h}_{j-1}} \right\| \leq (\gamma \cdot \lambda_1)^{t-k}$$

- **Consequence:** Vanilla RNNs struggle to learn **long-range dependencies** — the gradient signal from distant time steps is lost
- **Exploding gradients** can be mitigated by *gradient clipping*:  $\mathbf{g} \leftarrow \mathbf{g} \cdot \min \left( 1, \frac{c}{\|\mathbf{g}\|} \right)$  for some threshold  $c > 0$
- **Vanishing gradients** require *architectural* solutions  $\Rightarrow$  LSTM, GRU

# Long Short-Term Memory (LSTM)

## Definition 1.4 (LSTM — Hochreiter & Schmidhuber, 1997)

An LSTM cell maintains a *cell state*  $\mathbf{c}_t$  and *hidden state*  $\mathbf{h}_t$  via:

$$\mathbf{f}_t = \sigma_g(W_f[\mathbf{h}_{t-1}, \mathbf{x}_t] + \mathbf{b}_f) \quad (\text{forget gate}) \quad (1.15)$$

$$\mathbf{i}_t = \sigma_g(W_i[\mathbf{h}_{t-1}, \mathbf{x}_t] + \mathbf{b}_i) \quad (\text{input gate}) \quad (1.16)$$

$$\tilde{\mathbf{c}}_t = \tanh(W_c[\mathbf{h}_{t-1}, \mathbf{x}_t] + \mathbf{b}_c) \quad (\text{candidate cell state}) \quad (1.17)$$

$$\mathbf{c}_t = \mathbf{f}_t \odot \mathbf{c}_{t-1} + \mathbf{i}_t \odot \tilde{\mathbf{c}}_t \quad (\text{cell state update}) \quad (1.18)$$

$$\mathbf{o}_t = \sigma_g(W_o[\mathbf{h}_{t-1}, \mathbf{x}_t] + \mathbf{b}_o) \quad (\text{output gate}) \quad (1.19)$$

$$\mathbf{h}_t = \mathbf{o}_t \odot \tanh(\mathbf{c}_t) \quad (\text{hidden state}) \quad (1.20)$$

where  $\sigma_g$  is the sigmoid function and  $\odot$  denotes element-wise (Hadamard) product.

# LSTM: Why It Addresses Vanishing Gradients

- The **cell state update** (1.18) is the key design:

$$\mathbf{c}_t = \mathbf{f}_t \odot \mathbf{c}_{t-1} + \mathbf{i}_t \odot \tilde{\mathbf{c}}_t$$

# LSTM: Why It Addresses Vanishing Gradients

- The **cell state update** (1.18) is the key design:

$$\mathbf{c}_t = \mathbf{f}_t \odot \mathbf{c}_{t-1} + \mathbf{i}_t \odot \tilde{\mathbf{c}}_t$$

- The gradient of  $\mathbf{c}_t$  with respect to  $\mathbf{c}_{t-1}$  is:

$$\frac{\partial \mathbf{c}_t}{\partial \mathbf{c}_{t-1}} = \text{diag}(\mathbf{f}_t) + (\text{other terms})$$

# LSTM: Why It Addresses Vanishing Gradients

- The **cell state update** (1.18) is the key design:

$$\mathbf{c}_t = \mathbf{f}_t \odot \mathbf{c}_{t-1} + \mathbf{i}_t \odot \tilde{\mathbf{c}}_t$$

- The gradient of  $\mathbf{c}_t$  with respect to  $\mathbf{c}_{t-1}$  is:

$$\frac{\partial \mathbf{c}_t}{\partial \mathbf{c}_{t-1}} = \text{diag}(\mathbf{f}_t) + (\text{other terms})$$

- When  $\mathbf{f}_t \approx \mathbf{1}$  (forget gate open), the gradient flows *unattenuated* through the cell state — this creates a “**gradient highway**” across time steps

# LSTM: Why It Addresses Vanishing Gradients

- The **cell state update** (1.18) is the key design:

$$\mathbf{c}_t = \mathbf{f}_t \odot \mathbf{c}_{t-1} + \mathbf{i}_t \odot \tilde{\mathbf{c}}_t$$

- The gradient of  $\mathbf{c}_t$  with respect to  $\mathbf{c}_{t-1}$  is:

$$\frac{\partial \mathbf{c}_t}{\partial \mathbf{c}_{t-1}} = \text{diag}(\mathbf{f}_t) + (\text{other terms})$$

- When  $\mathbf{f}_t \approx \mathbf{1}$  (forget gate open), the gradient flows *unattenuated* through the cell state — this creates a “**gradient highway**” across time steps
- The three gates provide **learnable control** over information flow:
  - ▶ **Forget gate**  $\mathbf{f}_t$ : controls what to erase from memory
  - ▶ **Input gate**  $\mathbf{i}_t$ : controls what new information to store
  - ▶ **Output gate**  $\mathbf{o}_t$ : controls what to expose as hidden state



# LSTM: Why It Addresses Vanishing Gradients

- The **cell state update** (1.18) is the key design:

$$\mathbf{c}_t = \mathbf{f}_t \odot \mathbf{c}_{t-1} + \mathbf{i}_t \odot \tilde{\mathbf{c}}_t$$

- The gradient of  $\mathbf{c}_t$  with respect to  $\mathbf{c}_{t-1}$  is:

$$\frac{\partial \mathbf{c}_t}{\partial \mathbf{c}_{t-1}} = \text{diag}(\mathbf{f}_t) + (\text{other terms})$$

- When  $\mathbf{f}_t \approx \mathbf{1}$  (forget gate open), the gradient flows *unattenuated* through the cell state — this creates a “**gradient highway**” across time steps
- The three gates provide **learnable control** over information flow:
  - ▶ **Forget gate**  $\mathbf{f}_t$ : controls what to erase from memory
  - ▶ **Input gate**  $\mathbf{i}_t$ : controls what new information to store
  - ▶ **Output gate**  $\mathbf{o}_t$ : controls what to expose as hidden state
- **Empirically**, LSTMs can learn dependencies over sequences of length  $\sim 1000$ , far exceeding vanilla RNNs ( $\sim 10$ – $20$  steps)

# Part 4: The Transformer Architecture

**Goal:** Develop the complete mathematical description of the Transformer — the architecture underlying modern LLMs.

- Motivation: limitations of recurrence

## Part 4: The Transformer Architecture

**Goal:** Develop the complete mathematical description of the Transformer — the architecture underlying modern LLMs.

- Motivation: limitations of recurrence
- Token embeddings and positional encodings

# Part 4: The Transformer Architecture

**Goal:** Develop the complete mathematical description of the Transformer — the architecture underlying modern LLMs.

- Motivation: limitations of recurrence
- Token embeddings and positional encodings
- Scaled dot-product attention

## Part 4: The Transformer Architecture

**Goal:** Develop the complete mathematical description of the Transformer — the architecture underlying modern LLMs.

- Motivation: limitations of recurrence
- Token embeddings and positional encodings
- Scaled dot-product attention
- Multi-head attention

## Part 4: The Transformer Architecture

**Goal:** Develop the complete mathematical description of the Transformer — the architecture underlying modern LLMs.

- Motivation: limitations of recurrence
- Token embeddings and positional encodings
- Scaled dot-product attention
- Multi-head attention
- Feedforward layers, residual connections, layer normalisation

## Part 4: The Transformer Architecture

**Goal:** Develop the complete mathematical description of the Transformer — the architecture underlying modern LLMs.

- Motivation: limitations of recurrence
- Token embeddings and positional encodings
- Scaled dot-product attention
- Multi-head attention
- Feedforward layers, residual connections, layer normalisation
- Computational complexity

## Part 4: The Transformer Architecture

**Goal:** Develop the complete mathematical description of the Transformer — the architecture underlying modern LLMs.

- Motivation: limitations of recurrence
- Token embeddings and positional encodings
- Scaled dot-product attention
- Multi-head attention
- Feedforward layers, residual connections, layer normalisation
- Computational complexity
- Expressivity and computational limitations



# Motivation: From Recurrence to Attention

- Limitations of RNNs/LSTMs for language modelling:

# Motivation: From Recurrence to Attention

- Limitations of RNNs/LSTMs for language modelling:
  - ① Sequential computation: Hidden states must be computed in order  $\mathbf{h}_1 \rightarrow \mathbf{h}_2 \rightarrow \dots \rightarrow \mathbf{h}_T$ . This prevents parallelisation across time steps during training

# Motivation: From Recurrence to Attention

- Limitations of RNNs/LSTMs for language modelling:
  - 1 Sequential computation: Hidden states must be computed in order  $\mathbf{h}_1 \rightarrow \mathbf{h}_2 \rightarrow \dots \rightarrow \mathbf{h}_T$ . This prevents parallelisation across time steps during training
  - 2 Information bottleneck: All past information must be compressed into a fixed-dimensional hidden state  $\mathbf{h}_t \in \mathbb{R}^{d_h}$

# Motivation: From Recurrence to Attention

- Limitations of RNNs/LSTMs for language modelling:
  - 1 Sequential computation: Hidden states must be computed in order  $\mathbf{h}_1 \rightarrow \mathbf{h}_2 \rightarrow \dots \rightarrow \mathbf{h}_T$ . This prevents parallelisation across time steps during training
  - 2 Information bottleneck: All past information must be compressed into a fixed-dimensional hidden state  $\mathbf{h}_t \in \mathbb{R}^{d_h}$
  - 3 Long-range dependencies: Despite LSTMs, capturing very long-range dependencies remains difficult in practice

# Motivation: From Recurrence to Attention

- Limitations of RNNs/LSTMs for language modelling:
  - ① Sequential computation: Hidden states must be computed in order  $\mathbf{h}_1 \rightarrow \mathbf{h}_2 \rightarrow \dots \rightarrow \mathbf{h}_T$ . This prevents parallelisation across time steps during training
  - ② Information bottleneck: All past information must be compressed into a fixed-dimensional hidden state  $\mathbf{h}_t \in \mathbb{R}^{d_h}$
  - ③ Long-range dependencies: Despite LSTMs, capturing very long-range dependencies remains difficult in practice
- The Transformer (Vaswani et al., 2017) replaces recurrence entirely with an attention mechanism:
  - ▶ Every position can directly attend to every other position
  - ▶ Computation is fully parallelisable over sequence positions
  - ▶ “Attention is All You Need”

# Motivation: From Recurrence to Attention

- Limitations of RNNs/LSTMs for language modelling:
  - ① Sequential computation: Hidden states must be computed in order  $\mathbf{h}_1 \rightarrow \mathbf{h}_2 \rightarrow \dots \rightarrow \mathbf{h}_T$ . This prevents parallelisation across time steps during training
  - ② Information bottleneck: All past information must be compressed into a fixed-dimensional hidden state  $\mathbf{h}_t \in \mathbb{R}^{d_h}$
  - ③ Long-range dependencies: Despite LSTMs, capturing very long-range dependencies remains difficult in practice
- The Transformer (Vaswani et al., 2017) replaces recurrence entirely with an attention mechanism:
  - ▶ Every position can directly attend to every other position
  - ▶ Computation is fully parallelisable over sequence positions
  - ▶ “Attention is All You Need”
- Result: Dramatically better scalability, enabling training on much larger datasets and models (billions of parameters)

# Token Embeddings and Positional Encodings

- Each token  $x_t \in \mathcal{V}$  is mapped to a continuous vector via a learned **embedding matrix**  $E \in \mathbb{R}^{|\mathcal{V}| \times d}$ :

$$\mathbf{e}_t = E_{x_t} \in \mathbb{R}^d$$

# Token Embeddings and Positional Encodings

- Each token  $x_t \in \mathcal{V}$  is mapped to a continuous vector via a learned **embedding matrix**  $E \in \mathbb{R}^{|\mathcal{V}| \times d}$ :

$$\mathbf{e}_t = E_{x_t} \in \mathbb{R}^d$$

- Problem:** Unlike RNNs, the Transformer processes all positions simultaneously — there is no inherent notion of sequential order



# Token Embeddings and Positional Encodings

- Each token  $x_t \in \mathcal{V}$  is mapped to a continuous vector via a learned **embedding matrix**  $E \in \mathbb{R}^{|\mathcal{V}| \times d}$ :

$$\mathbf{e}_t = E_{x_t} \in \mathbb{R}^d$$

- Problem:** Unlike RNNs, the Transformer processes all positions simultaneously — there is no inherent notion of sequential order
- Solution:** Add **positional encodings** to inject position information:

$$\mathbf{x}_t = \mathbf{e}_t + \mathbf{p}_t$$

# Token Embeddings and Positional Encodings

- Each token  $x_t \in \mathcal{V}$  is mapped to a continuous vector via a learned **embedding matrix**  $E \in \mathbb{R}^{|\mathcal{V}| \times d}$ :

$$\mathbf{e}_t = E_{x_t} \in \mathbb{R}^d$$

- Problem:** Unlike RNNs, the Transformer processes all positions simultaneously — there is no inherent notion of sequential order
- Solution:** Add **positional encodings** to inject position information:

$$\mathbf{x}_t = \mathbf{e}_t + \mathbf{p}_t$$

- Vaswani et al. use sinusoidal positional encodings:

$$\text{PE}(\text{pos}, 2i) = \sin\left(\frac{\text{pos}}{10000^{2i/d}}\right) \quad (1.21)$$

$$\text{PE}(\text{pos}, 2i + 1) = \cos\left(\frac{\text{pos}}{10000^{2i/d}}\right) \quad (1.22)$$

for position  $\text{pos} = 1, \dots, T$  and dimension  $i = 0, \dots, d/2 - 1$

# Token Embeddings and Positional Encodings

- Each token  $x_t \in \mathcal{V}$  is mapped to a continuous vector via a learned **embedding matrix**  $E \in \mathbb{R}^{|\mathcal{V}| \times d}$ :

$$\mathbf{e}_t = E_{x_t} \in \mathbb{R}^d$$

- Problem:** Unlike RNNs, the Transformer processes all positions simultaneously — there is no inherent notion of sequential order
- Solution:** Add **positional encodings** to inject position information:

$$\mathbf{x}_t = \mathbf{e}_t + \mathbf{p}_t$$

- Vaswani et al. use sinusoidal positional encodings:

$$\text{PE}(\text{pos}, 2i) = \sin\left(\frac{\text{pos}}{10000^{2i/d}}\right) \quad (1.21)$$

$$\text{PE}(\text{pos}, 2i + 1) = \cos\left(\frac{\text{pos}}{10000^{2i/d}}\right) \quad (1.22)$$

for position  $\text{pos} = 1, \dots, T$  and dimension  $i = 0, \dots, d/2 - 1$

- Property:** For any fixed offset  $k$ ,  $\text{PE}(\text{pos} + k)$  is a linear function of  $\text{PE}(\text{pos})$ , allowing the model to learn relative positional relationships

# Why Sinusoidal Positional Encodings?

- **The core problem:** the Transformer processes all tokens simultaneously (no recurrence). Without positional information, it cannot distinguish “the cat sat on the mat” from “mat the on sat cat the”

# Why Sinusoidal Positional Encodings?

- **The core problem:** the Transformer processes all tokens simultaneously (no recurrence). Without positional information, it cannot distinguish “the cat sat on the mat” from “mat the on sat cat the”
- **Why sines and cosines?** Think of how we write integers in binary: position  $5 = 101_2$ . The least significant bit flips every step, the next every 2, the next every 4. Each bit operates at a different *frequency*

# Why Sinusoidal Positional Encodings?

- **The core problem:** the Transformer processes all tokens simultaneously (no recurrence). Without positional information, it cannot distinguish “the cat sat on the mat” from “mat the on sat cat the”
- **Why sines and cosines?** Think of how we write integers in binary: position  $5 = 101_2$ . The least significant bit flips every step, the next every 2, the next every 4. Each bit operates at a different *frequency*
- Sinusoidal PE does the same but with *smooth* oscillations: dimension pair  $(2i, 2i+1)$  uses frequency  $\omega_i = 1/10000^{2i/d}$ 
  - ▶ Small  $i$ :  $\omega_i$  large  $\rightarrow$  fast oscillation  $\rightarrow$  distinguishes nearby positions
  - ▶ Large  $i$ :  $\omega_i$  small  $\rightarrow$  slow oscillation  $\rightarrow$  distinguishes distant positions

# Why Sinusoidal Positional Encodings?

- **The core problem:** the Transformer processes all tokens simultaneously (no recurrence). Without positional information, it cannot distinguish “the cat sat on the mat” from “mat the on sat cat the”
- **Why sines and cosines?** Think of how we write integers in binary: position  $5 = 101_2$ . The least significant bit flips every step, the next every 2, the next every 4. Each bit operates at a different *frequency*
- Sinusoidal PE does the same but with *smooth* oscillations: dimension pair  $(2i, 2i+1)$  uses frequency  $\omega_i = 1/10000^{2i/d}$ 
  - ▶ Small  $i$ :  $\omega_i$  large  $\rightarrow$  fast oscillation  $\rightarrow$  distinguishes nearby positions
  - ▶ Large  $i$ :  $\omega_i$  small  $\rightarrow$  slow oscillation  $\rightarrow$  distinguishes distant positions
- Together, the  $d/2$  frequencies give each position a *unique fingerprint*, just as  $d$  binary digits uniquely encode  $2^d$  integers — but continuously

# Relative Positions and Alternatives

- **Key property:** for any offset  $k$ ,  $\text{PE}(\text{pos} + k)$  is a linear function of  $\text{PE}(\text{pos})$  via a rotation:

$$\begin{pmatrix} \sin(\omega_i(\text{pos} + k)) \\ \cos(\omega_i(\text{pos} + k)) \end{pmatrix} = \begin{pmatrix} \cos(\omega_i k) & \sin(\omega_i k) \\ -\sin(\omega_i k) & \cos(\omega_i k) \end{pmatrix} \begin{pmatrix} \sin(\omega_i \text{pos}) \\ \cos(\omega_i \text{pos}) \end{pmatrix}$$

- ▶ The rotation matrix depends only on  $k$ , not on  $\text{pos}$
- ▶ So the model can learn to attend to relative positions via linear projections



# Relative Positions and Alternatives

- **Key property:** for any offset  $k$ ,  $\text{PE}(\text{pos} + k)$  is a linear function of  $\text{PE}(\text{pos})$  via a rotation:

$$\begin{pmatrix} \sin(\omega_i(\text{pos} + k)) \\ \cos(\omega_i(\text{pos} + k)) \end{pmatrix} = \begin{pmatrix} \cos(\omega_i k) & \sin(\omega_i k) \\ -\sin(\omega_i k) & \cos(\omega_i k) \end{pmatrix} \begin{pmatrix} \sin(\omega_i \text{pos}) \\ \cos(\omega_i \text{pos}) \end{pmatrix}$$

- ▶ The rotation matrix depends only on  $k$ , not on  $\text{pos}$
- ▶ So the model can learn to attend to relative positions via linear projections
- **Alternatives used in modern LLMs:**
  - ▶ **Learned embeddings** (GPT-2): a trainable vector per position. Simple but limited to the maximum training length
  - ▶ **RoPE** (Su et al., 2021): applies the rotation above directly to  $Q, K$ . Used in LLaMA, Mistral, and most modern LLMs
  - ▶ **ALiBi** (Press et al., 2022): no positional encoding; adds a linear bias  $-m|i - j|$  to attention logits

# Scaled Dot-Product Attention

## Definition 1.5 (Scaled Dot-Product Attention)

Given an input matrix  $X \in \mathbb{R}^{T \times d}$  (rows are token representations), define:

$$Q = XW_Q, \quad K = XW_K, \quad V = XW_V \quad (1.23)$$

where  $W_Q, W_K \in \mathbb{R}^{d \times d_k}$  and  $W_V \in \mathbb{R}^{d \times d_v}$  are learned projection matrices. The *scaled dot-product attention* is:

$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^\top}{\sqrt{d_k}}\right) V \quad (1.24)$$

where the softmax is applied row-wise.

# Scaled Dot-Product Attention

## Definition 1.5 (Scaled Dot-Product Attention)

Given an input matrix  $X \in \mathbb{R}^{T \times d}$  (rows are token representations), define:

$$Q = XW_Q, \quad K = XW_K, \quad V = XW_V \quad (1.23)$$

where  $W_Q, W_K \in \mathbb{R}^{d \times d_k}$  and  $W_V \in \mathbb{R}^{d \times d_v}$  are learned projection matrices. The *scaled dot-product attention* is:

$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^\top}{\sqrt{d_k}}\right) V \quad (1.24)$$

where the softmax is applied row-wise.

- $Q$  (queries): “what am I looking for?”
- $K$  (keys): “what do I contain?”
- $V$  (values): “what information do I provide?”

# Scaled Dot-Product Attention

## Definition 1.5 (Scaled Dot-Product Attention)

Given an input matrix  $X \in \mathbb{R}^{T \times d}$  (rows are token representations), define:

$$Q = XW_Q, \quad K = XW_K, \quad V = XW_V \quad (1.23)$$

where  $W_Q, W_K \in \mathbb{R}^{d \times d_k}$  and  $W_V \in \mathbb{R}^{d \times d_v}$  are learned projection matrices. The *scaled dot-product attention* is:

$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^\top}{\sqrt{d_k}}\right) V \quad (1.24)$$

where the softmax is applied row-wise.

- $Q$  (**queries**): “what am I looking for?”
- $K$  (**keys**): “what do I contain?”
- $V$  (**values**): “what information do I provide?”
- Row  $t$  of the output is a **weighted average** of all value vectors, where the weights are determined by the similarity of query  $t$  to all keys

## Why Scale by $\sqrt{d_k}$ ?

- Consider the dot product  $\mathbf{q}^\top \mathbf{k}$  where  $\mathbf{q}, \mathbf{k} \in \mathbb{R}^{d_k}$  with entries drawn independently from a distribution with mean 0 and variance 1

## Why Scale by $\sqrt{d_k}$ ?

- Consider the dot product  $\mathbf{q}^\top \mathbf{k}$  where  $\mathbf{q}, \mathbf{k} \in \mathbb{R}^{d_k}$  with entries drawn independently from a distribution with mean 0 and variance 1
- Then:

$$\mathbf{q}^\top \mathbf{k} = \sum_{i=1}^{d_k} q_i k_i \quad \Rightarrow \quad \mathbb{E}[\mathbf{q}^\top \mathbf{k}] = 0, \quad \text{Var}(\mathbf{q}^\top \mathbf{k}) = d_k$$

## Why Scale by $\sqrt{d_k}$ ?

- Consider the dot product  $\mathbf{q}^\top \mathbf{k}$  where  $\mathbf{q}, \mathbf{k} \in \mathbb{R}^{d_k}$  with entries drawn independently from a distribution with mean 0 and variance 1
- Then:

$$\mathbf{q}^\top \mathbf{k} = \sum_{i=1}^{d_k} q_i k_i \quad \Rightarrow \quad \mathbb{E}[\mathbf{q}^\top \mathbf{k}] = 0, \quad \text{Var}(\mathbf{q}^\top \mathbf{k}) = d_k$$

- For large  $d_k$ , the dot products  $\mathbf{q}^\top \mathbf{k}$  have large magnitude, pushing the softmax into **saturation regions** where gradients are extremely small

## Why Scale by $\sqrt{d_k}$ ?

- Consider the dot product  $\mathbf{q}^\top \mathbf{k}$  where  $\mathbf{q}, \mathbf{k} \in \mathbb{R}^{d_k}$  with entries drawn independently from a distribution with mean 0 and variance 1
- Then:

$$\mathbf{q}^\top \mathbf{k} = \sum_{i=1}^{d_k} q_i k_i \quad \Rightarrow \quad \mathbb{E}[\mathbf{q}^\top \mathbf{k}] = 0, \quad \text{Var}(\mathbf{q}^\top \mathbf{k}) = d_k$$

- For large  $d_k$ , the dot products  $\mathbf{q}^\top \mathbf{k}$  have large magnitude, pushing the softmax into **saturation regions** where gradients are extremely small
- Dividing by  $\sqrt{d_k}$  normalises the variance:

$$\text{Var}\left(\frac{\mathbf{q}^\top \mathbf{k}}{\sqrt{d_k}}\right) = \frac{d_k}{d_k} = 1$$



## Why Scale by $\sqrt{d_k}$ ?

- Consider the dot product  $\mathbf{q}^\top \mathbf{k}$  where  $\mathbf{q}, \mathbf{k} \in \mathbb{R}^{d_k}$  with entries drawn independently from a distribution with mean 0 and variance 1
- Then:

$$\mathbf{q}^\top \mathbf{k} = \sum_{i=1}^{d_k} q_i k_i \quad \Rightarrow \quad \mathbb{E}[\mathbf{q}^\top \mathbf{k}] = 0, \quad \text{Var}(\mathbf{q}^\top \mathbf{k}) = d_k$$

- For large  $d_k$ , the dot products  $\mathbf{q}^\top \mathbf{k}$  have large magnitude, pushing the softmax into **saturation regions** where gradients are extremely small
- Dividing by  $\sqrt{d_k}$  normalises the variance:

$$\text{Var}\left(\frac{\mathbf{q}^\top \mathbf{k}}{\sqrt{d_k}}\right) = \frac{d_k}{d_k} = 1$$

- This keeps the softmax inputs in a regime where the gradients are well-behaved, ensuring **stable training**

## Why Scale by $\sqrt{d_k}$ ?

- Consider the dot product  $\mathbf{q}^\top \mathbf{k}$  where  $\mathbf{q}, \mathbf{k} \in \mathbb{R}^{d_k}$  with entries drawn independently from a distribution with mean 0 and variance 1
- Then:

$$\mathbf{q}^\top \mathbf{k} = \sum_{i=1}^{d_k} q_i k_i \quad \Rightarrow \quad \mathbb{E}[\mathbf{q}^\top \mathbf{k}] = 0, \quad \text{Var}(\mathbf{q}^\top \mathbf{k}) = d_k$$

- For large  $d_k$ , the dot products  $\mathbf{q}^\top \mathbf{k}$  have large magnitude, pushing the softmax into **saturation regions** where gradients are extremely small
- Dividing by  $\sqrt{d_k}$  normalises the variance:

$$\text{Var}\left(\frac{\mathbf{q}^\top \mathbf{k}}{\sqrt{d_k}}\right) = \frac{d_k}{d_k} = 1$$

- This keeps the softmax inputs in a regime where the gradients are well-behaved, ensuring **stable training**
- Without scaling:** Attention weights tend to concentrate on a single key (near-one-hot), reducing the model's ability to attend to multiple positions simultaneously

# Causal Masking for Autoregressive Generation

- For **autoregressive language modelling**, position  $t$  must only attend to positions  $1, \dots, t$  (not future positions)

# Causal Masking for Autoregressive Generation

- For **autoregressive language modelling**, position  $t$  must only attend to positions  $1, \dots, t$  (not future positions)
- This is enforced via a **causal mask**: before applying softmax, set future entries to  $-\infty$ :

$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^\top}{\sqrt{d_k}} + M\right) V \quad (1.25)$$

where  $M \in \mathbb{R}^{T \times T}$  is the mask matrix:

$$M_{ij} = \begin{cases} 0 & \text{if } i \geq j \\ -\infty & \text{if } i < j \end{cases}$$

# Causal Masking for Autoregressive Generation

- For **autoregressive language modelling**, position  $t$  must only attend to positions  $1, \dots, t$  (not future positions)
- This is enforced via a **causal mask**: before applying softmax, set future entries to  $-\infty$ :

$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^\top}{\sqrt{d_k}} + M\right) V \quad (1.25)$$

where  $M \in \mathbb{R}^{T \times T}$  is the mask matrix:

$$M_{ij} = \begin{cases} 0 & \text{if } i \geq j \\ -\infty & \text{if } i < j \end{cases}$$

- After applying softmax, the  $-\infty$  entries become 0 (since  $e^{-\infty} = 0$ )

# Causal Masking for Autoregressive Generation

- For **autoregressive language modelling**, position  $t$  must only attend to positions  $1, \dots, t$  (not future positions)
- This is enforced via a **causal mask**: before applying softmax, set future entries to  $-\infty$ :

$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^\top}{\sqrt{d_k}} + M\right) V \quad (1.25)$$

where  $M \in \mathbb{R}^{T \times T}$  is the mask matrix:

$$M_{ij} = \begin{cases} 0 & \text{if } i \geq j \\ -\infty & \text{if } i < j \end{cases}$$

- After applying softmax, the  $-\infty$  entries become 0 (since  $e^{-\infty} = 0$ )
- **Result:** The output at position  $t$  depends only on tokens at positions  $\leq t$ , ensuring the autoregressive property:

$$P_\theta(x_t \mid x_1, \dots, x_{t-1})$$

# Causal Masking for Autoregressive Generation

- For **autoregressive language modelling**, position  $t$  must only attend to positions  $1, \dots, t$  (not future positions)
- This is enforced via a **causal mask**: before applying softmax, set future entries to  $-\infty$ :

$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^\top}{\sqrt{d_k}} + M\right) V \quad (1.25)$$

where  $M \in \mathbb{R}^{T \times T}$  is the mask matrix:

$$M_{ij} = \begin{cases} 0 & \text{if } i \geq j \\ -\infty & \text{if } i < j \end{cases}$$

- After applying softmax, the  $-\infty$  entries become 0 (since  $e^{-\infty} = 0$ )
- **Result:** The output at position  $t$  depends only on tokens at positions  $\leq t$ , ensuring the autoregressive property:

$$P_\theta(x_t \mid x_1, \dots, x_{t-1})$$

- **GPT-style models** (decoder-only Transformers) use causal masking throughout. This allows training on all positions simultaneously while respecting the autoregressive structure

# Multi-Head Attention

- A single attention head captures one type of relationship between tokens. **Multi-head attention** allows the model to jointly attend to information from different representation subspaces



# Multi-Head Attention

- A single attention head captures one type of relationship between tokens. **Multi-head attention** allows the model to jointly attend to information from different representation subspaces

## Definition 1.6 (Multi-Head Attention)

*Given  $h$  attention heads, the multi-head attention is:*

$$\text{MultiHead}(X) = \text{Concat}(\text{head}_1, \dots, \text{head}_h) W_O \quad (1.26)$$

$$\text{where } \text{head}_i = \text{Attention}(XW_Q^{(i)}, XW_K^{(i)}, XW_V^{(i)})$$

*with per-head projections  $W_Q^{(i)}, W_K^{(i)} \in \mathbb{R}^{d \times d_k}$ ,  $W_V^{(i)} \in \mathbb{R}^{d \times d_v}$ , and output projection  $W_O \in \mathbb{R}^{hd_v \times d}$ .*

# Multi-Head Attention

- A single attention head captures one type of relationship between tokens. **Multi-head attention** allows the model to jointly attend to information from different representation subspaces

## Definition 1.6 (Multi-Head Attention)

*Given  $h$  attention heads, the multi-head attention is:*

$$\text{MultiHead}(X) = \text{Concat}(\text{head}_1, \dots, \text{head}_h) W_O \quad (1.26)$$

$$\text{where } \text{head}_i = \text{Attention}(XW_Q^{(i)}, XW_K^{(i)}, XW_V^{(i)})$$

*with per-head projections  $W_Q^{(i)}, W_K^{(i)} \in \mathbb{R}^{d \times d_k}$ ,  $W_V^{(i)} \in \mathbb{R}^{d \times d_v}$ , and output projection  $W_O \in \mathbb{R}^{hd_v \times d}$ .*

- Typically  $d_k = d_v = d/h$ , so the total computational cost is similar to a single head with full dimensionality

# Multi-Head Attention

- A single attention head captures one type of relationship between tokens. **Multi-head attention** allows the model to jointly attend to information from different representation subspaces

## Definition 1.6 (Multi-Head Attention)

*Given  $h$  attention heads, the multi-head attention is:*

$$\text{MultiHead}(X) = \text{Concat}(\text{head}_1, \dots, \text{head}_h) W_O \quad (1.26)$$

$$\text{where } \text{head}_i = \text{Attention}(XW_Q^{(i)}, XW_K^{(i)}, XW_V^{(i)})$$

*with per-head projections  $W_Q^{(i)}, W_K^{(i)} \in \mathbb{R}^{d \times d_k}$ ,  $W_V^{(i)} \in \mathbb{R}^{d \times d_v}$ , and output projection  $W_O \in \mathbb{R}^{hd_v \times d}$ .*

- Typically  $d_k = d_v = d/h$ , so the total computational cost is similar to a single head with full dimensionality
- **Different heads can specialise:** e.g. one head may attend to syntactic structure, another to semantic similarity, another to positional proximity

# Position-wise Feedforward Network

- After multi-head attention, each position is independently processed by a **position-wise feedforward network** (the same network applied to every position):

$$\text{FFN}(\mathbf{x}) = W_2 \text{ReLU}(W_1 \mathbf{x} + \mathbf{b}_1) + \mathbf{b}_2 \quad (1.27)$$

where  $W_1 \in \mathbb{R}^{d_{\text{ff}} \times d}$ ,  $W_2 \in \mathbb{R}^{d \times d_{\text{ff}}}$ , and typically  $d_{\text{ff}} = 4d$

# Position-wise Feedforward Network

- After multi-head attention, each position is independently processed by a **position-wise feedforward network** (the same network applied to every position):

$$\text{FFN}(\mathbf{x}) = W_2 \text{ReLU}(W_1 \mathbf{x} + \mathbf{b}_1) + \mathbf{b}_2 \quad (1.27)$$

where  $W_1 \in \mathbb{R}^{d_{\text{ff}} \times d}$ ,  $W_2 \in \mathbb{R}^{d \times d_{\text{ff}}}$ , and typically  $d_{\text{ff}} = 4d$

- **Role:** The FFN acts as a **per-token nonlinear transformation**. It processes each token's representation independently (no interaction between positions)

# Position-wise Feedforward Network

- After multi-head attention, each position is independently processed by a **position-wise feedforward network** (the same network applied to every position):

$$\text{FFN}(\mathbf{x}) = W_2 \text{ReLU}(W_1 \mathbf{x} + \mathbf{b}_1) + \mathbf{b}_2 \quad (1.27)$$

where  $W_1 \in \mathbb{R}^{d_{\text{ff}} \times d}$ ,  $W_2 \in \mathbb{R}^{d \times d_{\text{ff}}}$ , and typically  $d_{\text{ff}} = 4d$

- **Role:** The FFN acts as a **per-token nonlinear transformation**. It processes each token's representation independently (no interaction between positions)
- The attention layer handles *cross-position* interactions; the FFN handles *within-position* computation

# Position-wise Feedforward Network

- After multi-head attention, each position is independently processed by a **position-wise feedforward network** (the same network applied to every position):

$$\text{FFN}(\mathbf{x}) = W_2 \text{ReLU}(W_1 \mathbf{x} + \mathbf{b}_1) + \mathbf{b}_2 \quad (1.27)$$

where  $W_1 \in \mathbb{R}^{d_{\text{ff}} \times d}$ ,  $W_2 \in \mathbb{R}^{d \times d_{\text{ff}}}$ , and typically  $d_{\text{ff}} = 4d$

- **Role:** The FFN acts as a **per-token nonlinear transformation**. It processes each token's representation independently (no interaction between positions)
- The attention layer handles *cross-position* interactions; the FFN handles *within-position* computation
- **Interpretation** (Geva et al., 2021): The FFN layers can be viewed as **key-value memories**, where the first layer computes pattern-matching scores and the second layer retrieves associated information

# Position-wise Feedforward Network

- After multi-head attention, each position is independently processed by a **position-wise feedforward network** (the same network applied to every position):

$$\text{FFN}(\mathbf{x}) = W_2 \text{ReLU}(W_1 \mathbf{x} + \mathbf{b}_1) + \mathbf{b}_2 \quad (1.27)$$

where  $W_1 \in \mathbb{R}^{d_{\text{ff}} \times d}$ ,  $W_2 \in \mathbb{R}^{d \times d_{\text{ff}}}$ , and typically  $d_{\text{ff}} = 4d$

- **Role:** The FFN acts as a **per-token nonlinear transformation**. It processes each token's representation independently (no interaction between positions)
- The attention layer handles *cross-position* interactions; the FFN handles *within-position* computation
- **Interpretation** (Geva et al., 2021): The FFN layers can be viewed as **key-value memories**, where the first layer computes pattern-matching scores and the second layer retrieves associated information
- Modern variants use **SwiGLU** (Shazeer, 2020) instead of ReLU:

$$\text{SwiGLU}(\mathbf{x}) = (\text{Swish}(W_1 \mathbf{x}) \odot W_3 \mathbf{x}) W_2$$



# Residual Connections

- **Problem:** stacking  $L$  layers means the gradient must pass through  $L$  composed nonlinear functions — the same vanishing gradient issue as in RNNs

# Residual Connections

- **Problem:** stacking  $L$  layers means the gradient must pass through  $L$  composed nonlinear functions — the same vanishing gradient issue as in RNNs
- **Residual connection** (He et al., 2016): instead of  $\mathbf{x}^{(\ell+1)} = F_\ell(\mathbf{x}^{(\ell)})$ , compute

$$\mathbf{x}^{(\ell+1)} = \mathbf{x}^{(\ell)} + F_\ell(\mathbf{x}^{(\ell)})$$

where  $F_\ell$  is the sub-layer (attention or FFN). The network only needs to learn a *correction*  $F_\ell$ , not the full mapping

# Residual Connections

- **Problem:** stacking  $L$  layers means the gradient must pass through  $L$  composed nonlinear functions — the same vanishing gradient issue as in RNNs
- **Residual connection** (He et al., 2016): instead of  $\mathbf{x}^{(\ell+1)} = F_\ell(\mathbf{x}^{(\ell)})$ , compute

$$\mathbf{x}^{(\ell+1)} = \mathbf{x}^{(\ell)} + F_\ell(\mathbf{x}^{(\ell)})$$

where  $F_\ell$  is the sub-layer (attention or FFN). The network only needs to learn a *correction*  $F_\ell$ , not the full mapping

- **Why this helps — a two-layer example.** Without residuals:

$$\mathbf{x}^{(2)} = F_2(F_1(\mathbf{x}^{(0)})) \quad \Rightarrow \quad \frac{\partial \mathbf{x}^{(2)}}{\partial \mathbf{x}^{(0)}} = \underbrace{J_{F_2}}_{\text{can be small}} \cdot \underbrace{J_{F_1}}_{\text{can be small}}$$

With residuals:

$$\begin{aligned} \mathbf{x}^{(2)} &= \mathbf{x}^{(0)} + F_1(\mathbf{x}^{(0)}) + F_2(\mathbf{x}^{(0)} + F_1(\mathbf{x}^{(0)})) \\ \Rightarrow \quad \frac{\partial \mathbf{x}^{(2)}}{\partial \mathbf{x}^{(0)}} &= \underbrace{I}_{\text{always present}} + J_{F_1} + J_{F_2}(I + J_{F_1}) \end{aligned}$$

# Residual Connections

- **Problem:** stacking  $L$  layers means the gradient must pass through  $L$  composed nonlinear functions — the same vanishing gradient issue as in RNNs
- **Residual connection** (He et al., 2016): instead of  $\mathbf{x}^{(\ell+1)} = F_\ell(\mathbf{x}^{(\ell)})$ , compute

$$\mathbf{x}^{(\ell+1)} = \mathbf{x}^{(\ell)} + F_\ell(\mathbf{x}^{(\ell)})$$

where  $F_\ell$  is the sub-layer (attention or FFN). The network only needs to learn a *correction*  $F_\ell$ , not the full mapping

- **Why this helps — a two-layer example.** Without residuals:

$$\mathbf{x}^{(2)} = F_2(F_1(\mathbf{x}^{(0)})) \quad \Rightarrow \quad \frac{\partial \mathbf{x}^{(2)}}{\partial \mathbf{x}^{(0)}} = \underbrace{J_{F_2}}_{\text{can be small}} \cdot \underbrace{J_{F_1}}_{\text{can be small}}$$

With residuals:

$$\begin{aligned} \mathbf{x}^{(2)} &= \mathbf{x}^{(0)} + F_1(\mathbf{x}^{(0)}) + F_2(\mathbf{x}^{(0)} + F_1(\mathbf{x}^{(0)})) \\ \Rightarrow \quad \frac{\partial \mathbf{x}^{(2)}}{\partial \mathbf{x}^{(0)}} &= \underbrace{I}_{\text{always present}} + J_{F_1} + J_{F_2}(I + J_{F_1}) \end{aligned}$$

- The  $I$  term guarantees the gradient is *at least* the identity — it cannot vanish to zero, regardless of how small  $J_{F_1}$  and  $J_{F_2}$  are

# Layer Normalisation: The Problem

- **Problem:** after many layers, the entries of  $\mathbf{x}^{(\ell)} \in \mathbb{R}^d$  can grow or shrink in scale. If some dimensions become very large, the softmax in attention saturates; if very small, information is lost

# Layer Normalisation: The Problem

- **Problem:** after many layers, the entries of  $\mathbf{x}^{(\ell)} \in \mathbb{R}^d$  can grow or shrink in scale. If some dimensions become very large, the softmax in attention saturates; if very small, information is lost
- **Concrete example:** suppose  $\mathbf{x} = (0.1, 200, -150, 0.3)^\top$ . The large entries dominate any dot product or linear transformation, making the network insensitive to the small entries

# Layer Normalisation: The Problem

- **Problem:** after many layers, the entries of  $\mathbf{x}^{(\ell)} \in \mathbb{R}^d$  can grow or shrink in scale. If some dimensions become very large, the softmax in attention saturates; if very small, information is lost
- **Concrete example:** suppose  $\mathbf{x} = (0.1, 200, -150, 0.3)^\top$ . The large entries dominate any dot product or linear transformation, making the network insensitive to the small entries
- **Solution:** before each sub-layer, re-centre and re-scale the representation to have zero mean and unit variance across the  $d$  dimensions:

$$\text{LayerNorm}(\mathbf{x}) = \gamma \odot \frac{\mathbf{x} - \mu}{\sqrt{\sigma^2 + \epsilon}} + \beta \quad (1.28)$$

- ▶  $\mu = \frac{1}{d} \sum_{i=1}^d x_i$  (mean across the  $d$  dimensions of this token)
- ▶  $\sigma^2 = \frac{1}{d} \sum_{i=1}^d (x_i - \mu)^2$  (variance across the  $d$  dimensions)
- ▶  $\gamma, \beta \in \mathbb{R}^d$  are *learnable* scale and shift parameters
- ▶  $\epsilon > 0$  is a small constant for numerical stability

# Layer Normalisation: The Problem

- **Problem:** after many layers, the entries of  $\mathbf{x}^{(\ell)} \in \mathbb{R}^d$  can grow or shrink in scale. If some dimensions become very large, the softmax in attention saturates; if very small, information is lost
- **Concrete example:** suppose  $\mathbf{x} = (0.1, 200, -150, 0.3)^\top$ . The large entries dominate any dot product or linear transformation, making the network insensitive to the small entries
- **Solution:** before each sub-layer, re-centre and re-scale the representation to have zero mean and unit variance across the  $d$  dimensions:

$$\text{LayerNorm}(\mathbf{x}) = \gamma \odot \frac{\mathbf{x} - \mu}{\sqrt{\sigma^2 + \epsilon}} + \beta \quad (1.28)$$

- ▶  $\mu = \frac{1}{d} \sum_{i=1}^d x_i$  (mean across the  $d$  dimensions of this token)
  - ▶  $\sigma^2 = \frac{1}{d} \sum_{i=1}^d (x_i - \mu)^2$  (variance across the  $d$  dimensions)
  - ▶  $\gamma, \beta \in \mathbb{R}^d$  are *learnable* scale and shift parameters
  - ▶  $\epsilon > 0$  is a small constant for numerical stability
- After normalisation:  $\mathbf{x} = (0.1, 200, -150, 0.3)^\top \rightarrow (-0.56, 1.13, -1.12, -0.55)^\top$  — all dimensions are now on a comparable scale



# Layer Normalisation: Where and Why

- **Key distinction from BatchNorm:** LayerNorm normalises across the *feature dimension  $d$*  (independently per token). BatchNorm normalises across the *batch dimension* (across different examples)

# Layer Normalisation: Where and Why

- **Key distinction from BatchNorm:** LayerNorm normalises across the *feature dimension  $d$*  (independently per token). BatchNorm normalises across the *batch dimension* (across different examples)
  - ▶ BatchNorm: statistics depend on what other examples are in the mini-batch
  - ▶ LayerNorm: statistics depend only on the token's own representation
  - ▶ For autoregressive generation (one token at a time, batch size 1), BatchNorm is ill-defined. LayerNorm works regardless of batch size

# Layer Normalisation: Where and Why

- **Key distinction from BatchNorm:** LayerNorm normalises across the *feature dimension*  $d$  (independently per token). BatchNorm normalises across the *batch dimension* (across different examples)
  - ▶ BatchNorm: statistics depend on what other examples are in the mini-batch
  - ▶ LayerNorm: statistics depend only on the token's own representation
  - ▶ For autoregressive generation (one token at a time, batch size 1), BatchNorm is ill-defined. LayerNorm works regardless of batch size
- **Where to place it?** Two conventions:
  - ▶ **Post-norm** (Vaswani et al., 2017):  $\mathbf{x} \leftarrow \text{LayerNorm}(\mathbf{x} + \text{SubLayer}(\mathbf{x}))$
  - ▶ **Pre-norm** (GPT-2 and later):  $\mathbf{x} \leftarrow \mathbf{x} + \text{SubLayer}(\text{LayerNorm}(\mathbf{x}))$

# Layer Normalisation: Where and Why

- **Key distinction from BatchNorm:** LayerNorm normalises across the *feature dimension  $d$*  (independently per token). BatchNorm normalises across the *batch dimension* (across different examples)
  - ▶ BatchNorm: statistics depend on what other examples are in the mini-batch
  - ▶ LayerNorm: statistics depend only on the token's own representation
  - ▶ For autoregressive generation (one token at a time, batch size 1), BatchNorm is ill-defined. **LayerNorm works regardless of batch size**
- **Where to place it?** Two conventions:
  - ▶ **Post-norm** (Vaswani et al., 2017):  $\mathbf{x} \leftarrow \text{LayerNorm}(\mathbf{x} + \text{SubLayer}(\mathbf{x}))$
  - ▶ **Pre-norm** (GPT-2 and later):  $\mathbf{x} \leftarrow \mathbf{x} + \text{SubLayer}(\text{LayerNorm}(\mathbf{x}))$
- **Why pre-norm is preferred:** in post-norm, the LayerNorm sits *on the residual path* — the gradient must pass through its Jacobian. In pre-norm, the residual path  $\mathbf{x} \rightarrow \mathbf{x}$  is clean — the gradient highway from the residual connection is unobstructed

# Layer Normalisation: Where and Why

- **Key distinction from BatchNorm:** LayerNorm normalises across the *feature dimension  $d$*  (independently per token). BatchNorm normalises across the *batch dimension* (across different examples)
  - ▶ BatchNorm: statistics depend on what other examples are in the mini-batch
  - ▶ LayerNorm: statistics depend only on the token's own representation
  - ▶ For autoregressive generation (one token at a time, batch size 1), BatchNorm is ill-defined. **LayerNorm works regardless of batch size**
- **Where to place it?** Two conventions:
  - ▶ **Post-norm** (Vaswani et al., 2017):  $\mathbf{x} \leftarrow \text{LayerNorm}(\mathbf{x} + \text{SubLayer}(\mathbf{x}))$
  - ▶ **Pre-norm** (GPT-2 and later):  $\mathbf{x} \leftarrow \mathbf{x} + \text{SubLayer}(\text{LayerNorm}(\mathbf{x}))$
- **Why pre-norm is preferred:** in post-norm, the LayerNorm sits *on the residual path* — the gradient must pass through its Jacobian. In pre-norm, the residual path  $\mathbf{x} \rightarrow \mathbf{x}$  is clean — the gradient highway from the residual connection is unobstructed
- **Modern variants:** RMSNorm (Zhang & Sennrich, 2019) drops the mean subtraction and uses only root-mean-square normalisation — slightly faster, used in LLaMA

# The Transformer Decoder Block

A single **Transformer decoder block** composes the following operations. Given input  $X \in \mathbb{R}^{T \times d}$ :

④ **Layer Norm + Causal Multi-Head Attention + Residual:**

$$X' = X + \text{MultiHead}(\text{LayerNorm}(X))$$

# The Transformer Decoder Block

A single **Transformer decoder block** composes the following operations. Given input  $X \in \mathbb{R}^{T \times d}$ :

- ① Layer Norm + Causal Multi-Head Attention + Residual:

$$X' = X + \text{MultiHead}(\text{LayerNorm}(X))$$

- ② Layer Norm + FFN + Residual:

$$X'' = X' + \text{FFN}(\text{LayerNorm}(X'))$$

# The Transformer Decoder Block

A single **Transformer decoder block** composes the following operations. Given input  $X \in \mathbb{R}^{T \times d}$ :

- ① **Layer Norm + Causal Multi-Head Attention + Residual:**

$$X' = X + \text{MultiHead}(\text{LayerNorm}(X))$$

- ② **Layer Norm + FFN + Residual:**

$$X'' = X' + \text{FFN}(\text{LayerNorm}(X'))$$

A full **decoder-only Transformer** (e.g. GPT) stacks  $L$  such blocks:

$$X^{(0)} = \text{TokenEmbed}(x_1, \dots, x_T) + \text{PosEncode}(1, \dots, T)$$

$$X^{(\ell)} = \text{TransformerBlock}_{\ell}(X^{(\ell-1)}), \quad \ell = 1, \dots, L$$

$$\mathbf{y}_t = W_{\text{out}} \text{LayerNorm}(X_t^{(L)})$$

$$P(x_{t+1} \mid x_{\leq t}) = \text{softmax}(\mathbf{y}_t)$$



# The Transformer Decoder Block

A single **Transformer decoder block** composes the following operations. Given input  $X \in \mathbb{R}^{T \times d}$ :

- ① **Layer Norm + Causal Multi-Head Attention + Residual:**

$$X' = X + \text{MultiHead}(\text{LayerNorm}(X))$$

- ② **Layer Norm + FFN + Residual:**

$$X'' = X' + \text{FFN}(\text{LayerNorm}(X'))$$

A full **decoder-only Transformer** (e.g. GPT) stacks  $L$  such blocks:

$$X^{(0)} = \text{TokenEmbed}(x_1, \dots, x_T) + \text{PosEncode}(1, \dots, T)$$

$$X^{(\ell)} = \text{TransformerBlock}_{\ell}(X^{(\ell-1)}), \quad \ell = 1, \dots, L$$

$$\mathbf{y}_t = W_{\text{out}} \text{LayerNorm}(X_t^{(L)})$$

$$P(x_{t+1} \mid x_{\leq t}) = \text{softmax}(\mathbf{y}_t)$$

**Example scales:** GPT-3 has  $L = 96$  layers,  $d = 12288$ ,  $h = 96$  heads,  $d_{\text{ff}} = 49152$ , totalling 175 billion parameters.

# Computational Complexity of the Transformer

- Let  $T$  = sequence length,  $d$  = model dimension,  $d_{ff}$  = FFN hidden dimension,  $h$  = number of heads,  $d_k = d/h$

# Computational Complexity of the Transformer

- Let  $T$  = sequence length,  $d$  = model dimension,  $d_{ff}$  = FFN hidden dimension,  $h$  = number of heads,  $d_k = d/h$
- Self-attention:
  - ▶ Computing  $QK^\top$ : matrix multiplication  $\mathbb{R}^{T \times d_k} \times \mathbb{R}^{d_k \times T}$  costs  $O(T^2 d_k)$
  - ▶ Over  $h$  heads and including value projection:  $O(T^2 d)$

# Computational Complexity of the Transformer

- Let  $T$  = sequence length,  $d$  = model dimension,  $d_{ff}$  = FFN hidden dimension,  $h$  = number of heads,  $d_k = d/h$
- Self-attention:
  - ▶ Computing  $QK^\top$ : matrix multiplication  $\mathbb{R}^{T \times d_k} \times \mathbb{R}^{d_k \times T}$  costs  $O(T^2 d_k)$
  - ▶ Over  $h$  heads and including value projection:  $O(T^2 d)$
- Feedforward network:
  - ▶ Two matrix multiplications:  $\mathbb{R}^{T \times d} \times \mathbb{R}^{d \times d_{ff}}$  and  $\mathbb{R}^{T \times d_{ff}} \times \mathbb{R}^{d_{ff} \times d}$
  - ▶ Total:  $O(T d d_{ff})$

# Computational Complexity of the Transformer

- Let  $T$  = sequence length,  $d$  = model dimension,  $d_{ff}$  = FFN hidden dimension,  $h$  = number of heads,  $d_k = d/h$
- Self-attention:
  - ▶ Computing  $QK^\top$ : matrix multiplication  $\mathbb{R}^{T \times d_k} \times \mathbb{R}^{d_k \times T}$  costs  $O(T^2 d_k)$
  - ▶ Over  $h$  heads and including value projection:  $O(T^2 d)$
- Feedforward network:
  - ▶ Two matrix multiplications:  $\mathbb{R}^{T \times d} \times \mathbb{R}^{d \times d_{ff}}$  and  $\mathbb{R}^{T \times d_{ff}} \times \mathbb{R}^{d_{ff} \times d}$
  - ▶ Total:  $O(T d d_{ff})$
- Memory for attention: Storing the  $T \times T$  attention matrix requires  $O(T^2)$  memory per head

# Computational Complexity of the Transformer

- Let  $T$  = sequence length,  $d$  = model dimension,  $d_{ff}$  = FFN hidden dimension,  $h$  = number of heads,  $d_k = d/h$
- Self-attention:
  - ▶ Computing  $QK^\top$ : matrix multiplication  $\mathbb{R}^{T \times d_k} \times \mathbb{R}^{d_k \times T}$  costs  $O(T^2 d_k)$
  - ▶ Over  $h$  heads and including value projection:  $O(T^2 d)$
- Feedforward network:
  - ▶ Two matrix multiplications:  $\mathbb{R}^{T \times d} \times \mathbb{R}^{d \times d_{ff}}$  and  $\mathbb{R}^{T \times d_{ff}} \times \mathbb{R}^{d_{ff} \times d}$
  - ▶ Total:  $O(T d d_{ff})$
- Memory for attention: Storing the  $T \times T$  attention matrix requires  $O(T^2)$  memory per head
- The  $O(T^2)$  scaling with sequence length is the primary bottleneck of the Transformer architecture:
  - ▶ GPT-3:  $T = 2048$ ; GPT-4:  $T = 8192$  (or 128,000 with extensions)
  - ▶ Techniques to mitigate: FlashAttention (hardware-aware), sparse attention, linear attention approximations

# The Quadratic Bottleneck: Training vs. Inference

- The  $O(T^2)$  cost of attention manifests differently in **training** vs. **inference**:

# The Quadratic Bottleneck: Training vs. Inference

- The  $O(T^2)$  cost of attention manifests differently in **training** vs. **inference**:
- **Training (parallel)**: All  $T$  tokens are known. The full  $T \times T$  attention matrix is computed in one batched matrix multiplication. This is *embarrassingly parallel* on GPUs — the bottleneck is memory, not serial computation



# The Quadratic Bottleneck: Training vs. Inference

- The  $O(T^2)$  cost of attention manifests differently in **training** vs. **inference**:
- **Training (parallel)**: All  $T$  tokens are known. The full  $T \times T$  attention matrix is computed in one batched matrix multiplication. This is *embarrassingly parallel* on GPUs — the bottleneck is memory, not serial computation
- **Inference (autoregressive)**: Tokens are generated one at a time. At step  $t$ , we need  $\mathbf{q}_t^\top \mathbf{k}_j$  for all  $j \leq t$ 
  - ▶ Naive: recompute all  $t$  dot products at each step  $\rightarrow$  total cost  $O(T^2d)$
  - ▶ **KV-cache**: store previously computed  $\mathbf{k}_j, \mathbf{v}_j$ . At step  $t$ , only compute  $\mathbf{q}_t$  and look up the cached keys/values  $\rightarrow$  cost per step is  $O(td)$ , total  $O(T^2d)$  but with much better constants

# The Quadratic Bottleneck: Training vs. Inference

- The  $O(T^2)$  cost of attention manifests differently in **training** vs. **inference**:
- **Training (parallel)**: All  $T$  tokens are known. The full  $T \times T$  attention matrix is computed in one batched matrix multiplication. This is *embarrassingly parallel* on GPUs — the bottleneck is memory, not serial computation
- **Inference (autoregressive)**: Tokens are generated one at a time. At step  $t$ , we need  $\mathbf{q}_t^\top \mathbf{k}_j$  for all  $j \leq t$ 
  - ▶ Naive: recompute all  $t$  dot products at each step  $\rightarrow$  total cost  $O(T^2d)$
  - ▶ **KV-cache**: store previously computed  $\mathbf{k}_j, \mathbf{v}_j$ . At step  $t$ , only compute  $\mathbf{q}_t$  and look up the cached keys/values  $\rightarrow$  cost per step is  $O(td)$ , total  $O(T^2d)$  but with much better constants
- **For long sequences** ( $T = 100,000+$ ), even the KV-cache becomes a memory bottleneck: storing  $T$  key-value pairs per layer per head

# The Quadratic Bottleneck: Training vs. Inference

- The  $O(T^2)$  cost of attention manifests differently in **training** vs. **inference**:
- **Training (parallel)**: All  $T$  tokens are known. The full  $T \times T$  attention matrix is computed in one batched matrix multiplication. This is *embarrassingly parallel* on GPUs — the bottleneck is memory, not serial computation
- **Inference (autoregressive)**: Tokens are generated one at a time. At step  $t$ , we need  $\mathbf{q}_t^\top \mathbf{k}_j$  for all  $j \leq t$ 
  - ▶ Naive: recompute all  $t$  dot products at each step  $\rightarrow$  total cost  $O(T^2d)$
  - ▶ **KV-cache**: store previously computed  $\mathbf{k}_j, \mathbf{v}_j$ . At step  $t$ , only compute  $\mathbf{q}_t$  and look up the cached keys/values  $\rightarrow$  cost per step is  $O(td)$ , total  $O(T^2d)$  but with much better constants
- **For long sequences** ( $T = 100,000+$ ), even the KV-cache becomes a memory bottleneck: storing  $T$  key-value pairs per layer per head
- **This motivates two lines of research**:
  - ① Efficient attention: reduce the  $O(T^2)$  cost while keeping the Transformer architecture
  - ② Alternative architectures: replace attention entirely with  $O(T)$  mechanisms

# Linear Attention

- **Key observation:** standard attention computes

$$\text{Attn}(Q, K, V)_t = \frac{\sum_{j=1}^t \exp(\mathbf{q}_t^\top \mathbf{k}_j) \mathbf{v}_j}{\sum_{j=1}^t \exp(\mathbf{q}_t^\top \mathbf{k}_j)}$$

The softmax couples all positions, preventing factorisation

# Linear Attention

- **Key observation:** standard attention computes

$$\text{Attn}(Q, K, V)_t = \frac{\sum_{j=1}^t \exp(\mathbf{q}_t^\top \mathbf{k}_j) \mathbf{v}_j}{\sum_{j=1}^t \exp(\mathbf{q}_t^\top \mathbf{k}_j)}$$

The softmax couples all positions, preventing factorisation

- **Linear attention** (Katharopoulos et al., 2020): replace  $\exp(\mathbf{q}^\top \mathbf{k})$  with a kernel  $\phi(\mathbf{q})^\top \phi(\mathbf{k})$  for some feature map  $\phi$ :

$$\text{LinAttn}(Q, K, V)_t = \frac{\phi(\mathbf{q}_t)^\top \sum_{j=1}^t \phi(\mathbf{k}_j) \mathbf{v}_j^\top}{\phi(\mathbf{q}_t)^\top \sum_{j=1}^t \phi(\mathbf{k}_j)}$$

# Linear Attention

- **Key observation:** standard attention computes

$$\text{Attn}(Q, K, V)_t = \frac{\sum_{j=1}^t \exp(\mathbf{q}_t^\top \mathbf{k}_j) \mathbf{v}_j}{\sum_{j=1}^t \exp(\mathbf{q}_t^\top \mathbf{k}_j)}$$

The softmax couples all positions, preventing factorisation

- **Linear attention** (Katharopoulos et al., 2020): replace  $\exp(\mathbf{q}^\top \mathbf{k})$  with a kernel  $\phi(\mathbf{q})^\top \phi(\mathbf{k})$  for some feature map  $\phi$ :

$$\text{LinAttn}(Q, K, V)_t = \frac{\phi(\mathbf{q}_t)^\top \sum_{j=1}^t \phi(\mathbf{k}_j) \mathbf{v}_j^\top}{\phi(\mathbf{q}_t)^\top \sum_{j=1}^t \phi(\mathbf{k}_j)}$$

- **The trick:** define  $\mathbf{S}_t = \sum_{j=1}^t \phi(\mathbf{k}_j) \mathbf{v}_j^\top \in \mathbb{R}^{d_k \times d_v}$  and  $\mathbf{z}_t = \sum_{j=1}^t \phi(\mathbf{k}_j) \in \mathbb{R}^{d_k}$ . These can be updated *recurrently*:

$$\mathbf{S}_t = \mathbf{S}_{t-1} + \phi(\mathbf{k}_t) \mathbf{v}_t^\top, \quad \mathbf{z}_t = \mathbf{z}_{t-1} + \phi(\mathbf{k}_t)$$

# Linear Attention

- **Key observation:** standard attention computes

$$\text{Attn}(Q, K, V)_t = \frac{\sum_{j=1}^t \exp(\mathbf{q}_t^\top \mathbf{k}_j) \mathbf{v}_j}{\sum_{j=1}^t \exp(\mathbf{q}_t^\top \mathbf{k}_j)}$$

The softmax couples all positions, preventing factorisation

- **Linear attention** (Katharopoulos et al., 2020): replace  $\exp(\mathbf{q}^\top \mathbf{k})$  with a kernel  $\phi(\mathbf{q})^\top \phi(\mathbf{k})$  for some feature map  $\phi$ :

$$\text{LinAttn}(Q, K, V)_t = \frac{\phi(\mathbf{q}_t)^\top \sum_{j=1}^t \phi(\mathbf{k}_j) \mathbf{v}_j^\top}{\phi(\mathbf{q}_t)^\top \sum_{j=1}^t \phi(\mathbf{k}_j)}$$

- **The trick:** define  $\mathbf{S}_t = \sum_{j=1}^t \phi(\mathbf{k}_j) \mathbf{v}_j^\top \in \mathbb{R}^{d_k \times d_v}$  and  $\mathbf{z}_t = \sum_{j=1}^t \phi(\mathbf{k}_j) \in \mathbb{R}^{d_k}$ . These can be updated *recurrently*:

$$\mathbf{S}_t = \mathbf{S}_{t-1} + \phi(\mathbf{k}_t) \mathbf{v}_t^\top, \quad \mathbf{z}_t = \mathbf{z}_{t-1} + \phi(\mathbf{k}_t)$$

- Each step costs  $O(d^2)$  (update  $\mathbf{S}_t$ ) instead of  $O(td)$  (attend to all  $t$  keys)
- Total cost:  $O(Td^2)$  instead of  $O(T^2d)$  — **linear in sequence length**

# Linear Attention

- **Key observation:** standard attention computes

$$\text{Attn}(Q, K, V)_t = \frac{\sum_{j=1}^t \exp(\mathbf{q}_t^\top \mathbf{k}_j) \mathbf{v}_j}{\sum_{j=1}^t \exp(\mathbf{q}_t^\top \mathbf{k}_j)}$$

The softmax couples all positions, preventing factorisation

- **Linear attention** (Katharopoulos et al., 2020): replace  $\exp(\mathbf{q}^\top \mathbf{k})$  with a kernel  $\phi(\mathbf{q})^\top \phi(\mathbf{k})$  for some feature map  $\phi$ :

$$\text{LinAttn}(Q, K, V)_t = \frac{\phi(\mathbf{q}_t)^\top \sum_{j=1}^t \phi(\mathbf{k}_j) \mathbf{v}_j}{\phi(\mathbf{q}_t)^\top \sum_{j=1}^t \phi(\mathbf{k}_j)}$$

- **The trick:** define  $\mathbf{S}_t = \sum_{j=1}^t \phi(\mathbf{k}_j) \mathbf{v}_j^\top \in \mathbb{R}^{d_k \times d_v}$  and  $\mathbf{z}_t = \sum_{j=1}^t \phi(\mathbf{k}_j) \in \mathbb{R}^{d_k}$ . These can be updated *recurrently*:

$$\mathbf{S}_t = \mathbf{S}_{t-1} + \phi(\mathbf{k}_t) \mathbf{v}_t^\top, \quad \mathbf{z}_t = \mathbf{z}_{t-1} + \phi(\mathbf{k}_t)$$

- Each step costs  $O(d^2)$  (update  $\mathbf{S}_t$ ) instead of  $O(td)$  (attend to all  $t$  keys)
- Total cost:  $O(Td^2)$  instead of  $O(T^2d)$  — **linear in sequence length**
- **Trade-off:** the feature map  $\phi$  is an approximation; linear attention typically underperforms softmax attention on language modelling benchmarks



# State Space Models (SSMs) and Mamba

- An alternative to attention: model the sequence via a **continuous-time linear dynamical system**:

$$\begin{aligned}\dot{\mathbf{h}}(t) &= A\mathbf{h}(t) + Bx(t) \\ y(t) &= C\mathbf{h}(t)\end{aligned}$$

where  $A \in \mathbb{R}^{N \times N}$ ,  $B \in \mathbb{R}^{N \times 1}$ ,  $C \in \mathbb{R}^{1 \times N}$  are learnable, and  $\mathbf{h}(t) \in \mathbb{R}^N$  is the hidden state

# State Space Models (SSMs) and Mamba

- An alternative to attention: model the sequence via a **continuous-time linear dynamical system**:

$$\begin{aligned}\dot{\mathbf{h}}(t) &= A\mathbf{h}(t) + Bx(t) \\ y(t) &= C\mathbf{h}(t)\end{aligned}$$

where  $A \in \mathbb{R}^{N \times N}$ ,  $B \in \mathbb{R}^{N \times 1}$ ,  $C \in \mathbb{R}^{1 \times N}$  are learnable, and  $\mathbf{h}(t) \in \mathbb{R}^N$  is the hidden state

- After discretisation (zero-order hold with step  $\Delta$ ):  $\mathbf{h}_t = \bar{A}\mathbf{h}_{t-1} + \bar{B}x_t$ ,  $y_t = C\mathbf{h}_t$ 
  - ▶ This is a *linear RNN* — can be computed recurrently in  $O(T)$  at inference
  - ▶ But also admits a *convolution* form:  $y = \bar{K} * x$  where  $\bar{K}_t = C\bar{A}^t\bar{B}$ . This enables  $O(T \log T)$  parallel training via FFT

# State Space Models (SSMs) and Mamba

- An alternative to attention: model the sequence via a **continuous-time linear dynamical system**:

$$\begin{aligned}\dot{\mathbf{h}}(t) &= A\mathbf{h}(t) + Bx(t) \\ y(t) &= C\mathbf{h}(t)\end{aligned}$$

where  $A \in \mathbb{R}^{N \times N}$ ,  $B \in \mathbb{R}^{N \times 1}$ ,  $C \in \mathbb{R}^{1 \times N}$  are learnable, and  $\mathbf{h}(t) \in \mathbb{R}^N$  is the hidden state

- After discretisation (zero-order hold with step  $\Delta$ ):  $\mathbf{h}_t = \bar{A}\mathbf{h}_{t-1} + \bar{B}x_t$ ,  $y_t = C\mathbf{h}_t$ 
  - ▶ This is a *linear RNN* — can be computed recurrently in  $O(T)$  at inference
  - ▶ But also admits a *convolution* form:  $y = \bar{K} * x$  where  $\bar{K}_t = C\bar{A}^t\bar{B}$ . This enables  $O(T \log T)$  parallel training via FFT
- **S4** (Gu et al., 2022): structured state space with HiPPO initialisation of  $A$ . First SSM competitive with Transformers on long-range benchmarks

# State Space Models (SSMs) and Mamba

- An alternative to attention: model the sequence via a **continuous-time linear dynamical system**:

$$\begin{aligned}\dot{\mathbf{h}}(t) &= A\mathbf{h}(t) + Bx(t) \\ y(t) &= C\mathbf{h}(t)\end{aligned}$$

where  $A \in \mathbb{R}^{N \times N}$ ,  $B \in \mathbb{R}^{N \times 1}$ ,  $C \in \mathbb{R}^{1 \times N}$  are learnable, and  $\mathbf{h}(t) \in \mathbb{R}^N$  is the hidden state

- After discretisation (zero-order hold with step  $\Delta$ ):  $\mathbf{h}_t = \bar{A}\mathbf{h}_{t-1} + \bar{B}x_t$ ,  $y_t = C\mathbf{h}_t$ 
  - ▶ This is a *linear RNN* — can be computed recurrently in  $O(T)$  at inference
  - ▶ But also admits a *convolution* form:  $y = \bar{K} * x$  where  $\bar{K}_t = C\bar{A}^t\bar{B}$ . This enables  $O(T \log T)$  parallel training via FFT
- **S4** (Gu et al., 2022): structured state space with HiPPO initialisation of  $A$ . First SSM competitive with Transformers on long-range benchmarks
- **Mamba** (Gu & Dao, 2024): makes  $B$ ,  $C$ ,  $\Delta$  *input-dependent* (selective SSM). This breaks the convolution form but enables content-based reasoning like attention
  - ▶ Inference:  $O(T)$  recurrence (like an RNN), no KV-cache needed
  - ▶ Training:  $O(T)$  via a hardware-aware parallel scan
  - ▶ Matches Transformer quality at small-to-medium scale; used in Jamba, Zamba, Codestral Mamba

# State Space Models (SSMs) and Mamba

- An alternative to attention: model the sequence via a **continuous-time linear dynamical system**:

$$\begin{aligned}\dot{\mathbf{h}}(t) &= A\mathbf{h}(t) + Bx(t) \\ y(t) &= C\mathbf{h}(t)\end{aligned}$$

where  $A \in \mathbb{R}^{N \times N}$ ,  $B \in \mathbb{R}^{N \times 1}$ ,  $C \in \mathbb{R}^{1 \times N}$  are learnable, and  $\mathbf{h}(t) \in \mathbb{R}^N$  is the hidden state

- After discretisation (zero-order hold with step  $\Delta$ ):  $\mathbf{h}_t = \bar{A}\mathbf{h}_{t-1} + \bar{B}x_t$ ,  $y_t = C\mathbf{h}_t$ 
  - ▶ This is a *linear RNN* — can be computed recurrently in  $O(T)$  at inference
  - ▶ But also admits a *convolution* form:  $y = \bar{K} * x$  where  $\bar{K}_t = C\bar{A}^t\bar{B}$ . This enables  $O(T \log T)$  parallel training via FFT
- **S4** (Gu et al., 2022): structured state space with HiPPO initialisation of  $A$ . First SSM competitive with Transformers on long-range benchmarks
- **Mamba** (Gu & Dao, 2024): makes  $B$ ,  $C$ ,  $\Delta$  *input-dependent* (selective SSM). This breaks the convolution form but enables content-based reasoning like attention
  - ▶ Inference:  $O(T)$  recurrence (like an RNN), no KV-cache needed
  - ▶ Training:  $O(T)$  via a hardware-aware parallel scan
  - ▶ Matches Transformer quality at small-to-medium scale; used in Jamba, Zamba, Codestral Mamba
- **Open question**: do SSMs scale as well as Transformers to hundreds of billions of parameters? The scaling law evidence is still limited

# Attention, Linear Attention, and SSMs: Summary

- Three approaches to sequence modelling, each with different trade-offs:

	Softmax Attention	Linear Attention	SSMs (Mamba)
Training cost	$O(T^2d)$	$O(Td^2)$	$O(T)^*$
Inference (per step)	$O(td)$ + KV-cache	$O(d^2)$	$O(d)^*$
Memory at inference	$O(T \cdot d)$ KV-cache	$O(d^2)$ fixed	$O(d)$ fixed
Content-based routing	Yes (softmax)	Approximate	Yes (selective)
Long-range	Direct (any pair)	Via recurrent state	Via recurrent state
Proven at scale	Yes (GPT-4, etc.)	Limited	Emerging

\*Ignoring state dimension  $N$  for clarity; actual cost is  $O(TNd)$ .

# Attention, Linear Attention, and SSMs: Summary

- Three approaches to sequence modelling, each with different trade-offs:

	Softmax Attention	Linear Attention	SSMs (Mamba)
Training cost	$O(T^2 d)$	$O(T d^2)$	$O(T)^*$
Inference (per step)	$O(td)$ + KV-cache	$O(d^2)$	$O(d)^*$
Memory at inference	$O(T \cdot d)$ KV-cache	$O(d^2)$ fixed	$O(d)$ fixed
Content-based routing	Yes (softmax)	Approximate	Yes (selective)
Long-range	Direct (any pair)	Via recurrent state	Via recurrent state
Proven at scale	Yes (GPT-4, etc.)	Limited	Emerging

\*Ignoring state dimension  $N$  for clarity; actual cost is  $O(TNd)$ .

- Current landscape:** Transformers with softmax attention dominate large-scale LLMs. SSMs are a promising  $O(T)$  alternative, especially for very long contexts

# Attention, Linear Attention, and SSMs: Summary

- Three approaches to sequence modelling, each with different trade-offs:

	Softmax Attention	Linear Attention	SSMs (Mamba)
Training cost	$O(T^2d)$	$O(Td^2)$	$O(T)^*$
Inference (per step)	$O(td)$ + KV-cache	$O(d^2)$	$O(d)^*$
Memory at inference	$O(T \cdot d)$ KV-cache	$O(d^2)$ fixed	$O(d)$ fixed
Content-based routing	Yes (softmax)	Approximate	Yes (selective)
Long-range	Direct (any pair)	Via recurrent state	Via recurrent state
Proven at scale	Yes (GPT-4, etc.)	Limited	Emerging

\*Ignoring state dimension  $N$  for clarity; actual cost is  $O(TNd)$ .

- Current landscape:** Transformers with softmax attention dominate large-scale LLMs. SSMs are a promising  $O(T)$  alternative, especially for very long contexts
- Hybrid architectures** (Jamba, Zamba): interleave Transformer layers with Mamba layers, getting the best of both worlds



# Expressivity: Universal Approximation for Transformers

## Theorem 1.7 (Yun et al., 2020)

*Let  $1 \leq p < \infty$  and let  $\mathcal{F}^p$  denote the class of continuous, permutation-equivariant functions  $f : \mathbb{R}^{T \times d} \rightarrow \mathbb{R}^{T \times d}$  on compact domains. Then for any  $f \in \mathcal{F}^p$  and any  $\varepsilon > 0$ , there exists a Transformer network  $g$  such that:*

$$\|f - g\|_p < \varepsilon$$

*More precisely, Transformers with  $O(1)$  heads,  $O(1)$  layers, and sufficient width are universal approximators for sequence-to-sequence functions.*

# Expressivity: Universal Approximation for Transformers

## Theorem 1.7 (Yun et al., 2020)

Let  $1 \leq p < \infty$  and let  $\mathcal{F}^p$  denote the class of continuous, permutation-equivariant functions  $f : \mathbb{R}^{T \times d} \rightarrow \mathbb{R}^{T \times d}$  on compact domains. Then for any  $f \in \mathcal{F}^p$  and any  $\varepsilon > 0$ , there exists a Transformer network  $g$  such that:

$$\|f - g\|_p < \varepsilon$$

More precisely, Transformers with  $O(1)$  heads,  $O(1)$  layers, and sufficient width are universal approximators for sequence-to-sequence functions.

- This extends the classical Universal Approximation Theorem (for FNNs) to the [sequence-to-sequence setting](#)

# Expressivity: Universal Approximation for Transformers

## Theorem 1.7 (Yun et al., 2020)

Let  $1 \leq p < \infty$  and let  $\mathcal{F}^p$  denote the class of continuous, permutation-equivariant functions  $f : \mathbb{R}^{T \times d} \rightarrow \mathbb{R}^{T \times d}$  on compact domains. Then for any  $f \in \mathcal{F}^p$  and any  $\varepsilon > 0$ , there exists a Transformer network  $g$  such that:

$$\|f - g\|_p < \varepsilon$$

More precisely, Transformers with  $O(1)$  heads,  $O(1)$  layers, and sufficient width are universal approximators for sequence-to-sequence functions.

- This extends the classical Universal Approximation Theorem (for FNNs) to the [sequence-to-sequence setting](#)
- The self-attention mechanism is crucial: it allows arbitrary interactions between positions, which pure FFNs applied independently to each position cannot achieve

# Expressivity: Universal Approximation for Transformers

## Theorem 1.7 (Yun et al., 2020)

Let  $1 \leq p < \infty$  and let  $\mathcal{F}^p$  denote the class of continuous, permutation-equivariant functions  $f : \mathbb{R}^{T \times d} \rightarrow \mathbb{R}^{T \times d}$  on compact domains. Then for any  $f \in \mathcal{F}^p$  and any  $\varepsilon > 0$ , there exists a Transformer network  $g$  such that:

$$\|f - g\|_p < \varepsilon$$

More precisely, Transformers with  $O(1)$  heads,  $O(1)$  layers, and sufficient width are universal approximators for sequence-to-sequence functions.

- This extends the classical Universal Approximation Theorem (for FNNs) to the [sequence-to-sequence setting](#)
- The self-attention mechanism is crucial: it allows arbitrary interactions between positions, which pure FFNs applied independently to each position cannot achieve
- [Key insight](#): Self-attention can implement *contextual mappings* — the representation of each token can depend on the entire input sequence

## Part 5: Scaling Laws

**Goal:** Understand the empirical relationships between model scale, data, compute, and performance, and their implications for LLM development.

- Neural scaling laws (Kaplan et al., 2020)

## Part 5: Scaling Laws

**Goal:** Understand the empirical relationships between model scale, data, compute, and performance, and their implications for LLM development.

- Neural scaling laws (Kaplan et al., 2020)
- Chinchilla scaling laws (Hoffmann et al., 2022)

## Part 5: Scaling Laws

**Goal:** Understand the empirical relationships between model scale, data, compute, and performance, and their implications for LLM development.

- Neural scaling laws (Kaplan et al., 2020)
- Chinchilla scaling laws (Hoffmann et al., 2022)
- Emergent abilities and their interpretation

# Neural Scaling Laws (Kaplan et al., 2020)

- **Setup:** Train a family of Transformer LMs of different sizes on different amounts of data. Measure test loss (cross-entropy, i.e.  $-\frac{1}{T} \sum_t \log P(x_t | x_{<t})$ ) as a function of three variables:
  - ▶  $N$  = number of non-embedding parameters
  - ▶  $D$  = number of training tokens
  - ▶  $C$  = compute budget (in FLOPs)



# Neural Scaling Laws (Kaplan et al., 2020)

- **Setup:** Train a family of Transformer LMs of different sizes on different amounts of data. Measure test loss (cross-entropy, i.e.  $-\frac{1}{T} \sum_t \log P(x_t | x_{<t})$ ) as a function of three variables:
  - ▶  $N$  = number of non-embedding parameters
  - ▶  $D$  = number of training tokens
  - ▶  $C$  = compute budget (in FLOPs)
- **Empirical finding:** on log-log axes, the relationship is approximately *linear* — i.e. a **power law**:

$$L(N) \approx \left( \frac{N_c}{N} \right)^{\alpha_N}, \quad \alpha_N \approx 0.076 \quad (1.29)$$

$$L(D) \approx \left( \frac{D_c}{D} \right)^{\alpha_D}, \quad \alpha_D \approx 0.095 \quad (1.30)$$

$$L(C) \approx \left( \frac{C_c}{C} \right)^{\alpha_C}, \quad \alpha_C \approx 0.050 \quad (1.31)$$

where  $N_c, D_c, C_c$  are constants (determined by the other non-bottleneck variables being sufficient)

# Neural Scaling Laws (Kaplan et al., 2020)

- **Setup:** Train a family of Transformer LMs of different sizes on different amounts of data. Measure test loss (cross-entropy, i.e.  $-\frac{1}{T} \sum_t \log P(x_t | x_{<t})$ ) as a function of three variables:
  - ▶  $N$  = number of non-embedding parameters
  - ▶  $D$  = number of training tokens
  - ▶  $C$  = compute budget (in FLOPs)
- **Empirical finding:** on log-log axes, the relationship is approximately *linear* — i.e. a **power law**:

$$L(N) \approx \left( \frac{N_c}{N} \right)^{\alpha_N}, \quad \alpha_N \approx 0.076 \quad (1.29)$$

$$L(D) \approx \left( \frac{D_c}{D} \right)^{\alpha_D}, \quad \alpha_D \approx 0.095 \quad (1.30)$$

$$L(C) \approx \left( \frac{C_c}{C} \right)^{\alpha_C}, \quad \alpha_C \approx 0.050 \quad (1.31)$$

where  $N_c, D_c, C_c$  are constants (determined by the other non-bottleneck variables being sufficient)

- **Interpretation:**  $\alpha_N \approx 0.076$  means that to halve the loss, you need to increase  $N$  by a factor of  $2^{1/0.076} \approx 2^{13} \approx 8,000$ . Progress is real but expensive

# Scaling Laws: What Matters and What Doesn't

- Surprising finding 1: Model **shape** matters far less than model **size**
  - ▶ Varying depth vs. width, number of attention heads, FFN dimension — as long as total  $N$  is the same, loss is approximately the same
  - ▶ This justifies measuring progress by parameter count alone

# Scaling Laws: What Matters and What Doesn't

- **Surprising finding 1:** Model **shape** matters far less than model **size**
  - ▶ Varying depth vs. width, number of attention heads, FFN dimension — as long as total  $N$  is the same, loss is approximately the same
  - ▶ This justifies measuring progress by parameter count alone
- **Surprising finding 2:** Larger models are more **sample-efficient**
  - ▶ A  $10\times$  larger model reaches the same loss with  $\sim 10\times$  fewer training tokens
  - ▶ **But:** it costs  $10\times$  more FLOPs per token, so total compute is similar

# Scaling Laws: What Matters and What Doesn't

- **Surprising finding 1:** Model **shape** matters far less than model **size**
  - ▶ Varying depth vs. width, number of attention heads, FFN dimension — as long as total  $N$  is the same, loss is approximately the same
  - ▶ This justifies measuring progress by parameter count alone
- **Surprising finding 2:** Larger models are more **sample-efficient**
  - ▶ A  $10\times$  larger model reaches the same loss with  $\sim 10\times$  fewer training tokens
  - ▶ **But:** it costs  $10\times$  more FLOPs per token, so total compute is similar
- **Surprising finding 3:** Power laws hold over **many orders of magnitude**
  - ▶ Kaplan et al. tested models from  $\sim 1\text{K}$  to  $\sim 1\text{B}$  parameters — 6 orders of magnitude
  - ▶ The same power-law exponents fit the entire range with no sign of saturating
  - ▶ **This is unusual** — most empirical scaling relationships break down outside a narrow range

# Joint Scaling and Predictability

- When both  $N$  and  $D$  are limited, Kaplan et al. proposed a [joint scaling law](#):

$$L(N, D) \approx \left[ \left( \frac{N_c}{N} \right)^{\alpha_N / \alpha_D} + \frac{D_c}{D} \right]^{\alpha_D}$$

# Joint Scaling and Predictability

- When both  $N$  and  $D$  are limited, Kaplan et al. proposed a **joint scaling law**:

$$L(N, D) \approx \left[ \left( \frac{N_c}{N} \right)^{\alpha_N / \alpha_D} + \frac{D_c}{D} \right]^{\alpha_D}$$

- Interpretation:**  $L$  is dominated by whichever bottleneck is worse (smaller  $N$  or smaller  $D$ ). When  $N \gg N_c$ , the first term vanishes and  $L(D) \sim D^{-\alpha_D}$ . Symmetrically for  $D \gg D_c$

# Joint Scaling and Predictability

- When both  $N$  and  $D$  are limited, Kaplan et al. proposed a **joint scaling law**:

$$L(N, D) \approx \left[ \left( \frac{N_c}{N} \right)^{\alpha_N / \alpha_D} + \frac{D_c}{D} \right]^{\alpha_D}$$

- Interpretation:**  $L$  is dominated by whichever bottleneck is worse (smaller  $N$  or smaller  $D$ ). When  $N \gg N_c$ , the first term vanishes and  $L(D) \sim D^{-\alpha_D}$ . Symmetrically for  $D \gg D_c$
- Why this is practically important:** you can *predict* the performance of a large model **before** training it
  - ▶ Train a family of small models (e.g. 10M, 50M, 100M, 500M parameters)
  - ▶ Fit the power-law exponents  $\alpha_N, \alpha_D$  on these small runs
  - ▶ Extrapolate to predict the loss of a 70B or 175B model
  - ▶ This saves millions of dollars in wasted compute on bad configurations



# Joint Scaling and Predictability

- When both  $N$  and  $D$  are limited, Kaplan et al. proposed a **joint scaling law**:

$$L(N, D) \approx \left[ \left( \frac{N_c}{N} \right)^{\alpha_N / \alpha_D} + \frac{D_c}{D} \right]^{\alpha_D}$$

- Interpretation:**  $L$  is dominated by whichever bottleneck is worse (smaller  $N$  or smaller  $D$ ). When  $N \gg N_c$ , the first term vanishes and  $L(D) \sim D^{-\alpha_D}$ . Symmetrically for  $D \gg D_c$
- Why this is practically important:** you can *predict* the performance of a large model **before** training it
  - ▶ Train a family of small models (e.g. 10M, 50M, 100M, 500M parameters)
  - ▶ Fit the power-law exponents  $\alpha_N, \alpha_D$  on these small runs
  - ▶ Extrapolate to predict the loss of a 70B or 175B model
  - ▶ This saves millions of dollars in wasted compute on bad configurations
- Real-world example:** GPT-4's performance was reportedly predicted accurately from scaling laws fitted on much smaller models (OpenAI, 2023)

# The Compute Budget: Where Do the FLOPs Go?

- The total compute cost of training is approximately:

$$C \approx 6ND \text{ FLOPs}$$

# The Compute Budget: Where Do the FLOPs Go?

- The total compute cost of training is approximately:

$$C \approx 6ND \text{ FLOPs}$$

- Where does the factor of 6 come from?
  - ▶ Each token in the forward pass requires  $\sim 2N$  multiply-adds (one for each weight, applied to each input)
  - ▶ The backward pass is approximately  $2\times$  the forward pass (computing gradients w.r.t. both activations and weights)
  - ▶ Total:  $\sim 2N + 4N = 6N$  FLOPs per token, times  $D$  tokens

# The Compute Budget: Where Do the FLOPs Go?

- The total compute cost of training is approximately:

$$C \approx 6ND \text{ FLOPs}$$

- Where does the factor of 6 come from?

- ▶ Each token in the forward pass requires  $\sim 2N$  multiply-adds (one for each weight, applied to each input)
- ▶ The backward pass is approximately  $2\times$  the forward pass (computing gradients w.r.t. both activations and weights)
- ▶ Total:  $\sim 2N + 4N = 6N$  FLOPs per token, times  $D$  tokens

- Concrete scale:

- ▶ GPT-3 (175B params, 300B tokens):  $C \approx 6 \times 175 \times 10^9 \times 300 \times 10^9 = 3.15 \times 10^{23}$  FLOPs
- ▶ On 1024 A100 GPUs at 312 TFLOPS each:  $\sim 10$  days of training
- ▶ Estimated cost:  $\sim \$4\text{--}12\text{M}$  (at 2023 cloud prices)

# The Compute Budget: Where Do the FLOPs Go?

- The total compute cost of training is approximately:

$$C \approx 6ND \text{ FLOPs}$$

- Where does the factor of 6 come from?

- ▶ Each token in the forward pass requires  $\sim 2N$  multiply-adds (one for each weight, applied to each input)
- ▶ The backward pass is approximately  $2\times$  the forward pass (computing gradients w.r.t. both activations and weights)
- ▶ Total:  $\sim 2N + 4N = 6N$  FLOPs per token, times  $D$  tokens

- Concrete scale:

- ▶ GPT-3 (175B params, 300B tokens):  $C \approx 6 \times 175 \times 10^9 \times 300 \times 10^9 = 3.15 \times 10^{23}$  FLOPs
- ▶ On 1024 A100 GPUs at 312 TFLOPS each:  $\sim 10$  days of training
- ▶ Estimated cost:  $\sim \$4\text{--}12\text{M}$  (at 2023 cloud prices)

- The central question of scaling laws: Given a budget of  $C$  FLOPs, what is the best split between  $N$  and  $D = C/(6N)$ ?

# Compute-Optimal Training (Hoffmann et al., 2022)

- Kaplan et al. (2020) answer: Scale  $N$  faster than  $D$ 
  - ▶ Their analysis suggested  $N_{\text{opt}} \propto C^{0.73}$ ,  $D_{\text{opt}} \propto C^{0.27}$
  - ▶ In words: spend most of your budget on a bigger model, even if it sees less data

# Compute-Optimal Training (Hoffmann et al., 2022)

- [Kaplan et al. \(2020\) answer](#): Scale  $N$  faster than  $D$ 
  - ▶ Their analysis suggested  $N_{\text{opt}} \propto C^{0.73}$ ,  $D_{\text{opt}} \propto C^{0.27}$
  - ▶ In words: spend most of your budget on a bigger model, even if it sees less data
- [Hoffmann et al. \(2022\) answer](#): This was wrong. They proposed a refined loss model:

$$L(N, D) = E + \frac{A}{N^\alpha} + \frac{B}{D^\beta} \quad (1.32)$$

where  $E \approx 1.69$  nats is the [irreducible entropy](#) of natural language,  $\alpha \approx 0.34$ ,  $\beta \approx 0.28$

# Compute-Optimal Training (Hoffmann et al., 2022)

- Kaplan et al. (2020) answer: Scale  $N$  faster than  $D$ 
  - ▶ Their analysis suggested  $N_{\text{opt}} \propto C^{0.73}$ ,  $D_{\text{opt}} \propto C^{0.27}$
  - ▶ In words: spend most of your budget on a bigger model, even if it sees less data
- Hoffmann et al. (2022) answer: This was wrong. They proposed a refined loss model:

$$L(N, D) = E + \frac{A}{N^\alpha} + \frac{B}{D^\beta} \quad (1.32)$$

where  $E \approx 1.69$  nats is the **irreducible entropy** of natural language,  $\alpha \approx 0.34$ ,  $\beta \approx 0.28$

- Key insight: The three terms have clear interpretations:
  - ▶  $E$ : the entropy of the data — no model can beat this
  - ▶  $A/N^\alpha$ : the **approximation error** — the model is too small to represent the true distribution
  - ▶  $B/D^\beta$ : the **estimation error** — not enough data to learn the parameters well



# Compute-Optimal Training (Hoffmann et al., 2022)

- Kaplan et al. (2020) answer: Scale  $N$  faster than  $D$ 
  - ▶ Their analysis suggested  $N_{\text{opt}} \propto C^{0.73}$ ,  $D_{\text{opt}} \propto C^{0.27}$
  - ▶ In words: spend most of your budget on a bigger model, even if it sees less data
- Hoffmann et al. (2022) answer: This was wrong. They proposed a refined loss model:

$$L(N, D) = E + \frac{A}{N^\alpha} + \frac{B}{D^\beta} \quad (1.32)$$

where  $E \approx 1.69$  nats is the **irreducible entropy** of natural language,  $\alpha \approx 0.34$ ,  $\beta \approx 0.28$

- **Key insight:** The three terms have clear interpretations:
  - ▶  $E$ : the entropy of the data — no model can beat this
  - ▶  $A/N^\alpha$ : the **approximation error** — the model is too small to represent the true distribution
  - ▶  $B/D^\beta$ : the **estimation error** — not enough data to learn the parameters well
- Minimising  $L(N, D)$  subject to  $C = 6ND$  via Lagrange multipliers gives:

$$N_{\text{opt}} \propto C^{0.50}, \quad D_{\text{opt}} \propto C^{0.50}$$

Model size and data should be **scaled equally**

# The Chinchilla Result

- **The punchline:** Most large models before Chinchilla were *significantly undertrained* — too many parameters, too little data

# The Chinchilla Result

- **The punchline:** Most large models before Chinchilla were *significantly undertrained* — too many parameters, too little data
- **Concrete example:**
  - ▶ **Gopher** (DeepMind, 2021): 280B parameters, trained on 300B tokens
  - ▶ **Chinchilla** (DeepMind, 2022): 70B parameters, trained on 1.4T tokens
  - ▶ Same compute budget ( $\sim 5 \times 10^{23}$  FLOPs), but Chinchilla outperformed Gopher on nearly every benchmark

# The Chinchilla Result

- **The punchline:** Most large models before Chinchilla were *significantly undertrained* — too many parameters, too little data
- **Concrete example:**
  - ▶ **Gopher** (DeepMind, 2021): 280B parameters, trained on 300B tokens
  - ▶ **Chinchilla** (DeepMind, 2022): 70B parameters, trained on 1.4T tokens
  - ▶ Same compute budget ( $\sim 5 \times 10^{23}$  FLOPs), but Chinchilla outperformed Gopher on nearly every benchmark
- **Optimal data-to-parameters ratio:** approximately 20 tokens per parameter
  - ▶ GPT-3 (175B params, 300B tokens): ratio  $\approx 1.7$  — heavily undertrained
  - ▶ Chinchilla (70B params, 1.4T tokens): ratio  $\approx 20$  — compute-optimal
  - ▶ LLaMA (65B params, 1.4T tokens): ratio  $\approx 22$  — slightly over Chinchilla-optimal

# The Chinchilla Result

- **The punchline:** Most large models before Chinchilla were *significantly undertrained* — too many parameters, too little data
- **Concrete example:**
  - ▶ **Gopher** (DeepMind, 2021): 280B parameters, trained on 300B tokens
  - ▶ **Chinchilla** (DeepMind, 2022): 70B parameters, trained on 1.4T tokens
  - ▶ Same compute budget ( $\sim 5 \times 10^{23}$  FLOPs), but Chinchilla outperformed Gopher on nearly every benchmark
- **Optimal data-to-parameters ratio:** approximately 20 tokens per parameter
  - ▶ GPT-3 (175B params, 300B tokens): ratio  $\approx 1.7$  — heavily undertrained
  - ▶ Chinchilla (70B params, 1.4T tokens): ratio  $\approx 20$  — compute-optimal
  - ▶ LLaMA (65B params, 1.4T tokens): ratio  $\approx 22$  — slightly over Chinchilla-optimal
- **The “Chinchilla tax”:** Compute-optimal training demands far more data than previously assumed. For 175B parameters, the optimal dataset is  $\sim 3.5$ T tokens

# The Chinchilla Result

- **The punchline:** Most large models before Chinchilla were *significantly undertrained* — too many parameters, too little data
- **Concrete example:**
  - ▶ **Gopher** (DeepMind, 2021): 280B parameters, trained on 300B tokens
  - ▶ **Chinchilla** (DeepMind, 2022): 70B parameters, trained on 1.4T tokens
  - ▶ Same compute budget ( $\sim 5 \times 10^{23}$  FLOPs), but Chinchilla outperformed Gopher on nearly every benchmark
- **Optimal data-to-parameters ratio:** approximately 20 tokens per parameter
  - ▶ GPT-3 (175B params, 300B tokens): ratio  $\approx 1.7$  — heavily undertrained
  - ▶ Chinchilla (70B params, 1.4T tokens): ratio  $\approx 20$  — compute-optimal
  - ▶ LLaMA (65B params, 1.4T tokens): ratio  $\approx 22$  — slightly over Chinchilla-optimal
- **The “Chinchilla tax”:** Compute-optimal training demands far more data than previously assumed. For 175B parameters, the optimal dataset is  $\sim 3.5$ T tokens
- **Beyond Chinchilla:** Recent models (LLaMA-3, Gemma) train well *past* the Chinchilla-optimal point — more data than predicted optimal, because inference cost (which scales with  $N$ , not  $D$ ) matters in deployment

# Emergent Abilities

- [Wei et al. \(2022\)](#) observed that certain capabilities appear to “emerge” suddenly at specific model scales:
  - ▶ *Few-shot arithmetic*: Near-zero accuracy below 13B, then jumps to  $> 50\%$
  - ▶ *Multi-step reasoning*: Appears around 100B parameters
  - ▶ *Word unscrambling*: Absent below a threshold, then rapidly improves

# Emergent Abilities

- Wei et al. (2022) observed that certain capabilities appear to “emerge” suddenly at specific model scales:
  - ▶ *Few-shot arithmetic*: Near-zero accuracy below 13B, then jumps to  $> 50\%$
  - ▶ *Multi-step reasoning*: Appears around 100B parameters
  - ▶ *Word unscrambling*: Absent below a threshold, then rapidly improves
- An ability is called **emergent** if it is “not present in smaller models but is present in larger models” — a *sharp, unpredictable* transition



# Emergent Abilities

- Wei et al. (2022) observed that certain capabilities appear to “emerge” suddenly at specific model scales:
  - ▶ *Few-shot arithmetic*: Near-zero accuracy below 13B, then jumps to  $> 50\%$
  - ▶ *Multi-step reasoning*: Appears around 100B parameters
  - ▶ *Word unscrambling*: Absent below a threshold, then rapidly improves
- An ability is called **emergent** if it is “not present in smaller models but is present in larger models” — a *sharp, unpredictable* transition
- This is surprising because the scaling laws predict *smooth* improvement. If the underlying loss improves smoothly, why do specific capabilities appear to jump?

# Emergent Abilities: The Metric Artefact Debate

- Schaeffer et al. (2023) argued that emergence is a measurement artefact:

# Emergent Abilities: The Metric Artefact Debate

- Schaeffer et al. (2023) argued that emergence is a **measurement artefact**:
- **The argument**: Consider a task like 3-digit addition. The metric is exact-match accuracy (the answer is either exactly right or wrong). Suppose the per-token probability improves smoothly from 0.1 to 0.99 as the model scales:
  - ▶ Getting all 4 digits right requires  $\sim p^4$
  - ▶ At  $p = 0.5$ : accuracy  $\approx 0.5^4 = 6\%$  (looks like failure)
  - ▶ At  $p = 0.9$ : accuracy  $\approx 0.9^4 = 66\%$  (looks like sudden success)

# Emergent Abilities: The Metric Artefact Debate

- Schaeffer et al. (2023) argued that emergence is a **measurement artefact**:
- **The argument**: Consider a task like 3-digit addition. The metric is exact-match accuracy (the answer is either exactly right or wrong). Suppose the per-token probability improves smoothly from 0.1 to 0.99 as the model scales:
  - ▶ Getting all 4 digits right requires  $\sim p^4$
  - ▶ At  $p = 0.5$ : accuracy  $\approx 0.5^4 = 6\%$  (looks like failure)
  - ▶ At  $p = 0.9$ : accuracy  $\approx 0.9^4 = 66\%$  (looks like sudden success)
- The *underlying* capability (per-token accuracy) improved smoothly, but the *metric* (exact match) introduced a nonlinear threshold that created the appearance of a phase transition

# Emergent Abilities: The Metric Artefact Debate

- Schaeffer et al. (2023) argued that emergence is a **measurement artefact**:
- **The argument**: Consider a task like 3-digit addition. The metric is exact-match accuracy (the answer is either exactly right or wrong). Suppose the per-token probability improves smoothly from 0.1 to 0.99 as the model scales:
  - ▶ Getting all 4 digits right requires  $\sim p^4$
  - ▶ At  $p = 0.5$ : accuracy  $\approx 0.5^4 = 6\%$  (looks like failure)
  - ▶ At  $p = 0.9$ : accuracy  $\approx 0.9^4 = 66\%$  (looks like sudden success)
- The *underlying* capability (per-token accuracy) improved smoothly, but the *metric* (exact match) introduced a nonlinear threshold that created the appearance of a phase transition
- **Evidence**: When Schaeffer et al. re-evaluated the same tasks with continuous metrics (e.g. Brier score, token-level log-likelihood), the sharp transitions disappeared — performance improved smoothly and predictably with scale

# Emergent Abilities: The Metric Artefact Debate

- Schaeffer et al. (2023) argued that emergence is a **measurement artefact**:
- **The argument**: Consider a task like 3-digit addition. The metric is exact-match accuracy (the answer is either exactly right or wrong). Suppose the per-token probability improves smoothly from 0.1 to 0.99 as the model scales:
  - ▶ Getting all 4 digits right requires  $\sim p^4$
  - ▶ At  $p = 0.5$ : accuracy  $\approx 0.5^4 = 6\%$  (looks like failure)
  - ▶ At  $p = 0.9$ : accuracy  $\approx 0.9^4 = 66\%$  (looks like sudden success)
- The *underlying* capability (per-token accuracy) improved smoothly, but the *metric* (exact match) introduced a nonlinear threshold that created the appearance of a phase transition
- **Evidence**: When Schaeffer et al. re-evaluated the same tasks with continuous metrics (e.g. Brier score, token-level log-likelihood), the sharp transitions disappeared — performance improved smoothly and predictably with scale
- **Current consensus**: The underlying capabilities likely improve continuously with scale (consistent with smooth scaling laws), but certain *task-level metrics* can make this look like sudden emergence

# Summary

- ① **Statistical Language Modelling:** Language models assign probabilities to token sequences via the chain rule decomposition. Neural language models replace counting-based estimation with learned parameters

# Summary

- 1 **Statistical Language Modelling:** Language models assign probabilities to token sequences via the chain rule decomposition. Neural language models replace counting-based estimation with learned parameters
- 2 **Neural Networks:** Universal approximators (Cybenko, Hornik). Depth provides exponential efficiency gains. Trained via SGD and backpropagation



# Summary

- ① **Statistical Language Modelling:** Language models assign probabilities to token sequences via the chain rule decomposition. Neural language models replace counting-based estimation with learned parameters
- ② **Neural Networks:** Universal approximators (Cybenko, Hornik). Depth provides exponential efficiency gains. Trained via SGD and backpropagation
- ③ **Recurrent Neural Networks:** Process sequences via hidden states. Suffer from vanishing/exploding gradients. LSTMs partially address this with gating mechanisms. Theoretically Turing-complete but limited in practice

# Summary

- ① **Statistical Language Modelling:** Language models assign probabilities to token sequences via the chain rule decomposition. Neural language models replace counting-based estimation with learned parameters
- ② **Neural Networks:** Universal approximators (Cybenko, Hornik). Depth provides exponential efficiency gains. Trained via SGD and backpropagation
- ③ **Recurrent Neural Networks:** Process sequences via hidden states. Suffer from vanishing/exploding gradients. LSTMs partially address this with gating mechanisms. Theoretically Turing-complete but limited in practice
- ④ **Transformers:** Replace recurrence with self-attention. Enable full parallelisation and direct long-range interactions.  $O(T^2d)$  complexity. Universal approximators for sequence-to-sequence functions. Alternatives: linear attention, SSMs (Mamba)

# Summary

- ① **Statistical Language Modelling:** Language models assign probabilities to token sequences via the chain rule decomposition. Neural language models replace counting-based estimation with learned parameters
- ② **Neural Networks:** Universal approximators (Cybenko, Hornik). Depth provides exponential efficiency gains. Trained via SGD and backpropagation
- ③ **Recurrent Neural Networks:** Process sequences via hidden states. Suffer from vanishing/exploding gradients. LSTMs partially address this with gating mechanisms. Theoretically Turing-complete but limited in practice
- ④ **Transformers:** Replace recurrence with self-attention. Enable full parallelisation and direct long-range interactions.  $O(T^2d)$  complexity. Universal approximators for sequence-to-sequence functions. Alternatives: linear attention, SSMs (Mamba)
- ⑤ **Scaling Laws:** Test loss follows power laws in model size, data, and compute. Chinchilla-optimal training scales  $N$  and  $D$  equally. Emergent abilities are debated

# Optional Reading

- Douglas, M. R. (2023). *Large Language Models*. *arXiv:2307.05782*.
  - ▶ Primary reference for this lecture
- Vaswani, A. et al. (2017). Attention Is All You Need. *NeurIPS*.
  - ▶ The original Transformer paper
- Kaplan, J. et al. (2020). Scaling Laws for Neural Language Models. *arXiv:2001.08361*.
- Hoffmann, J. et al. (2022). Training Compute-Optimal Large Language Models. *NeurIPS* (Chinchilla paper).
- Yun, C. et al. (2020). Are Transformers Universal Approximators of Sequence-to-Sequence Functions? *ICLR*.
- Merrill, W. & Sabharwal, A. (2023). The Parallelism Tradeoff: Limitations of Log-Precision Transformers. *TACL*.
- Siegelmann, H. & Sontag, E. (1995). On the Computational Power of Neural Nets. *JCSS*, 50(1), 132–150.
- Schaeffer, R. et al. (2023). Are Emergent Abilities of Large Language Models a Mirage? *NeurIPS*.