Transformers

Self-Attention and BERT

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WHO ARE MY NEIGHBOURS?

Traditional domain in a windowed (ramp or otherwise) approach includes frequency counts (co-occurrence) and correlation measures[1]

- Frequency count - cooccurence
- Correlation

SVD Domain

- The transformation of the incidence matrix into SVD domain leads to define the relationship between two words based on the magnitude of the diagonal matrix Σ

$$A = \sum_{j=1}^{r} \sigma_j u_j v_j^T$$

σ_j capture the strength of latent semantic dimensions
The low-rank approximation captures as much information/energy as possible with respect to the word relationships

GloVe Domain

- GloVe is a global log-bilinear regression model capturing global corpus statistics. Ratio of the co-occuring word probabilities are transformed into word embeddings[2]

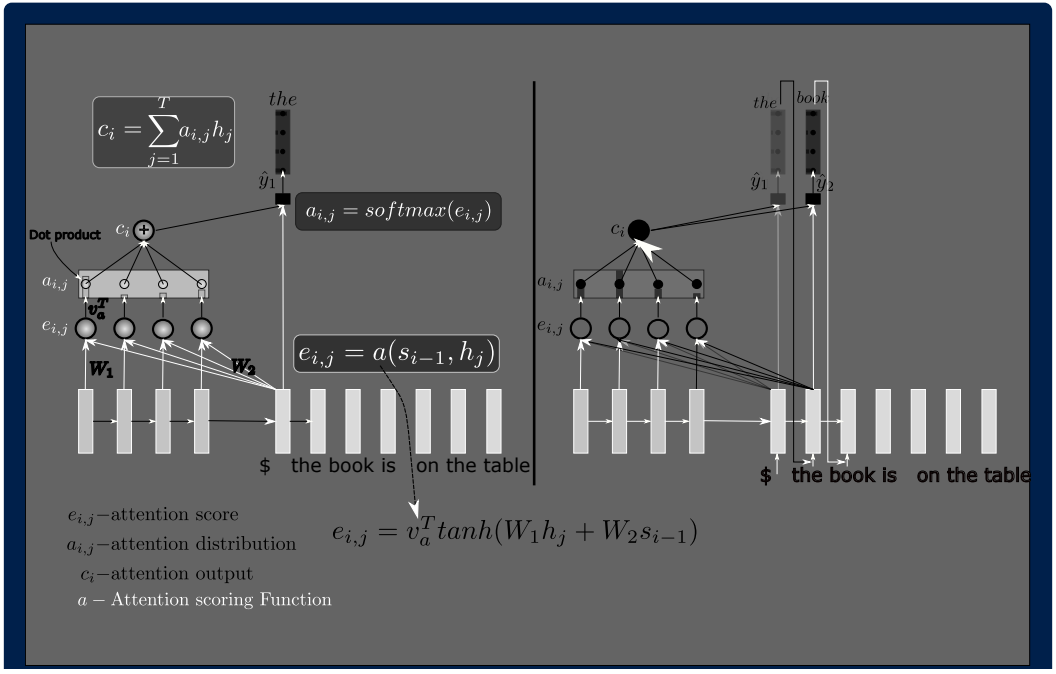
LANGUAGE MODELS

Useful in

- Auto-generation of sentences
- Auto-completion of sentences
- Creating contextualized word-vectors
- Machine Translation

ATTENTION: WHERE DID IT BEGIN? [3] I

ATTENTION: WHERE DID IT BEGIN? [3] II



DO I KNOW MORE ABOUT MYSELF AND MY NEIGHBORS?

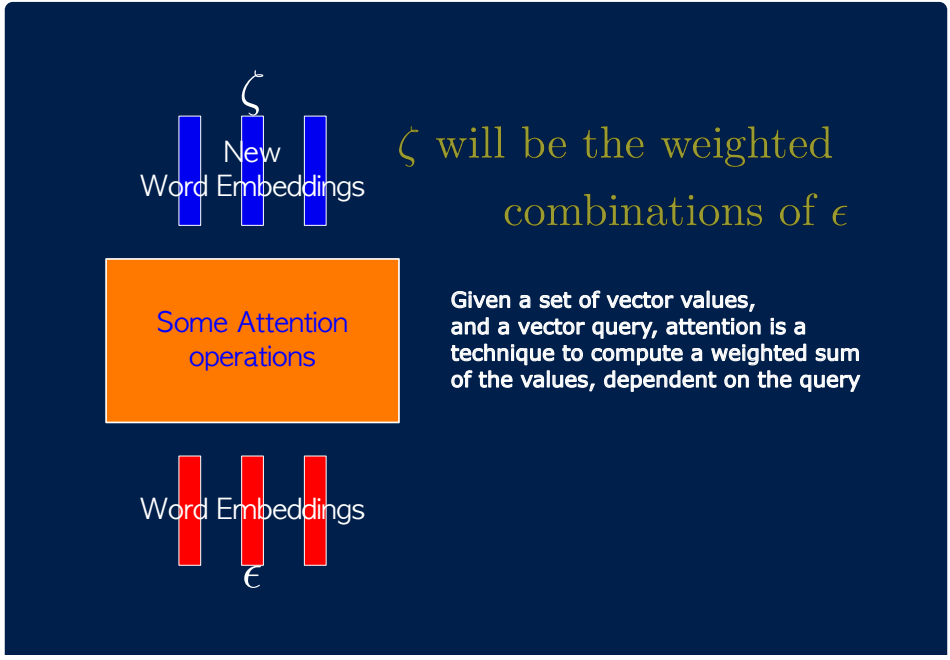
- How much influence should I receive from my neighboring words??
- How can I effectively capture information from my neighbors?

Ideally word embeddings aim to capture meaningful semantic relations beyond raw counts or co-occurrence frequencies

ANY CHANGE REQUIRED?

- Is it possible to encode the time series data differently?
- How can we manage the complexities of recurrent models (serial processing, vanishing/exploding gradient)?
- Is it possible to encode each word vector differently depending on its context?

IDEAL ENCODING OF EMBEDDING



QUERY-KEY INTERACTION

- Computes relevance scores for each query token by considering all keys from input tokens
- Evaluates its relationship with every other token in the sequence, including itself
- Enables a comprehensive assessment of contextual dependencies

MECHANISM

The process begins with the query matrix Q for a specific token being dot-producted with the entire key matrix K^T, where K encompasses representations from all tokens in the context, resulting in a score for each possible pair.
These scores are then scaled by $\sqrt{d_k}$ and passed through a softmax to produce attention weights, ensuring that the query's focus is distributed across all relevant keys without omission.
This full consideration promotes parallelism and captures global interactions, as opposed to local windows in other architectures, making it efficient for sequences of varying lengths.

MECHANISM OF CONSIDERATION (EQUATIONS)

The scaled dot-product computation:

$$s_{ij} = \frac{q_i \cdot k_j^T}{\sqrt{d_k}} \tag{1}$$

Attention weights via softmax:

$$\alpha = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right) \tag{2}$$

IMPLICATIONS FOR ATTENTION COMPUTATION

- Generates a weighted sum of value vectors based on the relevance of tokens in the context.
- Token Consideration: No token is excluded initially, allowing the model to prioritize relationships across the entire input.
- Dynamically prioritizes distant or subtle relationships, such as coreferences or syntactic dependencies.

IMPLICATIONS FOR ATTENTION COMPUTATION (CONTINUED)

In practice, for a sequence of length n, this leads to an $O(n^2)$ complexity per attention head, but optimizations like masking can limit it in decoder contexts without altering the core all-keys consideration principle.
The final output is:

$$\text{Output} = \alpha V \tag{3}$$

THE CAUSAL (DECODER) MASK

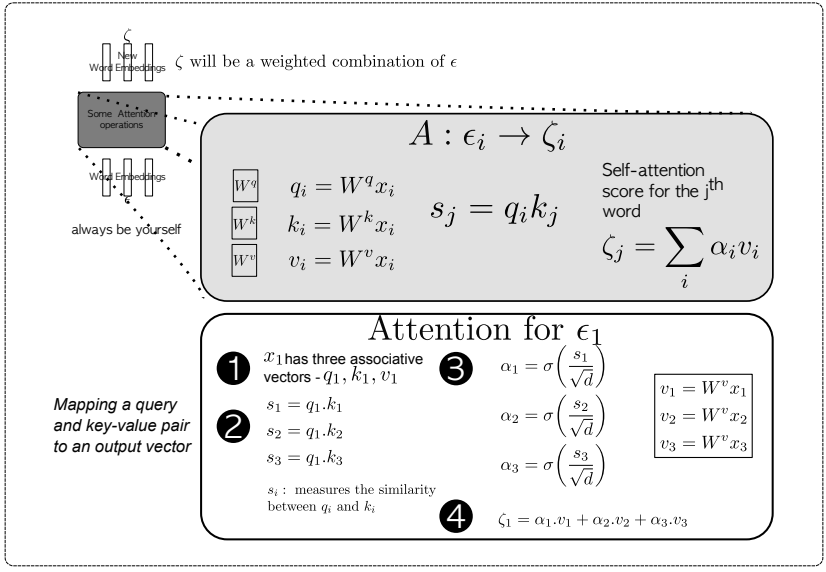
A language model must not see the future: when predicting token i, only positions $j \leq i$ may contribute. This is enforced *before* the softmax:

$$S_{ij} = \frac{(QK^\top)_{ij}}{\sqrt{d_k}}, \qquad S_{ij} \leftarrow -\infty \text{ for all } j > i \tag{4}$$

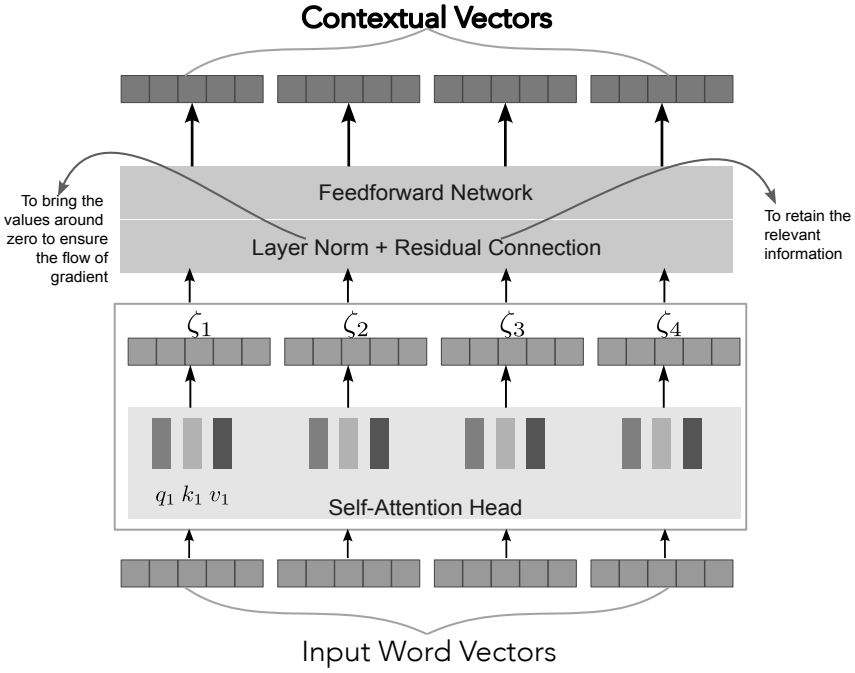
- $e^{-\infty} = 0$, so masked positions get **exactly zero** attention weight and each row still sums to 1 over the surviving entries
- Row 0 can attend only to itself, so its output is exactly V_0
- The *last* row is unchanged by the mask: it could already see everything
- Encoder (BERT-style) attention omits the mask; decoder (GPT-style) attention always applies it. This single matrix of $-\infty$s is the difference between "understanding" and "generating"

Masking, then softmax, never the other way round. Renormalisation is what redistributes the blocked probability mass over the visible tokens.

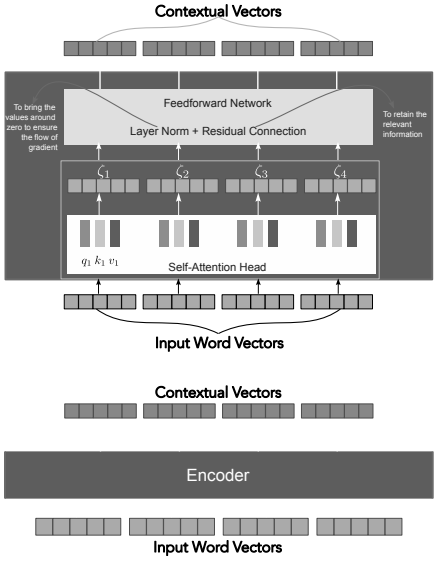
SELF-ATTENTION LAYER

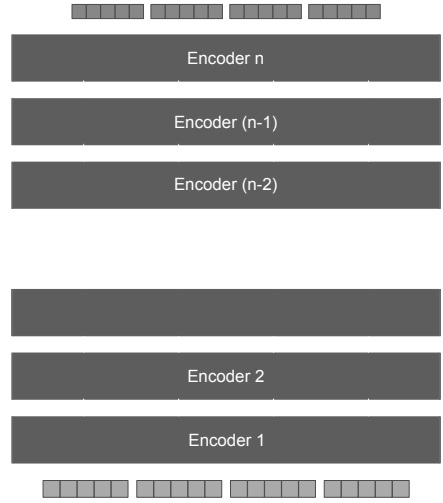


SINGLE TRANSFORMER LAYER



TRANSFORMER ENCODER





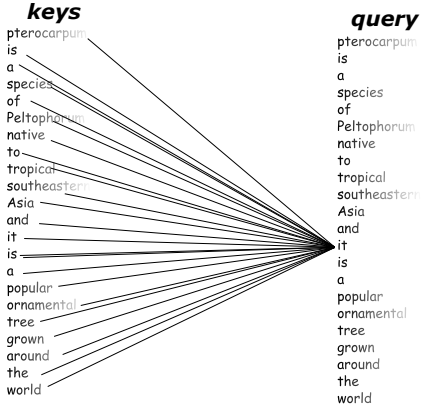
SELF-ATTENTION

Peltophorum pterocarpum is a species of **Peltophorum**, native to tropical southeastern Asia and **it** is a popular ornamental tree grown around the world

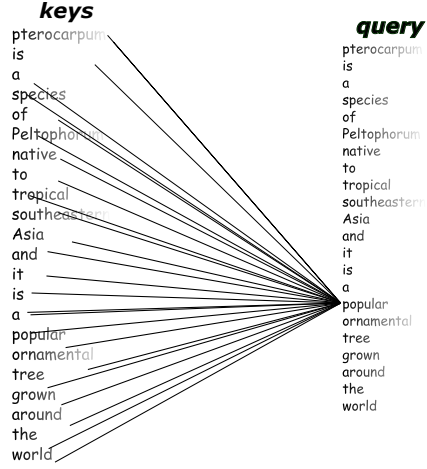
What does it refer to?

Self-attention allows us to associate *it* with Peltophorum pterocarpum

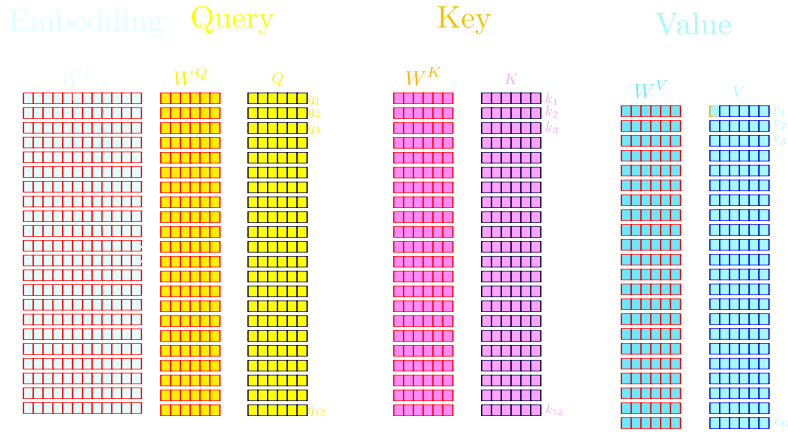
SELF-ATTENTION - WORD LEVEL



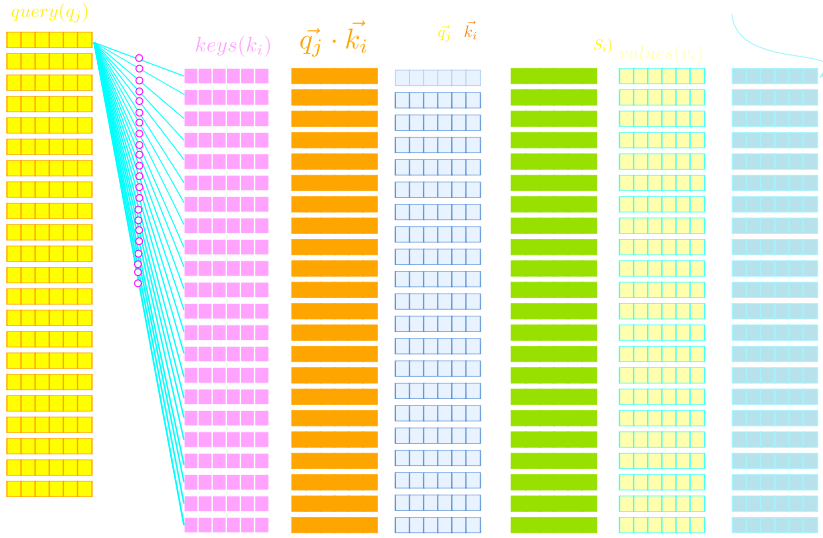
Self-attention allows each word to align itself to other words using their positions and looks for clues for a better contextul encoding



CREATING QUERY, KEY AND VALUES



COMPUTING ATTENTION(Q,K,V)

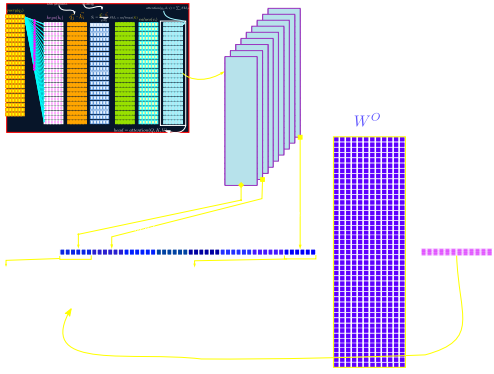


MULTI-HEAD ATTENTION

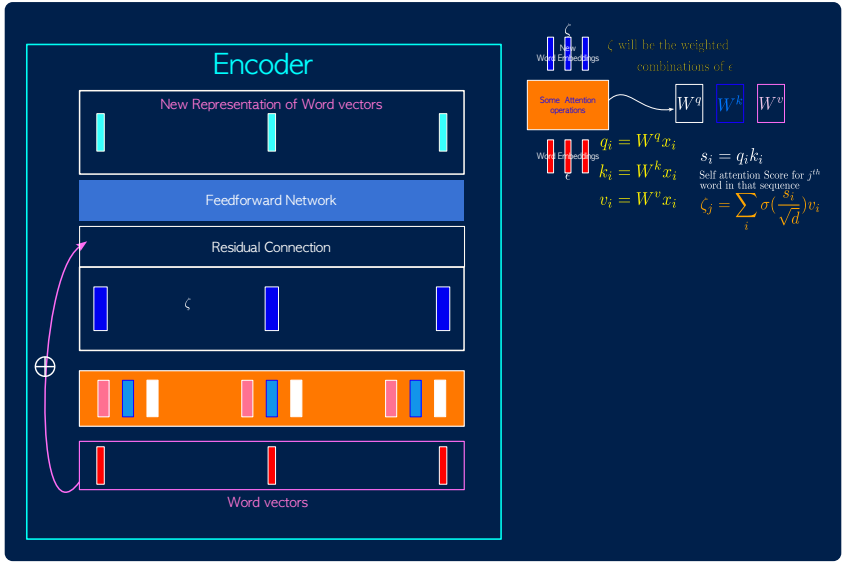
The summed attention score,

$$a(q, k_i, v_i) = \sum_i \left(\frac{e^{\frac{q \cdot k_i}{\sqrt{d_k}}}}{\sum_j e^{\frac{q \cdot k_j}{\sqrt{d_k}}}} \right) v_i$$

has information about all the word, but may have more information about words that have similarity scores higher than others in that context.



SELF-ATTENTION



ATTENTION COMPUTATION: A SIMPLIFIED EXAMPLE I

Let's compute attention using a simplified example with word embeddings. We'll use a small set of embeddings for demonstration purposes.
Assume we have the following word embeddings for simplicity:

- **Query (q)**: Embedding for "who"
- **Keys (k)**: Embeddings for "is", "the", "best"
- **Values (v)**: Same as Keys for simplicity, but in practice, they could be different.

SAMPLE SET OF WORDS

Let's say each embedding is a 3-dimensional vector:

$$
\begin{aligned}
&q : [0.1, 0.2, 0.3] \\
&k_1 \text{ (is)} : [0.4, 0.5, 0.6] \\
&k_2 \text{ (the)} : [0.2, 0.1, 0.3] \\
&k_3 \text{ (best)} : [0.6, 0.7, 0.8] \\
&v_1 \text{ (is)} : [0.4, 0.5, 0.6] \\
&v_2 \text{ (the)} : [0.2, 0.1, 0.3] \\
&v_3 \text{ (best)} : [0.6, 0.7, 0.8]
\end{aligned}
$$

Compute similarity scores - Dot Product

$$q \cdot k_1 = 0.1 \cdot 0.4 + 0.2 \cdot 0.5 + 0.3 \cdot 0.6 = 0.04 + 0.1 + 0.18 = 0.32$$
$$q \cdot k_2 = 0.1 \cdot 0.2 + 0.2 \cdot 0.1 + 0.3 \cdot 0.3 = 0.02 + 0.02 + 0.09 = 0.13$$
$$q \cdot k_3 = 0.1 \cdot 0.6 + 0.2 \cdot 0.7 + 0.3 \cdot 0.8 = 0.06 + 0.14 + 0.24 = 0.44$$

Apply Softmax Normalization

- **Exponentiation** $e^{0.32/\sqrt{3}} \approx 1.20, \quad e^{0.13/\sqrt{3}} \approx 1.08, \quad e^{0.44/\sqrt{3}} \approx 1.29$
- **Sum of exponents:** $1.20 + 1.08 + 1.29 = 3.57$
- **Attention weights:** $\alpha_1 = \frac{1.20}{3.57} \approx 0.34, \quad \alpha_2 = \frac{1.08}{3.57} \approx 0.30, \quad \alpha_3 = \frac{1.29}{3.57} \approx 0.36$

STEP 2: WEIGHTED SUM OF VALUE VECTORS ζ

$$\begin{aligned}\text{Attention}(q,k,v) &= \alpha_1 v_1 + \alpha_2 v_2 + \alpha_3 v_3 \\ &= 0.34 \cdot [0.4, 0.5, 0.6] + 0.3 \cdot [0.2, 0.1, 0.3] + 0.36 \cdot [0.6, 0.7, 0.8] \\ &= [0.41, 0.45, 0.58]\end{aligned}$$

The attention output for the query "who" given the keys and values "is", "the", "best" is approximately:

$$\zeta = [0.41, 0.45, 0.58]$$

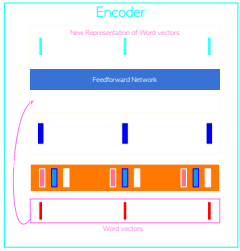
This vector represents a weighted combination of the input values, where the weights are determined by how relevant each key is to the query, as computed through the attention mechanism.

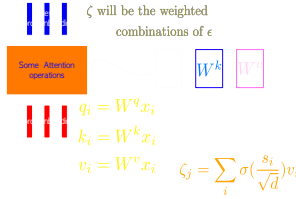
Note: This is a highly simplified example. In real-world scenarios, embeddings are much higher dimensional, and the attention mechanism is applied across all positions in the sequence, often in parallel for efficiency.

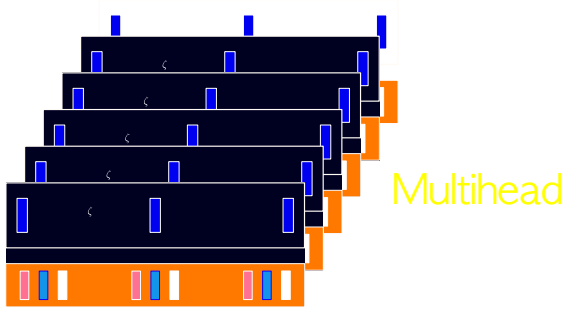
PYTHON CODE TO COMPUTE ζ

```
import numpy as np

def compute_attention(q, keys, values):
d = q.shape[0]
# Compute scaled dot products
dot_products = np.dot(keys, q) / np.sqrt(d)

exp_scores = np.exp(dot_products - np.max(dot_products))
attention_weights = exp_scores / np.sum(exp_scores)

zeta = np.sum(attention_weights[:, None] * values, axis=0)
return attention_weights, zeta
```

MULTIHEAD ATTENTION







POSITIONAL ENCODING

- RNN models encode the time signal in a sequential manner
- Positional encoding is important for contextual learning
- Transformers use a separate positional vector which is added to the embedding
- Positional encoding should be unique, not just a scalar
- Positional values should be bounded
- Positional values between any two positions should be consistent
- Sentence length should not be a constraint
- Deterministic

POSITIONAL ENCODING

$$\vec{pe}_t^{\,i} = \begin{cases} \sin(\omega_k \cdot t), & \text{if } i = 2k \\ \cos(\omega_k \cdot t), & \text{if } i = 2k+1 \end{cases}$$

where $\omega_k = \frac{1}{10000^{(2k/d)}}$.

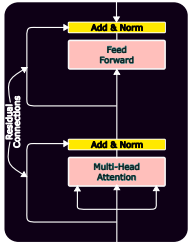
This positional vector will be a pair of sin and cos values and i is the index of the dimension in the word vector

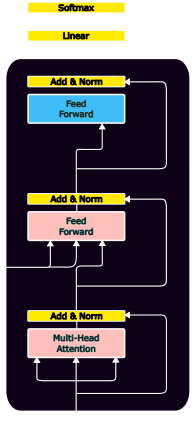
1. Good reference for Transformer - The Illustrated Transformer, Jay Alammar
2. The Annotated Transformer - Austin Huang et al

POSITIONAL ENCODING - PYTHON CODE

```
def positional_encoding(position, d_model):
    angle_rates = 1 / np.power(10000, \
    (2 * (np.arange(d_model) // 2)) / d_model)
    position = position.reshape(-1, 1)
    angle_rates = angle_rates.reshape(1, -1)
    angle_rates = position * angle_rates
    angle_rates[:, 0::2] = np.sin(angle_rates[:, 0::2])
    angle_rates[:, 1::2] = np.cos(angle_rates[:, 1::2])
    return angle_rates
```

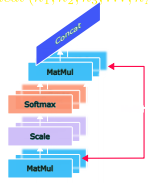
TRANSFORMER ARCHITECTURE





$$\text{Attention} = softmax\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$

$$MultiHead(Q,K,V) = Concat(h_1, h_2, h_3, \ldots, h_N)w^O$$



NUMBER OF PARAMETERS IN A TRANSFORMER

Embedding Layer - $N_{emb} = V \times D$
where N_{emb} is the number of parameters in the embedding layer, V is the vocabulary size and D is the embedding dimension

Multi-Head Attention - $N_{attn} = 3 \times D \times d_k \times h + h \times d_v \times d_k + 2 \times h \times d_k$ (biases)
where N_{attn} is the number of parameters in multi-head attention, D is the embedding dimension, d_k is the dimension of the key vector, h is the number of heads and d_v is the dimension of the value vector

Feed-Forward Network - $N_{ffn} = 2 \times D \times H + H + H \times D$
where N_{ffn} is the number of parameters in the feed-forward network, D is the embedding dimension and H is the hidden dimension

Layer Norm - $N_{ln} = 2 \times D$
where N_{ln} is the number of parameters in the layer normalization, D is the embedding dimension

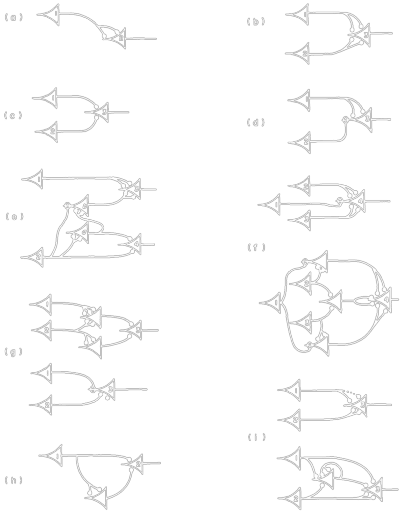
Total Number of Parameters per Encoder/Decoder Layer - $N_{layer} = N_{attn} + N_{ffn} + N_{ln}$

Total Number of Parameters in the Transformer - $N_{total} = N_{emb} + N_{layer} \times L$
where L is the number of layers

CHARACTERISTICS OF DIFFERENT LANGUAGE MODELS

Dependency Type	Dependency Structure	Models	
Independent Prediction	Does not depend on any token	Unigram	$P(X) = \prod_{i=1}^{M} P(x_i)$
Markov (Left2Right)	Depends on a fixed number of previous tokens	N-gram	$P(X) = \prod_{i=1}^{M} P(x_i \mid x_{i-n+1}, \ldots, x_{i-1})$
Unidirectional autoregressive	Depends on the previous tokens	RNN,GPT	$P(X) = \prod_{i=1}^{M} P(x_i \mid x_1, \ldots, x_{i-1})$
Bidirectional context	Left2Right /right2left Autoregressive	BERT	$P(X) = \prod_{i=1}^{M} P(x_i \mid x_{\neq i})$

MCCULLOCH-PITTS VS TRANSFORMER



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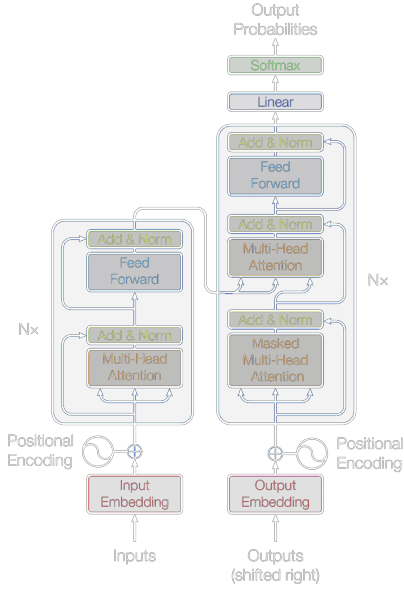


QUESTION: WHAT DO TRANSFORMER HEADS SPECIALIZE AT?

- All attention heads receive the same input embeddings.
- Heads start with random weights.
- How do they specialize in attending to different aspects of input?

RANDOM INITIALIZATION OF WEIGHTS

- Each head has unique weight matrices (W_Q, W_K, W_V, W_O).
- Random initialization leads to diverse transformations of input.
- Ensures heads start with distinct attention patterns.

SPECIALIZATION THROUGH TRAINING

- Heads specialize via backpropagation during training.
- Loss function guides heads to focus on:
  - Syntactic relationships (e.g., dependencies between words).
  - Semantic relationships (e.g., context or meaning).
  - Positional or structural patterns.

MULTI-HEAD ATTENTION MECHANISM

- Each head computes its own attention scores and representation.
- Representations are concatenated and linearly transformed.
- Enables model to aggregate diverse perspectives, such as:
  - Word-level dependencies.
  - Sentence-level context.
  - Positional relevance.

LAYER STACKING

- Outputs from one layer (all heads) serve as inputs to the next.
- Subsequent layers refine or build on earlier attention patterns.
- Hierarchical structure deepens specialization.

IMPLICIT COMPETITION

- Heads compete to minimize loss:
  - Redundant attention patterns provide diminishing returns.
  - Specialization maximizes each head's contribution.
- Encourages efficient use of capacity.

EXPERIMENTAL FINDINGS

- Certain heads consistently specialize across tasks and datasets:
  - Positional encoding.
  - Syntax parsing.
  - Semantic roles.
- Some heads act as:
  - **Generalists:** Broad attention across sequences.
  - **Specialists:** Focused attention on specific patterns.

SUMMARY

- Specialization arises from:
  - Random initialization of weights.
  - Differentiated learning through backpropagation.
  - Layer interactions and multi-head architecture.
- Leads to a division of labor among attention heads.
- Key to the power and flexibility of transformer models.

PURPOSE OF RESIDUAL CONNECTIONS

- **Mitigate Vanishing Gradients:**
  - Ensure gradients flow through deeper networks.
- **Enable Deeper Architectures:**
  - Support the use of multiple layers without degradation.
- **Easier Optimization:**
  - Simplify the training of complex models.

MECHANISM OF RESIDUAL CONNECTIONS

- **Post-Attention:**

$$\text{Output} = \text{LayerNorm}(\text{Input} + \text{SelfAttention}(\text{Input}))$$

- **Post-Feed-Forward:**

$$\text{Output} = \text{LayerNorm}(\text{PreviousOutput} + \text{FeedForward}(\text{PreviousOutput}))$$

BENEFITS OF RESIDUAL CONNECTIONS

- **Stability in Training:**
  - Prevents exploding or vanishing gradients in deep models.
- **Feature Preservation and Enhancement:**
  - Maintains input features while enhancing them through transformation.
- **Increased Model Expressiveness:**
  - Allows the model to learn complex representations.

WORD EMBEDDING

1. Word embedding is fundamental to Deep Learning of NLP
2. Contextual word embedding is now used in most of the downstream applications

CLOZE TEST

According to a report in yesterday's newspaper (1)——— police dog was taken to Raj Bhavan (2)——— Monday. This was to trace the (3)——— of the "very important horse" which (4)——— reported missing on Sunday. The dog picked (5)——— the scent on some traces of (6)——— and ran a few yards before losing the (7)———. The police have launched a vigorous (8)——— into the whole affair. They have (9)——— the services of a forensic expert, (10)——— fingerprint expert and a photographer. (11)——— are now fourteen horses at Raj Bhavan (12)——— are kept in a large shed near the gate.

1	once	a	new
2	at	next	on
3	police	killers	dogs
...	...	...	...
11	There	We	So
12	who	were	which

The purpose of the Cloze test is to measure the reading comprehension of a student with respect to grammar, usage, vocabulary, and contextual understanding.

MASKED LM[5]

Objectives

- Predict the masked word using the context
- Combine left and right contexts to predict the masked word
- Use sentence pairs to predict the next sentence
- Use the trained model for token-level and sentence-level tasks
- Mask some of the tokens from the input
- Predict the original token using its context
- Use Bidirectional deep transformer model fuse the left and right context and develop a contextual representation

HOW DO WE MASK?

- 15% of the words are randomly masked
- Perform the following operation on the the i^{th} token
  1. Replace with a $<MASK>$ 80% of the time
  2. Replace with a random token 10% of the time
  3. Retain the original 10% of the time

BIDIRECTIONAL ENCODER REPRESENTATIONS FROM TRANSFORMERS (BERT) - ARCHITECTURE

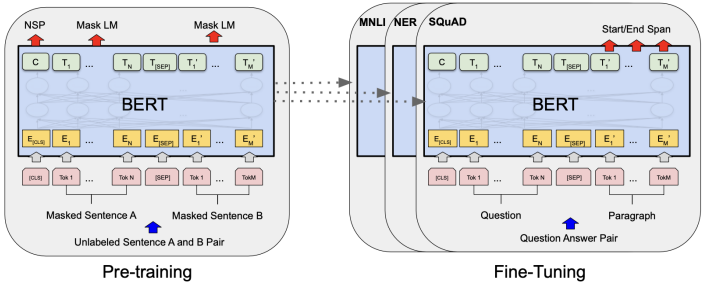


Figure: Overall pre-training and fine-tuning procedures for BERT. Apart from output layers, the same architec- tures are used in both pre-training and fine-tuning. The same pre-trained model parameters are used to initialize models for different down-stream tasks. During fine-tuning, all parameters are fine-tuned. [CLS] is a special symbol added in front of every input example, and [SEP] is a special separator token (e.g. separating questions/answers).Next Sentence Prediction (NSP) And Perturbation is a method used to assess or enhance the performance of BERT-like models by altering or analyzing their training dynamics, specifically in tasks involving next sentence prediction.

DOES BERT PREDICT THE "NEXT WORD"?

- **Unlike GPT-style models, BERT does not predict the next word in the sequence**
- Instead, BERT predicts the **original word at the masked position**, leveraging:
  - **Bidirectional context** from both preceding and following tokens.
- **Example:**
  - Input: `The [MASK] sat on the mat.`
  - BERT considers both sides of `[MASK]`:
    - Context: "The" and "sat on the mat."
    - Prediction: "cat."
- **Why is this effective?**
  - Bidirectional prediction enables **contextual understanding**.
  - Excels in tasks like **question answering** and **natural language inference**.

GENERATIVE PRE-TRAINED TRANSFORMER - GPT

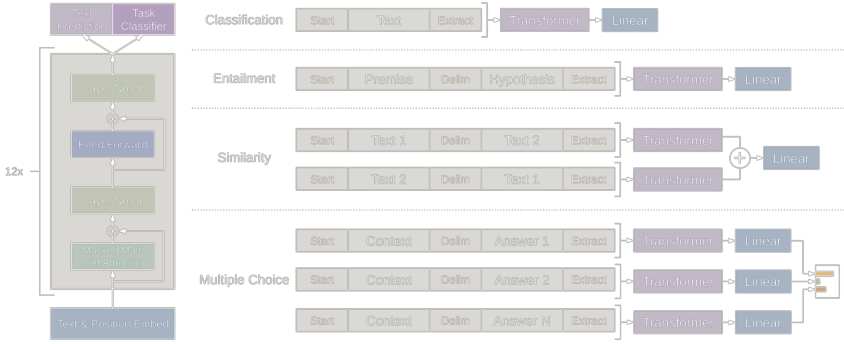
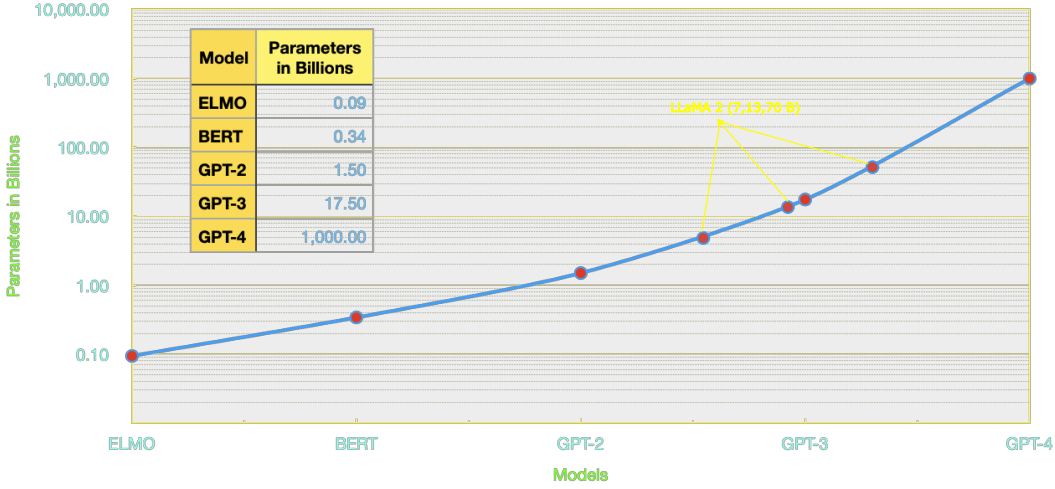


Figure: (left) Transformer architecture and training objectives used in this work. (right) Input transformations for fine-tuning on different tasks. We convert all structured inputs into token sequences to be processed by our pre-trained model, followed by a linear+softmax layer[6]

PARAMETERS OF LARGE LANGUAGE MODEL



LLAMA 2 OVERVIEW

- Open-source foundation model: Llama 2[7]
- Fine-tuned chat models for conversational AI
- Improves upon Llama 1 with new architectures and training methods
- Released by Meta AI
- Goals: Advance conversational AI, promote open research

KEY CONTRIBUTIONS

- Architecture: decoder-only Transformer with pre-normalization (RMSNorm), SwiGLU activations, and rotary positional embeddings (RoPE)
- Enhanced training: supervised fine-tuning followed by RLHF
- Large-scale pre-training: 2 trillion tokens; models of 7B, 13B, and 70B parameters; 4K-token context
- Grouped-query attention (in the 70B model) for faster inference
- Open-weights release: model weights and usage license (later Llama 3 models scaled to 15T training tokens and longer contexts)

TRAINING OF LLAMA 2-CHAT

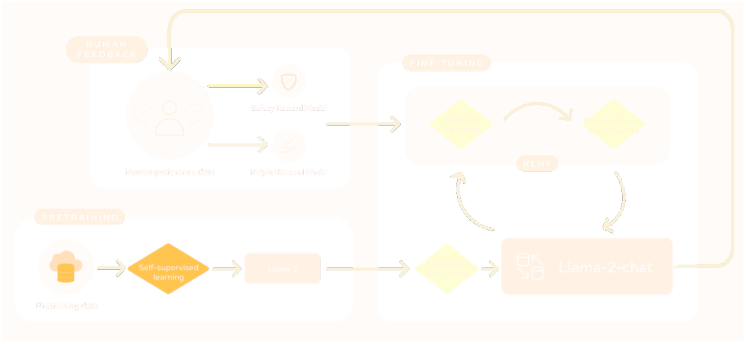


Figure: Thisprocessbeginswiththepretraining of Llama 2 usingpublicly availableonlinesources. Followingthis,wecreateaninitialversionof Llama 2-Chat throughtheapplication of supervised fine-tuning. Subsequently, the model is iteratively refined using Reinforcement Learning with Human Feedback (RLHF) methodologies, specifically through rejection sampling and Proximal Policy Optimization(PPO).ThroughouttheRLHFstage,theaccumulationof iterativerewardmodelingdata in parallel with model enhancements is crucial toensure thereward modelsremain within distribution[7].

IMPACT AND RESULTS

- State-of-the-art performance on conversational benchmarks
- Improved conversational flow and coherence
- Enhanced ability to understand context and nuance
- Demonstrates potential for real-world applications
- Opens doors for future research in conversational AI

SAMPLE TEXT GENERATION - MINIGPT

```
const LEARNING_RATE: f64 = 0.0003;
const BLOCK_SIZE: i64 = 128;
const BATCH_SIZE: i64 = 64;
const EPOCHS: i64 = 100;
const SAMPLING_LEN: i64 = 4096;
```

```
Config {
        vocab_size: 130,
        n_embd: 128,
        n_head: 8,
        n_layer: 8,
        block_size: 128,
        attn_pdrop: 0.1,
        resid_pdrop: 0.1,
        embd_pdrop: 0.1,
        };
```

Generated Text

for the gbr genome determines a comprehensive comparison from existing quality was commonly important to a lung w fusion if they can be a compared x-rayed, with the blood scenario of the lesion of t-cell support probability.in this later, the next for the first room of responses to materials and infection has classified a retrospective response of younger genes [138] .

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