STAT 453: Introduction to Deep Learning and Generative Models

Ben Lengerich

Lecture 21: GPT Architectures

November 17, 2025

Reading: See course homepage

From RNN…

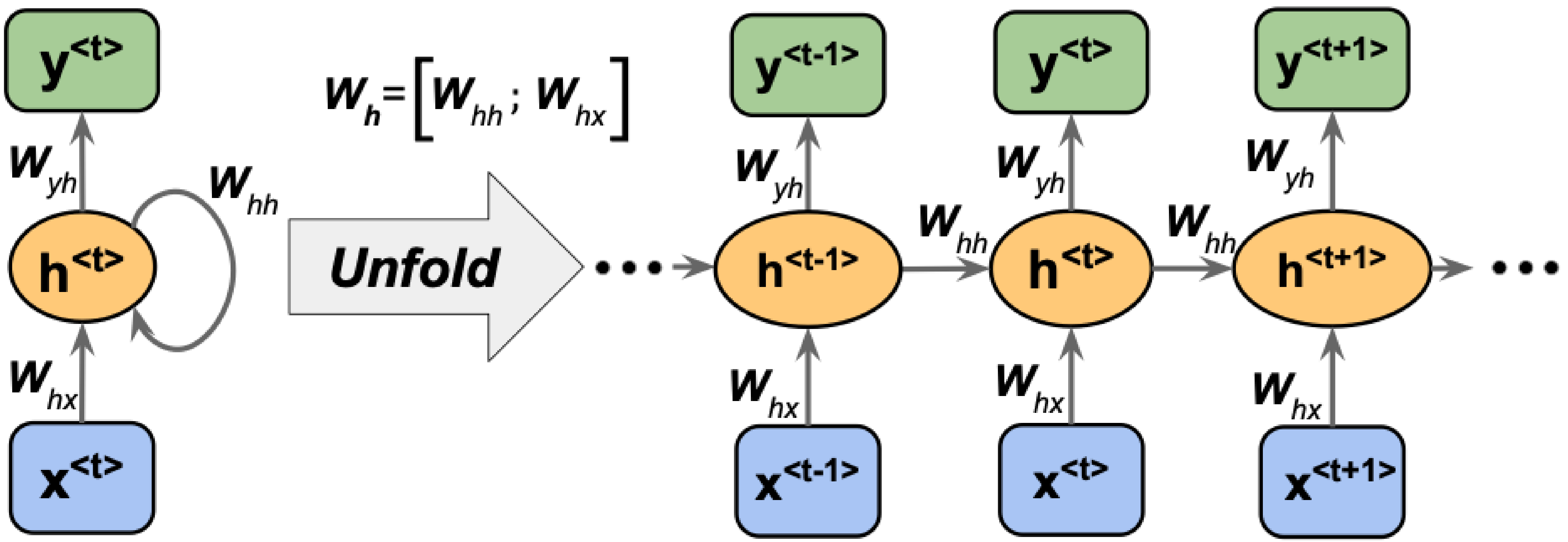
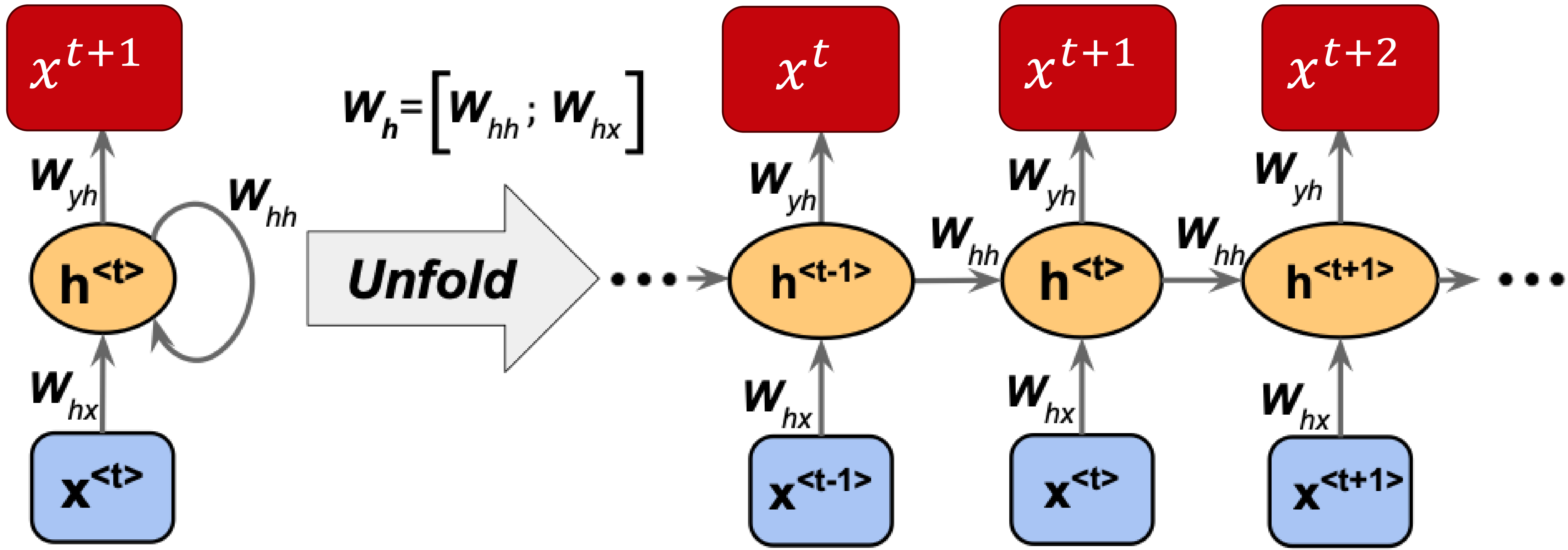


Image source: Sebastian Raschka, Vahid Mirjalili. Python Machine Learning. 3rd Edition. Packt, 2019

From RNN…to GPT



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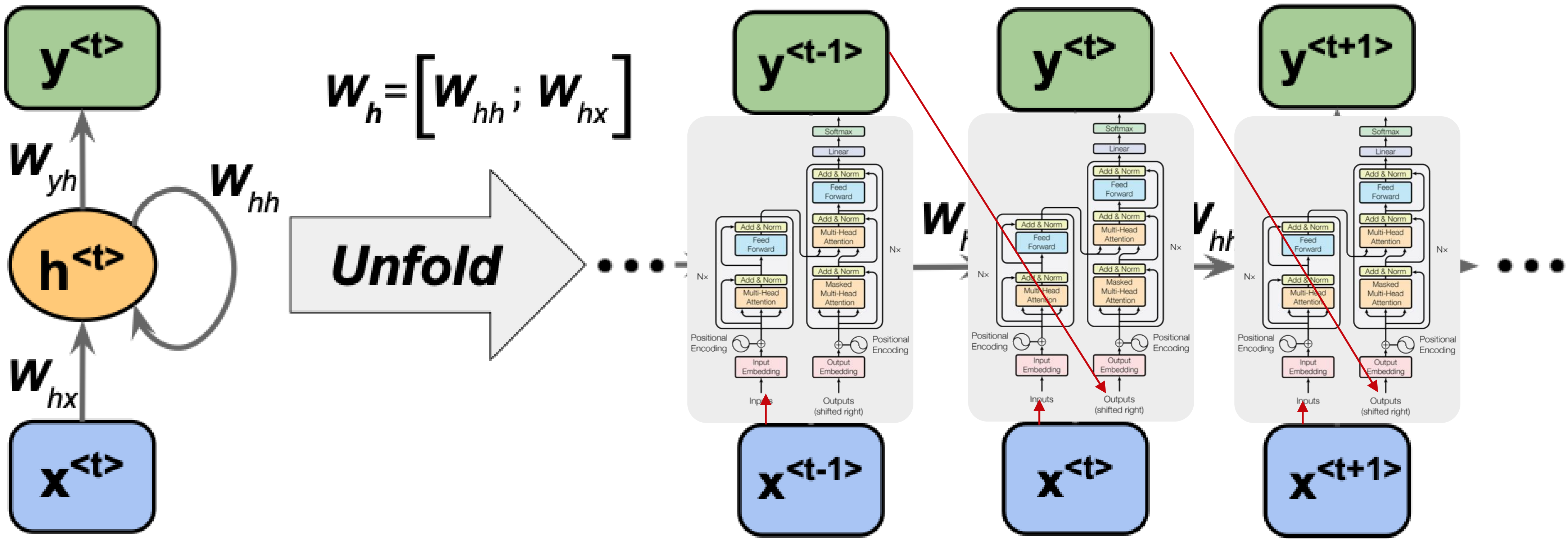
From RNN…to GPT…by Transformers



Vaswani, A., Shazeer, N., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A.N., Kaiser, L. and Polosukhin, I., 2017. Attention Is All You Need.

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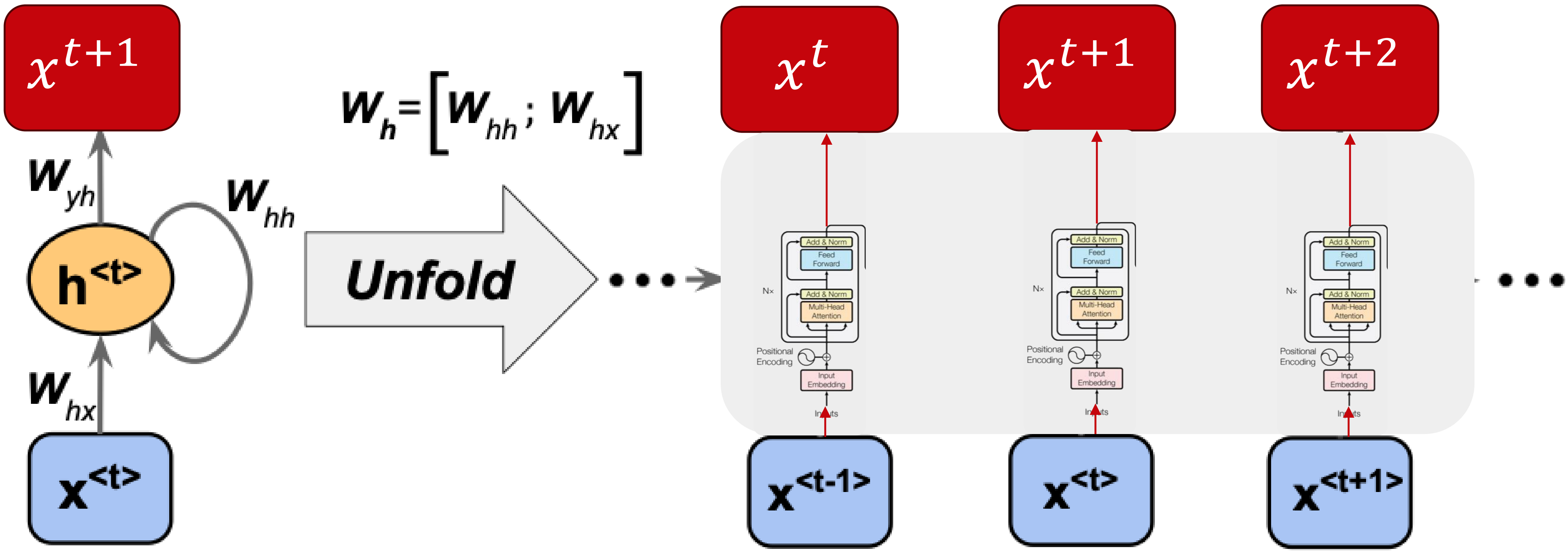

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Self-attention (very basic form)

No learnable parameters?

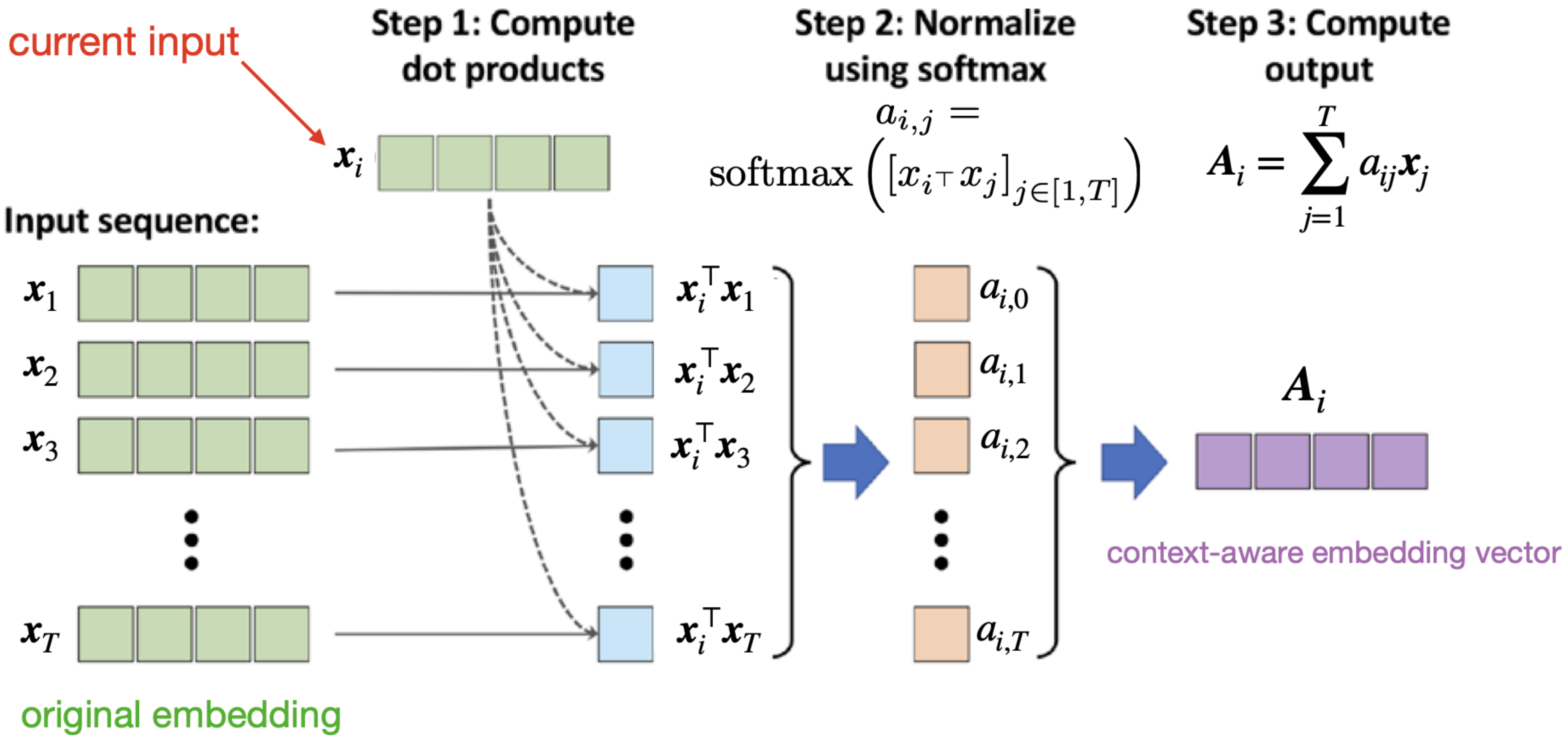


Image source: Raschka & Mirjalili 2019. Python Machine Learning, 3rd edition

Learnable Self-attention

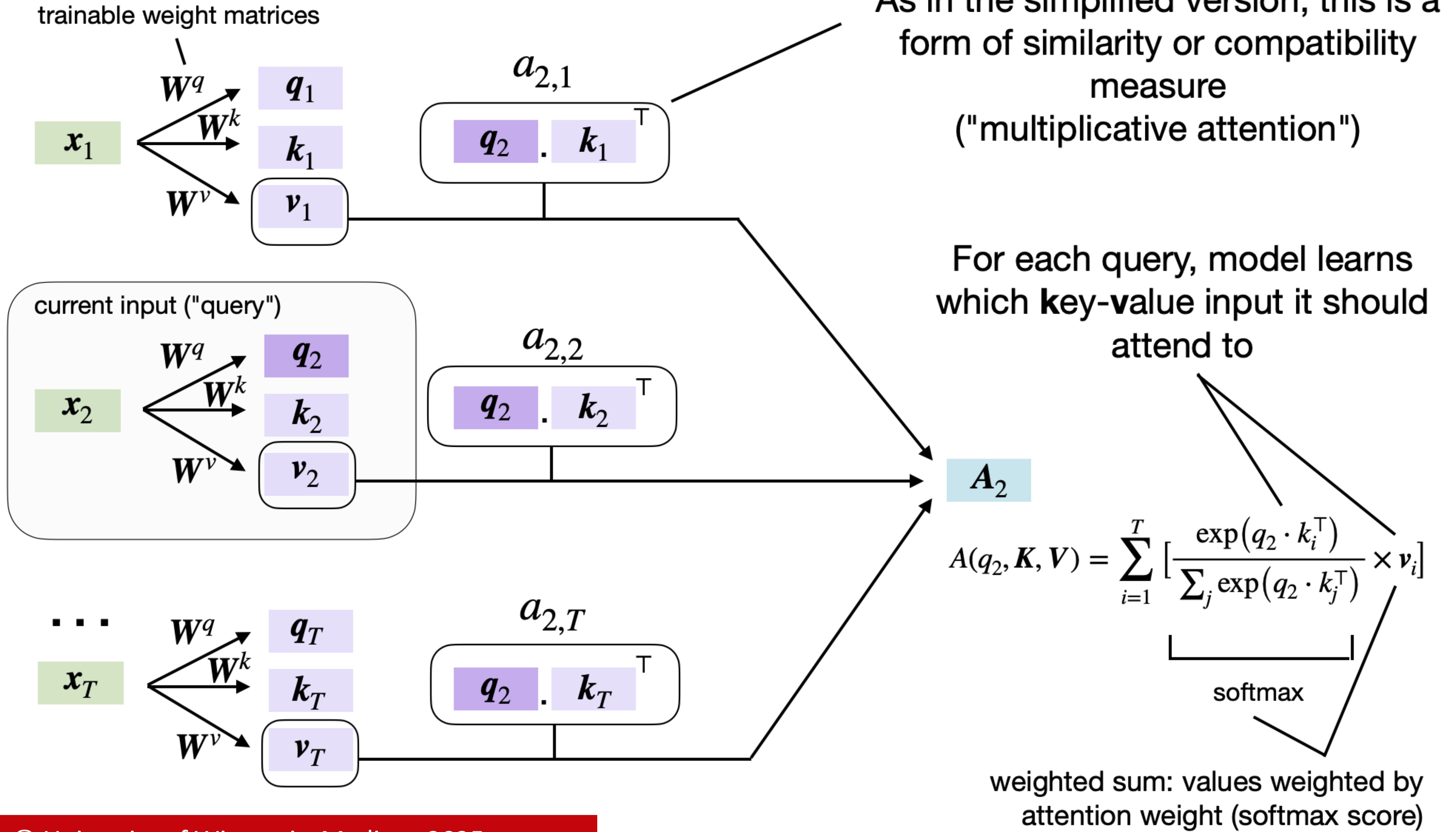
- Previous basic version did not involve any learnable parameters, so not very useful for learning a language model
- We are now adding 3 trainable weight matrices that are multiplied with the input sequence embeddings

$$\text{query} = \boldsymbol{W}^q \boldsymbol{x}_i$$

$$\text{key} = \boldsymbol{W}^k \boldsymbol{x}_i$$

$$\text{value} = \boldsymbol{W}^v \boldsymbol{x}_i$$

Learnable Self-attention



At the end of the day…

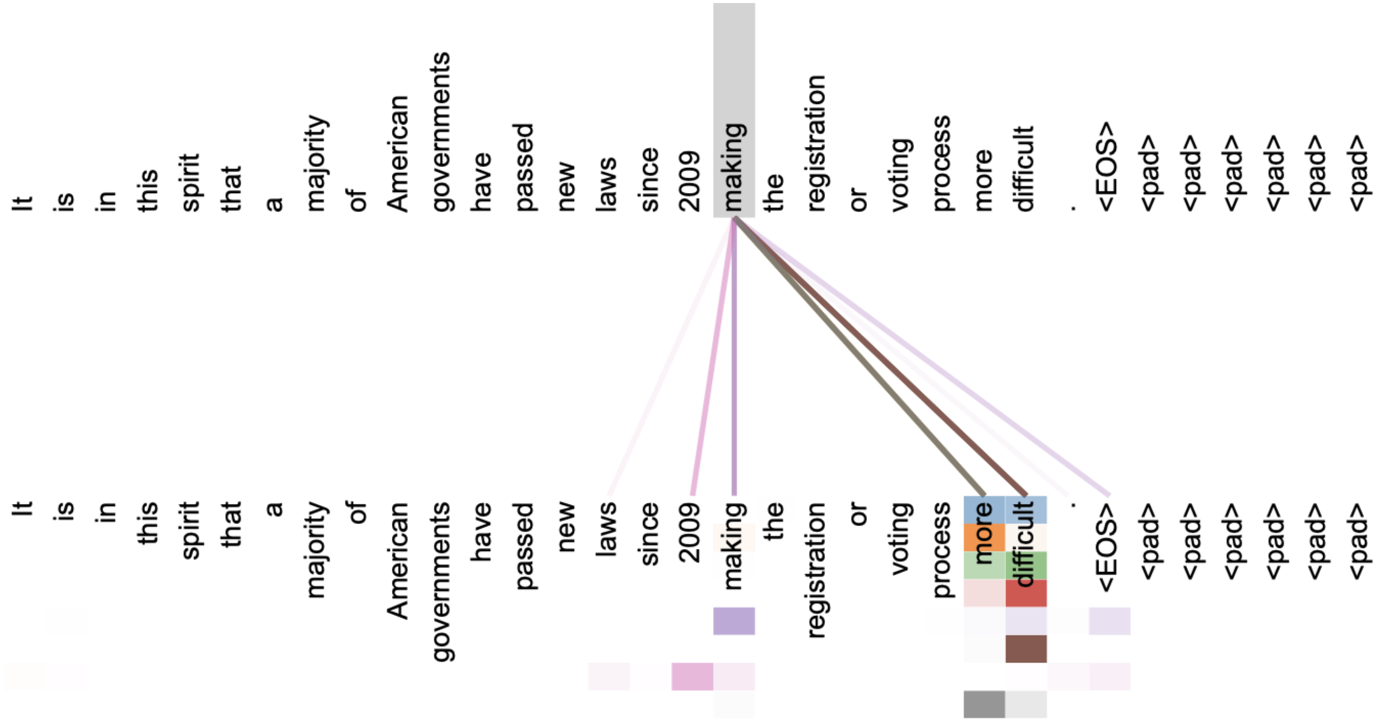


Figure 3: An example of the attention mechanism following long-distance dependencies in the encoder self-attention in layer 5 of 6. Many of the attention heads attend to a distant dependency of the verb ‘making’, completing the phrase ‘making...more difficult’. Attentions here shown only for the word ‘making’. Different colors represent different heads. Best viewed in color.

Vaswani, A., Shazeer, N., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A. N., ... & Polosukhin, I. (2017). Attention is all you need. In *Advances in neural information processing systems* (pp. 5998-6008).

The "Transformer"

Attention Is All You Need

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Attention is **all you need**
A Vaswani, N Shazeer, N Parmar… - Advances in neural …, 2017 - proceedings.neurips.cc
… to attend to **all** positions in the decoder up to and including that position. **We need** to prevent … **We** implement this inside of scaled dot-product **attention** by masking out (setting to −∞) …
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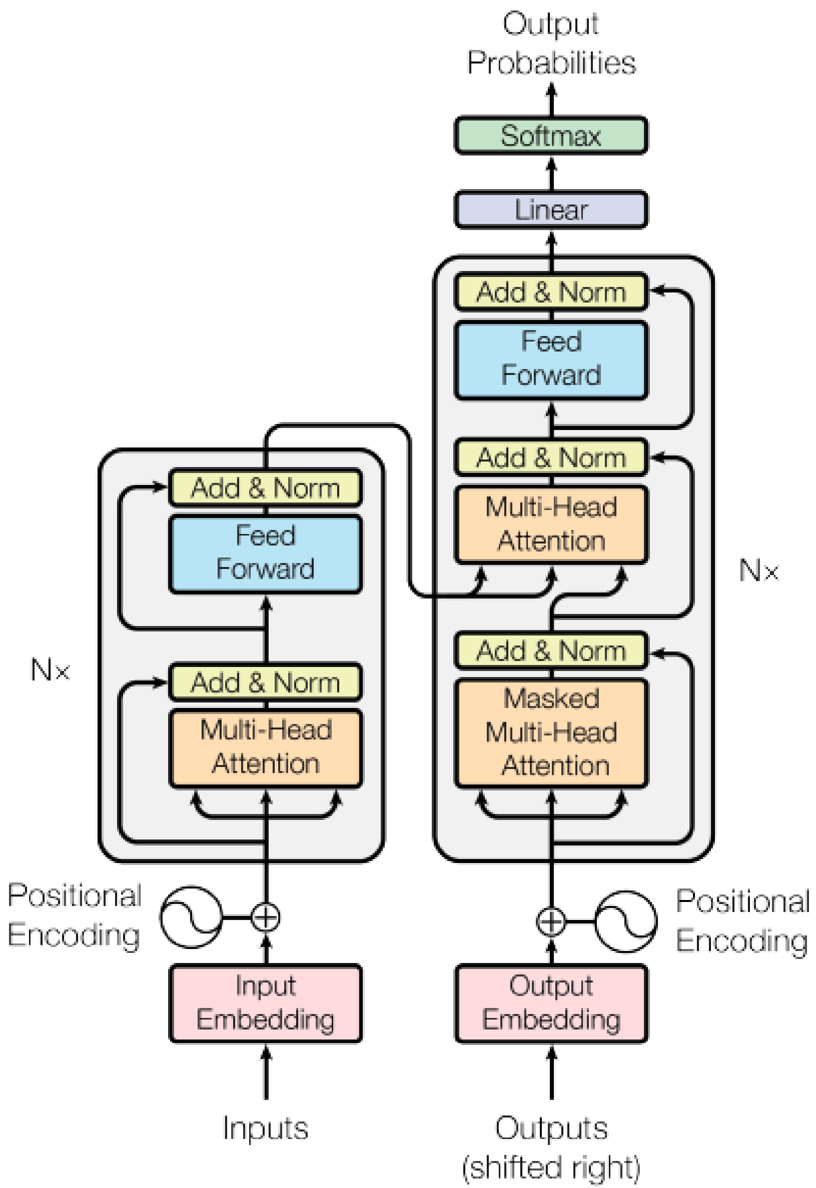
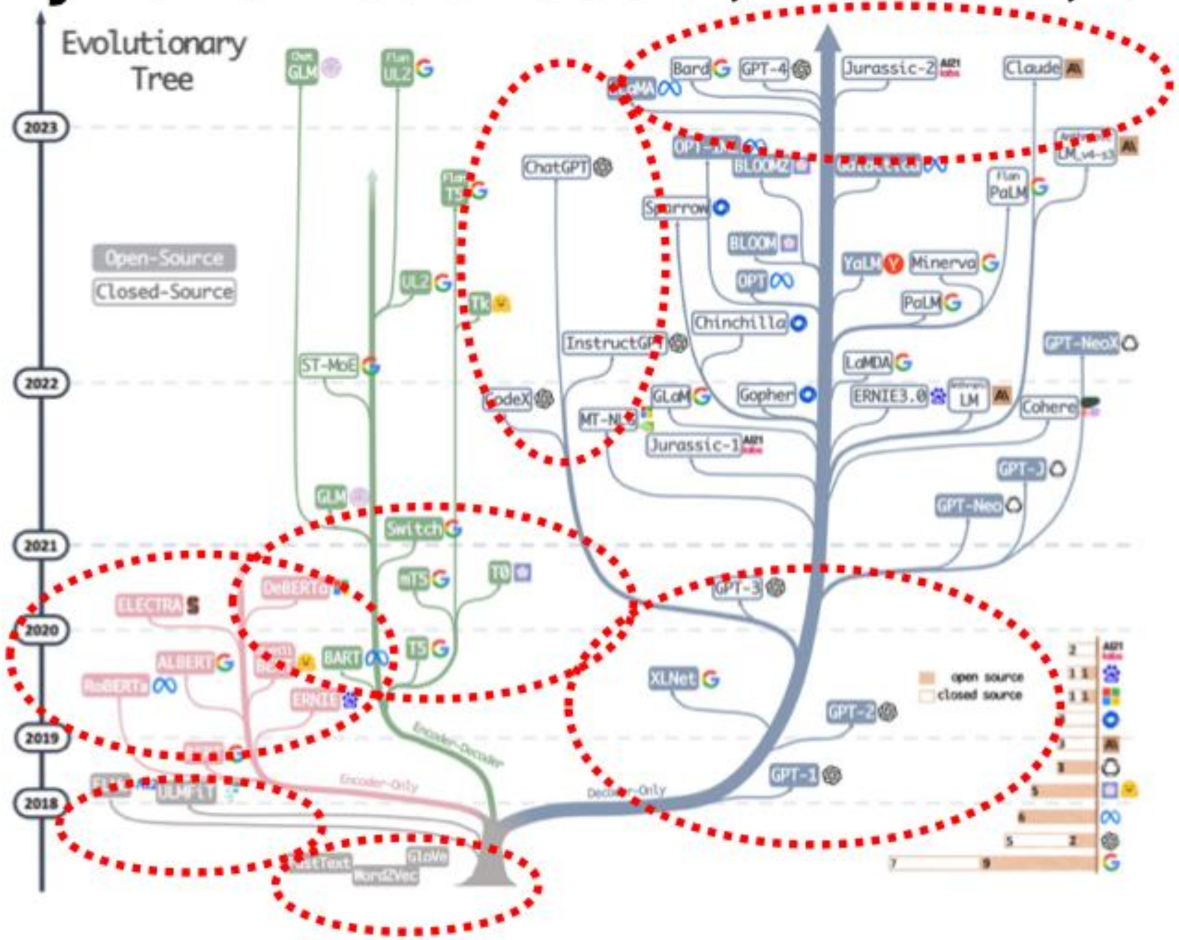


Figure 1: The Transformer - model architecture.

Many variants of transformer architectures

Many variants: encoder, decoder, or both



Yang et al., 2023, arxiv: 2304.13712

Many variants of transformer architectures

Some early transformer architectures

- **GPT-v1:** Generative Pre-Trained Transformer
- **BERT:** Bidirectional Encoder Representations from Transformers
- **GPT-v2:** Language Models are Unsupervised Multitask Learners
- **GPT-v3:** Language Models are Few-Shot Learners
- **BART:** Combining Bidirectional and Auto-Regressive Transformers
- Closing Words -- The Recent Growth of Language Transformers

Today: GPT

Generative Pre-Trained Transformer

From Transformer to GPT

Recall the "Transformer"

Attention Is All You Need

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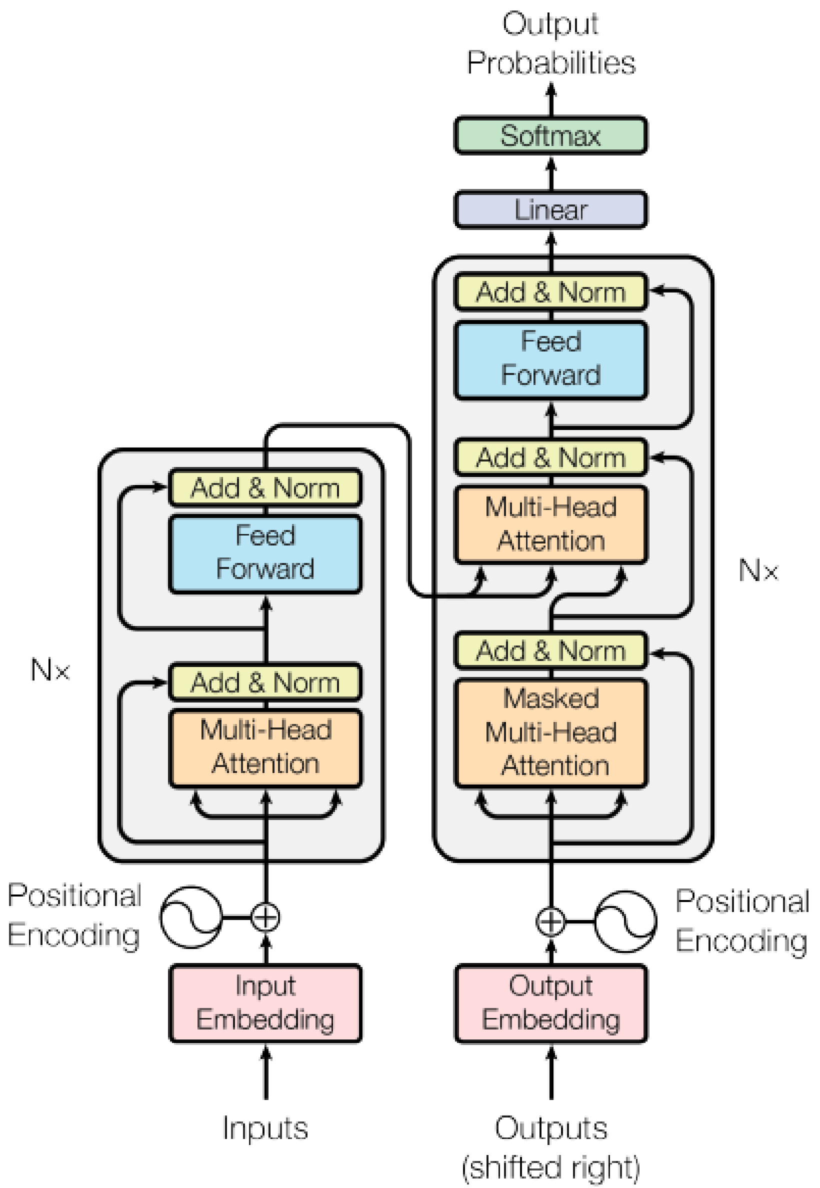


Figure 1: The Transformer - model architecture.

Recall the "Transformer"

- **Original Transformer** (Vaswani et al., 2017):
  - Encoder-decoder architecture for sequence-to-sequence tasks
  - Parallelizable self-attention instead of recurrence
  - Positional encodings enable order sensitivity
- **Encoder**: Processes input sequence
- **Decoder**: Generates output sequence using masked attention + encoder output
- Inspired by machine translation (observe full input sequence, predict full output sequence)

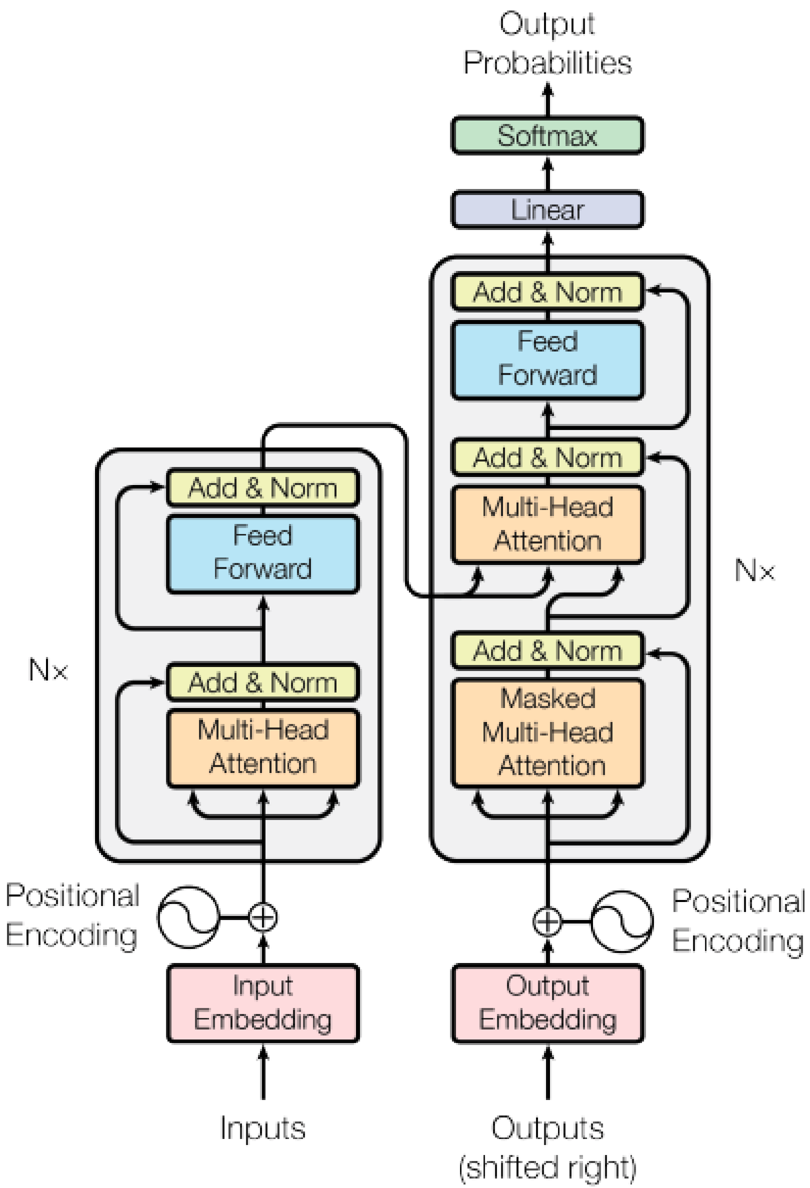


Figure 1: The Transformer - model architecture.

From Sequence Transduction to Sequence Modeling

- **Original Transformer** (Vaswani et al., 2017):

$$P(Y \mid X) = \prod_t P(Y_t \mid Y_{<t}, X)$$

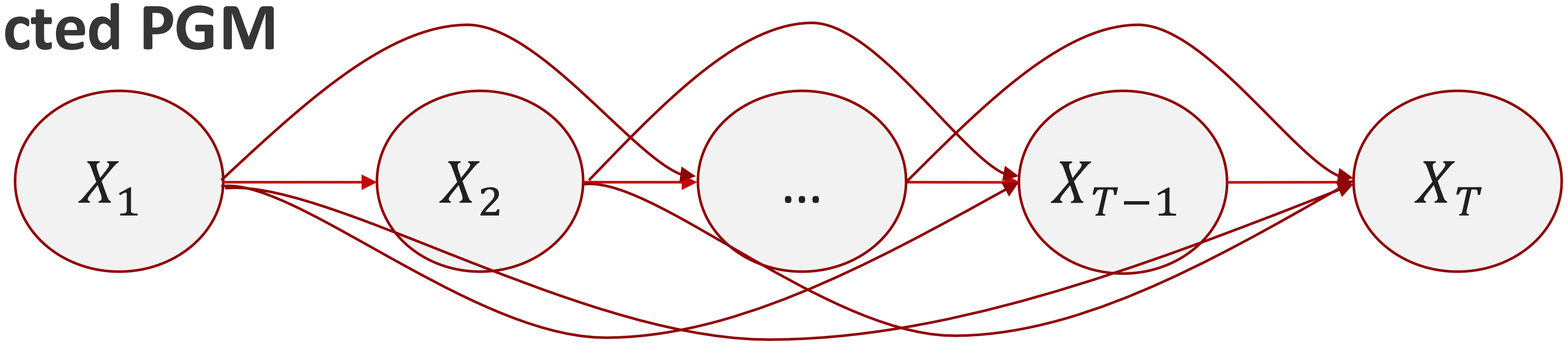
  - **Conditional** sequence model for tasks like translation (input → output)
- **Generative Pretrained Transformer (GPT)** Models:

$$P(X) = \prod_t P(X_t \mid X_{<t})$$

  - **Unconditional** generative model over raw text
- Architectural consequence: **no encoder**, only a decoder with causal structure

GPT = Probabilistic Model + Transformer Decoder

- **Directed PGM**



$$P_\theta(X) = \prod_i \prod_t P_\theta(X_{i,t} \mid X_{i,<t})$$

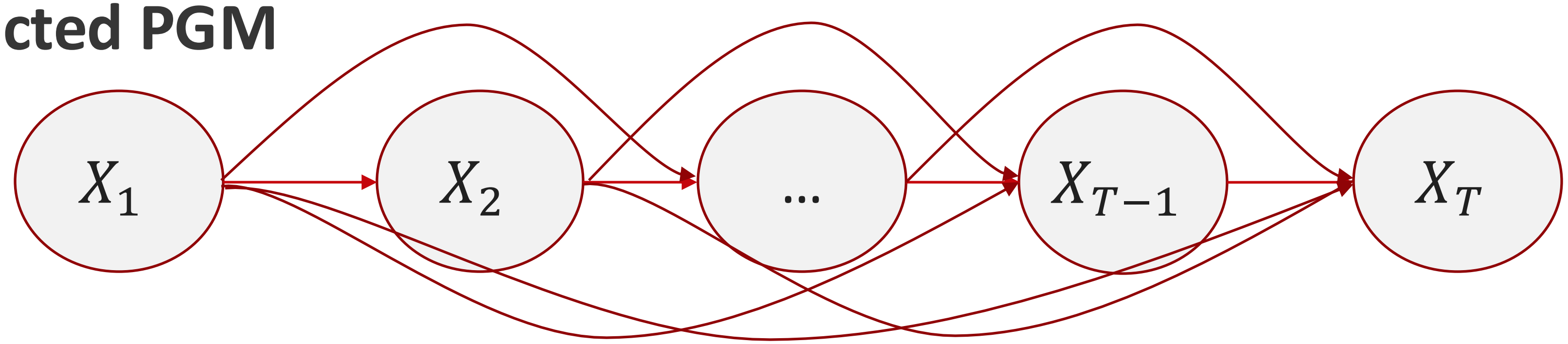
- **Probabilistic objective:** Max log-likelihood of observed seqs

$$\max_\theta \sum_i \sum_t \log P_\theta\left(X_{i,t} \mid X_{i,<t} \right)$$

[Radford et al., Improving Language Understanding by Generative Pre-Training]

GPT = Probabilistic Model + Transformer Decoder

- **Directed PGM**



$$P_\theta(X) = \prod_i \prod_t P_\theta(X_{i,t} \mid X_{i,<t})$$

- **Model structure:**
  - Input: token embeddings + positional encodings
  - Masked multi-head attention: Enforces “causality”
  - Decoder stack: Learns $P(X_t \mid X_{<t})$
  - Output: softmax over vocabulary

[Radford et al., Improving Language Understanding by Generative Pre-Training]

Let’s write a GPT

Let’s write a GPT

- EasyGPT repo
  - Adapted from Andrej Karpathy’s nanoGPT

From our “GPT” to GPT-4

From our “GPT-0” to GPT-1

- Architecture:
  - Tokenizer: Characters → “Byte-Pair Encoder” tokenizer
  - Activation: ReLU → GELU
  - Weight sharing for embedding / output
  - Scale (117M params):
    - Layers: 4 → 12
    - Attention Heads: 4 → 12
    - Block size (max context): 32 → 512
    - Vocab: 65 → 40000 BPE tokens
    - Embedding dim: 64 → 768
- Training:
  - Dataset: TinyShakespeare (1MB) → BookCorpus (5GB)
  - Initialization & normalization: Default → Carefully tuned
  - Optimizer: Vanilla Adam → Adam + learning rate warmup + weight decay
- Inference:
  - Sampling: Greedy → Top-k

From GPT-1 to GPT-2

GPT-2: [Radford et al., Language Models are Unsupervised Multitask Learners]

- Architecture:
  - Scale: Variety of options, with biggest (1.5B params):
    - Layers: 12 → 48
    - Attention Heads: 12 → 25
    - Embedding Dim: 768 → 1600
    - Block size (max context): 512 → 1024
    - Vocab: 40k → 50k tokens
- Training:
  - Dataset: BookCorpus (5GB) → WebText (40GB)

You can reproduce GPT-2 yourself:
https://github.com/karpathy/nanoGPT
(takes 4 days to train on an 8xA100 machine)

From GPT-2 to GPT-3

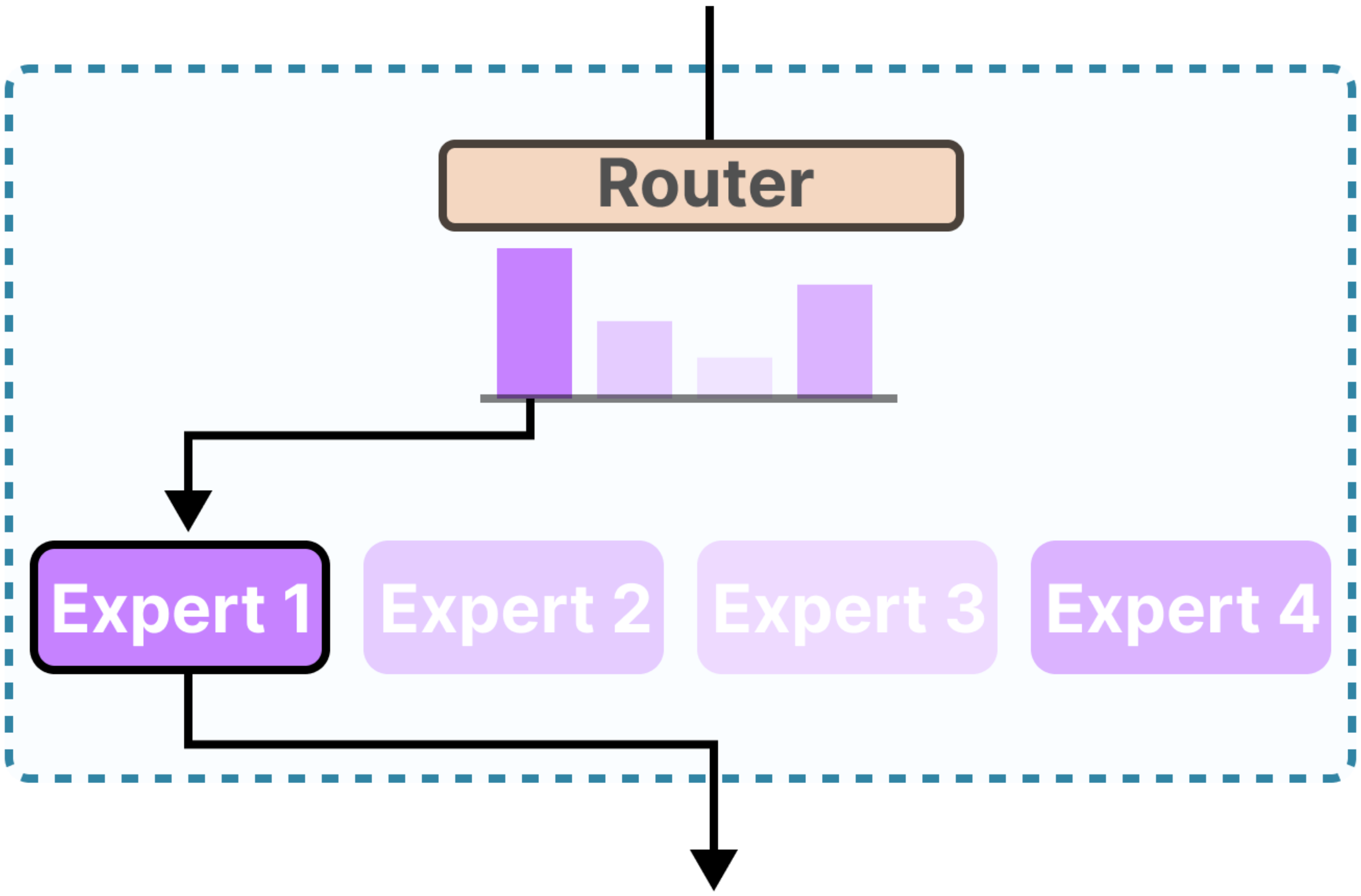
- Architecture:
  - Scale (1.5B → 175B params):
    - Block size (max context): 1024 → 2048
    - Layers: 48 → 96
    - Embedding Dim: 1600 → 12,288
    - Attention Heads: 25 → 96
- Training:
  - Dataset: WebText (40GB) → Common Crawl + books, Wikipedia, code, etc. (~570GB)

GPT-3: [Brown et al., Language Models are Few-Shot Learners]

From GPT-3 to GPT-4?

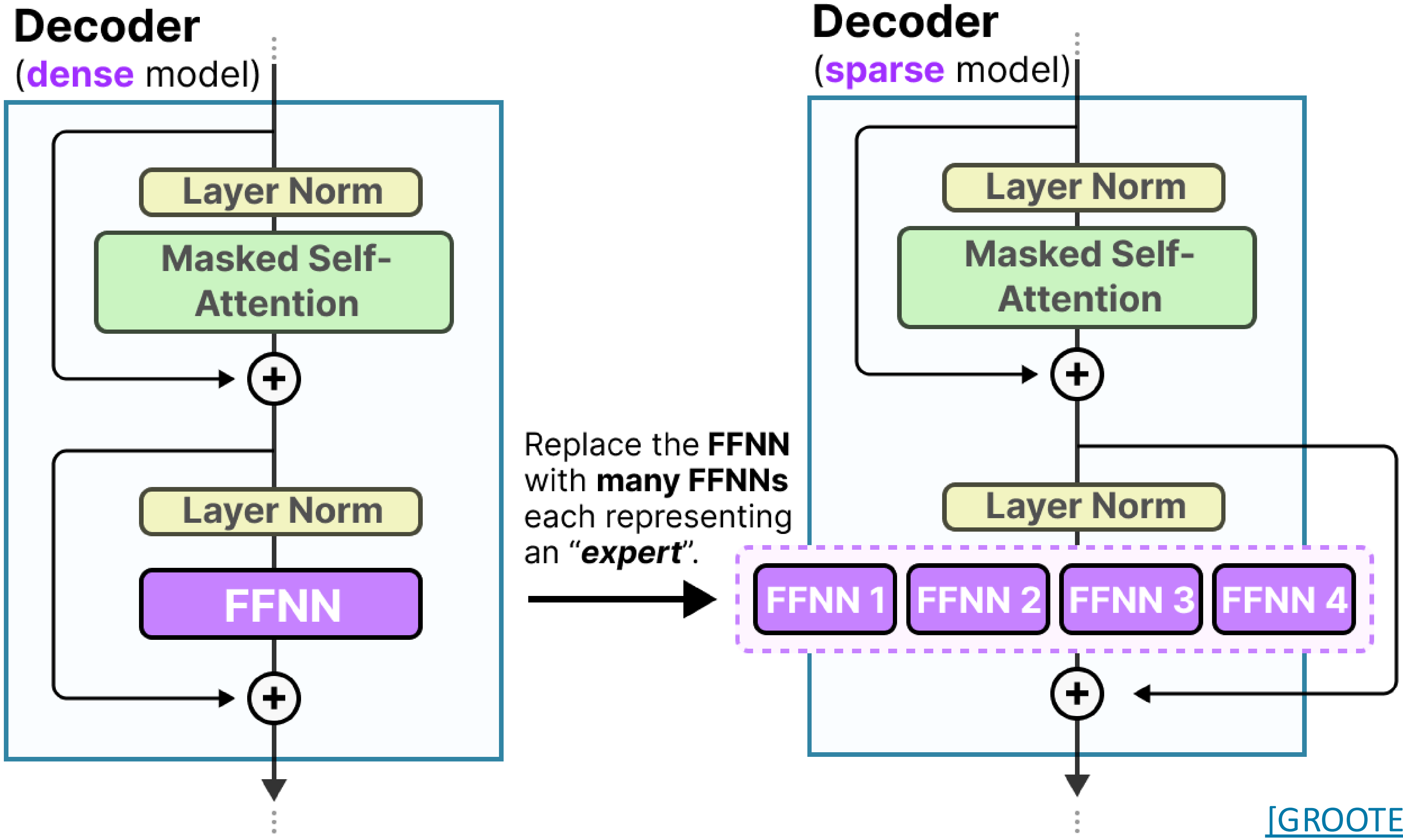
- Architecture:
  - Likely includes MoE
  - Tokenizer: Includes image patches for multi-modal
  - Scale:
    - Total parameters: 175B → Likely >1T
    - Block size (max context): 2048 → 128k
- Training:
  - Dataset: Common Crawl + books, Wikipedia, code, etc. (~570GB) → Larger, undisclosed data training. Reported 13T tokens (~50TB)
  - Alignment: Reinforcement learning + human feedback + system-level “safety”

Mixture of Experts



[GROOTENDORST]

Mixture of Experts inside Transformer Decoder



[GROOTENDORST]

Mixture of Experts: A probabilistic idea

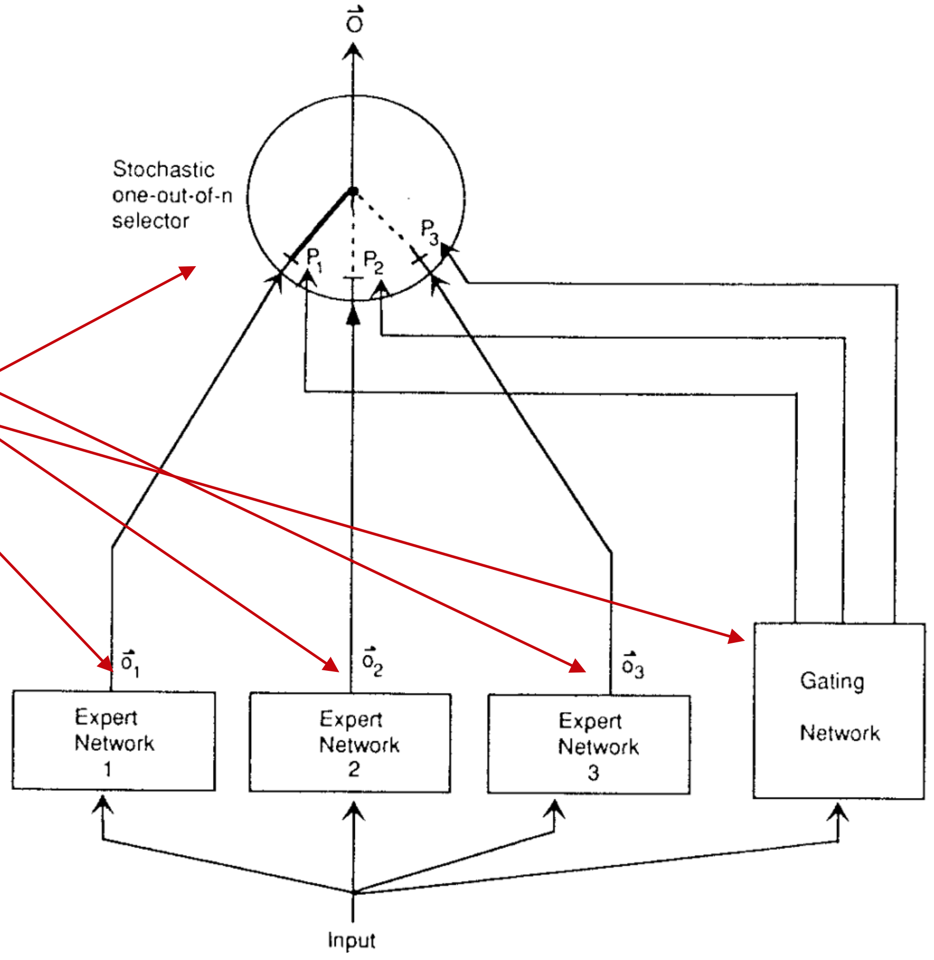
- Let

$$P(Y \mid X) = \sum_m g_m(X) \cdot P_m(Y \mid X)$$

- Constrain $\sum_m g_m(X) = 1$ and $g_m(X) \geq 0 \; \forall \, m, \mathrm{X}.$

How would you estimate these parameters?

[Hierarchical mixtures of experts and the EM algorithm, 1993]



"Adaptive Mixtures of Local Experts" Jacobs et al 1991

Mixture of Experts: Unifies Several Approaches

Let

$$P(Y \mid X) = \sum_m g_m(X) \cdot P_m(Y \mid X)$$

- **Mixture of Experts** [Jacobs et al 1991]: $g_m(X)$ is a learned gating function.
- **Bagging** [Breiman 1996]: $g_m(X) = \frac{1}{M}$ is a constant, uniform weighting.
- **Boosting** [Freund & Schapire 1997]: $g_m(X) = \alpha_m$ is a constant per-expert weight.

Bonus

Mixture of Experts: Some analysis

Let

$$P(Y \mid X) = \sum_m g_m(X) \cdot P_m(Y \mid X)$$

- Let's examine the mean functions. Define:

$$\bar{f}(x) \coloneqq \mathrm{E}[\,Y \mid X\,] = \sum_m g_m(X) E_m[\,Y \mid X\,] = \sum_m g_m(X)\, f_m(x)$$

- Let's compare:
  - $\epsilon(x) \coloneqq \left(Y - \bar{f}(x)\right)^2$ ← "Ensemble error"
  - $\bar{\epsilon}(x) \coloneqq \frac{1}{M} \sum_m \left(Y - f_m(x)\right)^2$ ← "Average expert error"

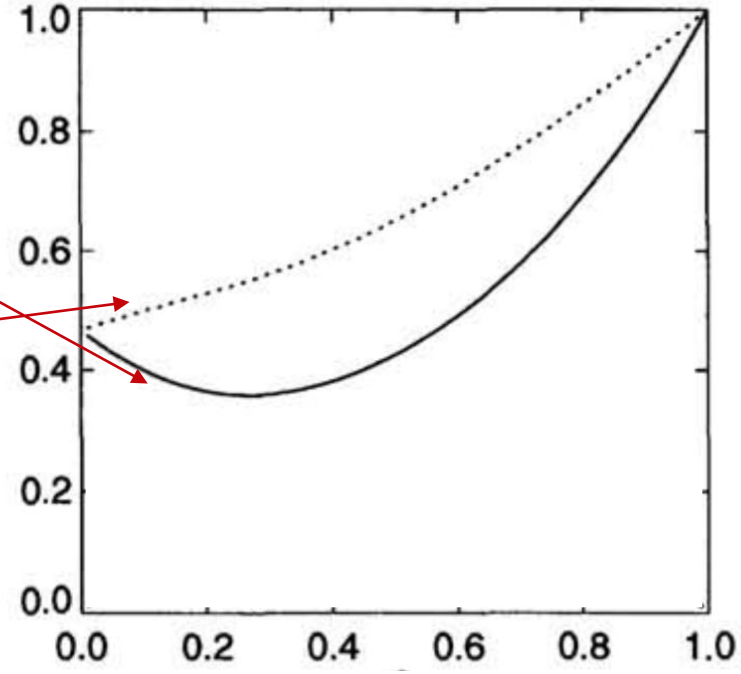
Will these be minimized for the same ensemble?

Bonus

Mixture of Experts: Some analysis

- $\epsilon(x) := \left(Y - \bar{f}(x)\right)^2$ "Ensemble error"
- $\bar{\epsilon}(x) := \frac{1}{M}\sum_m \left(Y - f_m(x)\right)^2$ "Average expert error"

Linear f_m



Diversity in Experts
(% Unique Training Data)

[Sollich & Krogh 1995]

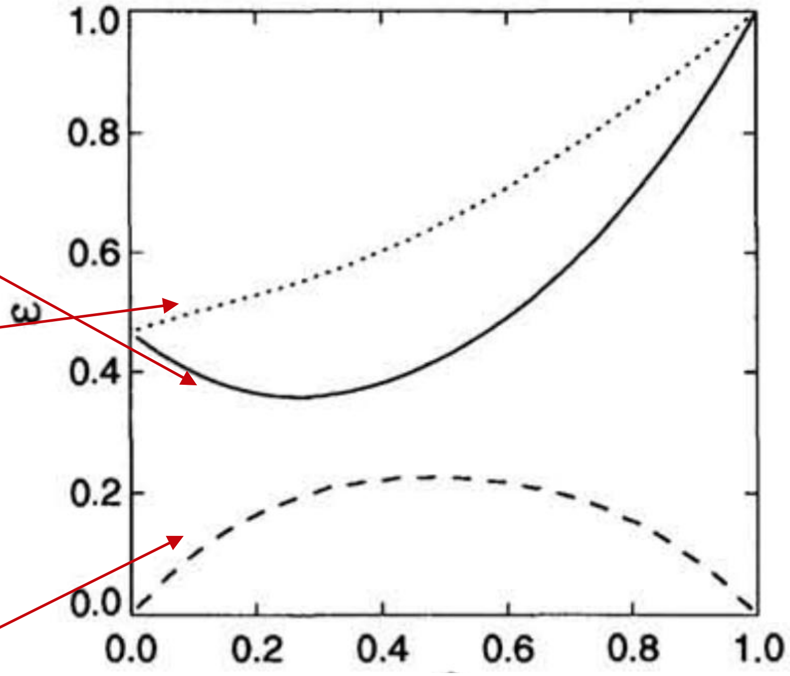
Bonus

Mixture of Experts: Some analysis

- $\epsilon(x) := \left(Y - \bar{f}(x)\right)^2$ "Ensemble error"
- $\bar{\epsilon}(x) := \frac{1}{M}\sum_m \left(Y - f_m(x)\right)^2$ "Average expert error"

"Disagreement between experts"

Linear f_m



Diversity in Experts
(% Unique Training Data)

[Sollich & Krogh 1995]

Intuition: Expert errors are wrong in individualized ways and cancel out through consensus.

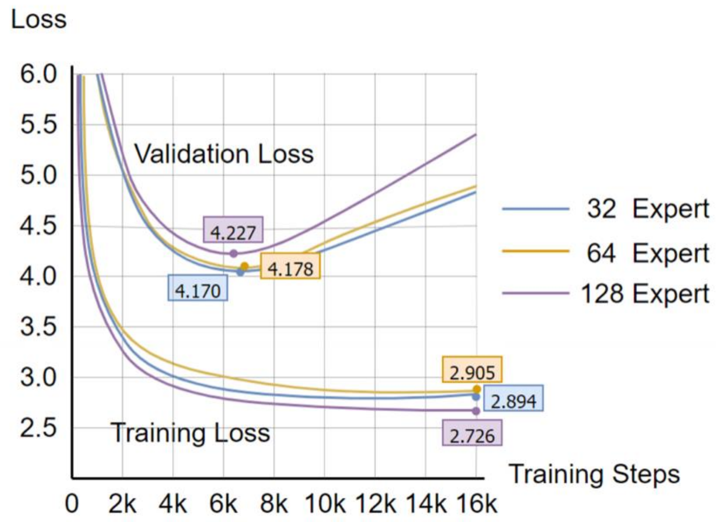
→ Slight "overfitting" of experts helps!

Mixture of Experts: In LLMs

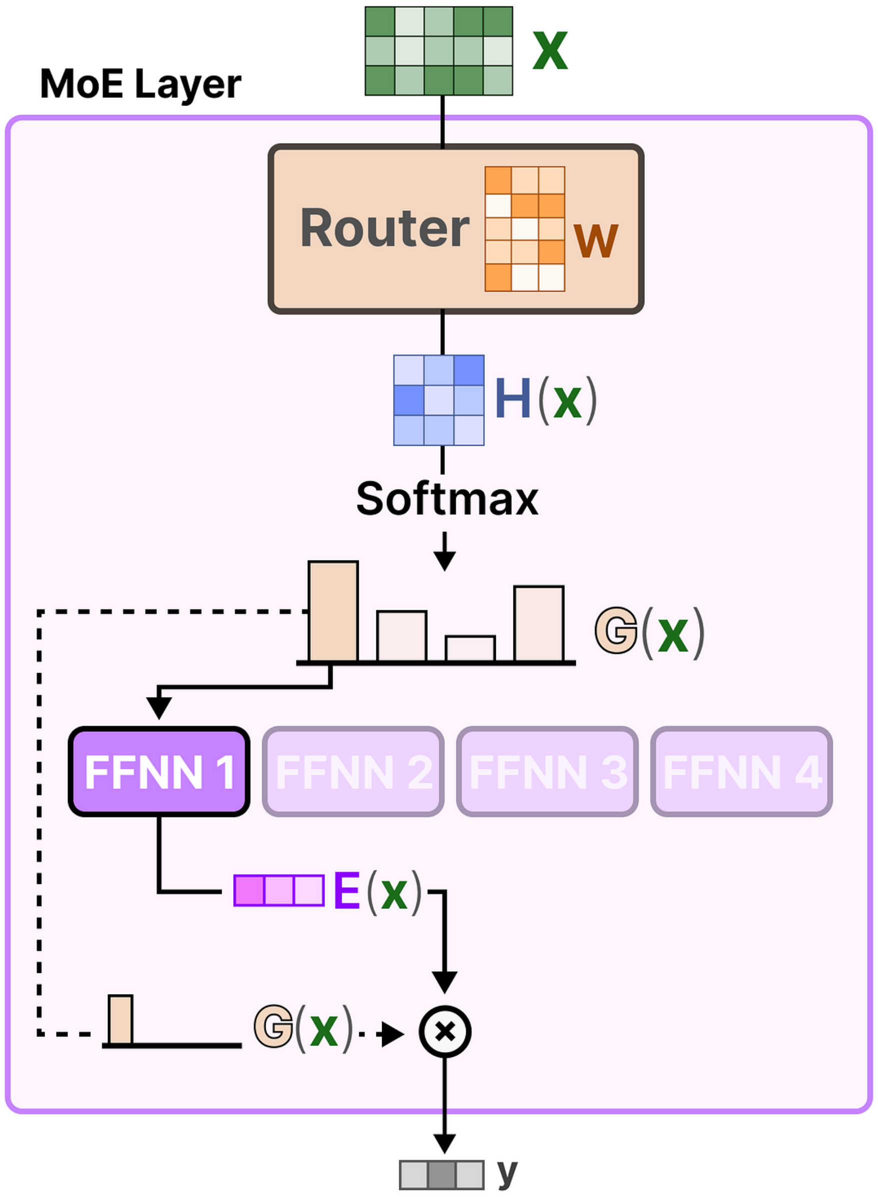
- Implications for serving?

- Implications for training?

Easy to have experts over-specialize



[XIE ET AL 2022]



[GROOTENDORST]

Summary: From Transformer to GPT

Component	Transformer	GPT
Architecture	Encoder-decoder (full)	Decoder-only
Attention	Full self-attention	Masked (causal) self-attention
Positional encoding	Sinusoidal (original)	Learned positional embeddings
Output	Task-specific	Next-token prediction
Training objective	Flexible (e.g., translation)	Language modeling (autoregressive)
Inference	Depends on task	Greedy / sampling for text gen

Summary: From GPT-1 to GPT-4

- **Architecture:**
  - **Scale:** Variety of options, with biggest (1.5B params → >1T params):
    - Block size (max context): 512 → 128k
    - Layers: 12 → >96
    - Attention Heads: 12 → >96
    - Embedding Dim: 768 → >12,288
    - Vocab: 40k → >50k tokens
  - Tokenizer: Includes image patches for multimodal
  - **Mixture-of-Experts**
- **Training:**
  - Dataset: BookCorpus (5GB) → Private 13T tokens (~50TB)
  - Reinforcement learning for alignment

Questions?

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