# Transformer Training Process

how transformer trained step by step

Training a Transformer model involves several well-defined steps, from preprocessing the data to optimizing the model. Here's a step-by-step explanation of the training process:

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### 1. Data Preparation

- **Input Data**: Collect text data for training (e.g., sentences, documents).
- **Tokenization**: Break the text into smaller units (tokens) using methods like Byte Pair Encoding (BPE) or WordPiece.
- **Vocabulary Building**: Create a vocabulary of tokens and map each token to an integer (token ID).
- **Padding/Truncation**: Ensure all sequences are of the same length by padding shorter sequences and truncating longer ones.
- **Attention Masking**: Create masks to ignore padded tokens during attention calculations.

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### 2. Model Initialization

- **Model Architecture**: Define the Transformer architecture (e.g., number of layers, heads, embedding size, feed-forward dimensions).
- **Parameter Initialization**: Initialize weights and biases (commonly using methods like Xavier or He initialization).

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### 3. Training Loop

**For each epoch (pass over the dataset):**

1. **Forward Pass**:
   - **Input Embeddings**: Convert token IDs to dense vectors using embedding layers.
   - **Positional Encoding**: Add positional information to embeddings to capture sequence order.
   - **Transformer Layers**:
     - **Multi-Head Self-Attention**: Compute attention scores for each token, considering all other tokens in the sequence.
     - **Feed-Forward Network**: Pass attention outputs through dense layers for feature extraction.
     - **Layer Normalization and Residual Connections**: Improve gradient flow and stability.
   - **Output Layer**: Generate predictions (e.g., probabilities for each token in a vocabulary for language modeling).
2. **Loss Calculation**:
   - Compute the loss using a loss function (e.g., Cross-Entropy for language modeling).
3. **Backward Pass**:
   - Compute gradients using backpropagation to determine how the weights should be updated.
4. **Optimization**:
   - Update model weights using an optimizer (e.g., Adam, AdamW).
   - Use a learning rate scheduler to adjust the learning rate dynamically.

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### 4. Validation

- Evaluate the model on a separate validation dataset after each epoch.
- Compute metrics like perplexity, accuracy, or BLEU scores (for translation tasks).

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### 5. Regularization

- Apply techniques like:
  - **Dropout**: Randomly deactivate neurons to prevent overfitting.
  - **Gradient Clipping**: Prevent exploding gradients by capping gradient values.

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### 6. Fine-Tuning (Optional)

- For specific tasks (e.g., text classification, translation), fine-tune the pretrained Transformer on task-specific data.
- Use transfer learning to adapt the model without training from scratch.

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### 7. Checkpointing and Saving

- Save the model periodically during training.
- Save the final model after training completes.

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### 8. Deployment

- Convert the model for inference using libraries like ONNX or TensorFlow Lite.
- Optimize for latency using techniques like quantization or pruning.

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Would you like more details on any of these steps?

details of Data preparation

### Details of Data Preparation for Training Transformers

Data preparation is a crucial step in ensuring that the Transformer model is fed clean, properly formatted, and contextually meaningful data. Here's a detailed breakdown:

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### 1. Data Collection

- **Source Identification**:
  - Gather data from text corpora (e.g., Wikipedia, Common Crawl, news articles, books).
  - For specific tasks, collect domain-specific datasets (e.g., medical records, programming documentation).
- **Data Format**:
  - Ensure the data is in a compatible format like plain text, JSON, or CSV.

## 2. Text Preprocessing

- **Cleaning**:
  - Remove unwanted characters, HTML tags, and metadata.
  - Normalize text (convert to lowercase if case sensitivity isn't required).
  - Handle special characters or emojis based on task relevance.
- **Tokenization**:
  - Split text into tokens (e.g., words, subwords, or characters).
  - Use algorithms like:
    - **Byte Pair Encoding (BPE)**.
    - **WordPiece** (used in BERT).
    - **SentencePiece** (used in T5 and ALBERT).
    - **Unigram Language Model**.
- **Removing Noise**:
  - Eliminate non-text elements such as numbers or URLs (if irrelevant).
  - Filter out short or meaningless text samples.
- **Sentence Segmentation**:
  - Break text into meaningful sentence units using tools like spaCy or NLTK.

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## 3. Vocabulary Building

- **Vocabulary Definition**:
  - Create a vocabulary of unique tokens (e.g., `{'hello': 1, 'world': 2, '[PAD]': 0}`).
- **Special Tokens**:
  - Add tokens for:
    - **[PAD]**: Padding sequences.
    - **[CLS]**: Classifier token (used in BERT for classification tasks).
    - **[SEP]**: Separator token (used for sentence pairs).
    - **[MASK]**: Masked token for masked language modeling tasks.
- **Size**:
  - Determine vocabulary size (e.g., 30k–50k tokens) balancing coverage and memory constraints.

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## 4. Sequence Management

- **Padding and Truncation**:
  - Pad shorter sequences with a special `[PAD]` token to ensure uniform length.
  - Truncate longer sequences to fit within the model's maximum sequence length.
  - Example:

```bash
```

```
Input:  [The, cat, sat]
Padded: [The, cat, sat, [PAD], [PAD]]
```

- **Attention Masking**:
  - Create attention masks to distinguish real tokens from padded tokens.
  - Example:

```makefile
Sequence: [The, cat, sat, [PAD], [PAD]]
Mask:     [1, 1, 1, 0, 0]
```

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## 5. Encoding

- **Integer Mapping**:
  - Convert tokens into integers using the vocabulary.
  - Example:

```vbnet
Input:  ["hello", "world"]
Output: [12, 45]
```

- **Positional Encoding**:
  - Encode token positions into vectors to provide order information.
  - Positional encoding can be:
    - **Fixed** (sinusoidal functions, as in the original Transformer paper).
    - **Learned** (learnable embedding vectors).

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## 6. Data Augmentation (Optional)

- **For Larger Datasets**:
  - Synonym replacement.
  - Back-translation (translate text to another language and back to the original).
  - Sentence shuffling for sequence-based tasks.
- **For Smaller Datasets**:
  - Duplicate samples with slight perturbations.

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## 7. Dataset Splitting

- Divide the data into:
  - **Training Set**: Majority of the data for model training (70–80%).
  - **Validation Set**: Used for hyperparameter tuning (10–15%).
  - **Test Set**: Used to evaluate model performance (10–15%).
- Ensure splits are representative and balanced across classes (for classification tasks).

### 8. Data Formatting

- Structure data for the training framework (e.g., PyTorch, TensorFlow).
- Use formats like TFRecord (for TensorFlow) or data loaders (for PyTorch).

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### 9. Handling Large Datasets

- **Sharding**: Split large datasets into smaller chunks for easier processing.
- **Streaming**: Load data in batches to avoid memory issues.
- **Preprocessing Pipelines**: Use tools like Hugging Face's `datasets` library or Apache Beam.

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### 10. Dataset Storage and Loading

- Save preprocessed datasets for reuse (e.g., in `.json`, `.csv`, or binary formats).
- Use efficient data loaders (e.g., PyTorch `DataLoader`, TensorFlow `tf.data.Dataset`) to fetch data in batches during training.

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Would you like a Python code example for tokenization or preprocessing?

details of Model initialization

## Details of Model Initialization for Transformers

Initializing a Transformer involves setting up the architecture, layers, and weights before training begins. Proper initialization is crucial for ensuring the model converges efficiently and performs well. Here are the detailed steps:

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### 1. Define the Transformer Architecture

- **Input Parameters**:
  - **Vocabulary Size (`V`)**: Number of unique tokens in the vocabulary.
  - **Maximum Sequence Length (`L`)**: Maximum number of tokens in a sequence.
  - **Embedding Dimension (`d_model`)**: Size of token embeddings and hidden representations.
  - **Number of Layers (`N`)**: Number of Transformer encoder/decoder layers.
  - **Number of Attention Heads (`h`)**: Number of heads in multi-head self-attention.
  - **Feedforward Dimension (`d_ff`)**: Size of the hidden layer in the feed-forward network.
  - **Dropout Rate (`p`)**: Dropout probability for regularization.
- **Key Components**:
  - **Embedding Layer**: Maps token IDs to dense vectors.
  - **Positional Encoding**: Adds positional information to embeddings.
  - **Multi-Head Self-Attention Mechanism**: Captures relationships between tokens.
  - **Feedforward Network**: Processes attention outputs to extract features.
  - **Residual Connections**: Helps with gradient flow and reduces vanishing gradients.

- **Layer Normalization**: Stabilizes training by normalizing intermediate outputs.
- **Output Layer**: Maps the final representation to desired outputs (e.g., logits for tokens).

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## 2. Initialize Model Weights

- **Weight Initialization Techniques**:
  - **Xavier Initialization**: Used for layers with linear activation functions.

$$W \sim \mathcal{U}(-\sqrt{\frac{6}{d_{in} + d_{out}}}, \sqrt{\frac{6}{d_{in} + d_{out}}})$$

  - **He Initialization**: Common for layers with ReLU activation.

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

  - **Embedding Initialization**:
    - Randomly initialize token embeddings with small values.
    - Optionally, pre-train embeddings using methods like Word2Vec or GloVe.
  - **Bias Initialization**:
    - Typically initialized to zero for simplicity.
- **Attention Mechanism Weights**:
  - Query, Key, and Value matrices are initialized as $W_Q, W_K, W_V$, often using Xavier initialization.
  - Output projection weights $W_O$ are similarly initialized.

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## 3. Create Positional Encoding

- **Purpose**: Since Transformers lack inherent sequence order, positional encodings provide this information.
- **Sinusoidal Positional Encoding** (used in the original Transformer paper):

$$PE_{(pos,2i)} = \sin\left(\frac{pos}{10000^{2i/d_{model}}}\right)$$

$$PE_{(pos,2i+1)} = \cos\left(\frac{pos}{10000^{2i/d_{model}}}\right)$$

  - **Fixed and Deterministic**: No learnable parameters.
  - **Adds to Token Embeddings**.

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## 4. Setup Multi-Head Self-Attention

- **Splitting Heads**:
  - Input embedding $X \in \mathbb{R}^{L \times d_{model}}$ is split into $h$ attention heads.
  - Each head has a dimension of $d_k = d_{model}/h$.
- **Attention Mechanism**:
  - Compute scaled dot-product attention for each head:

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

- **Concatenation and Projection**:

- Concatenate outputs from all heads and project back to $d_{model}$.

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### 5. Define Feedforward Network

- **Architecture**:
  - Two linear layers with a ReLU activation in between.
  - Input size: $d_{model}$, Hidden size: $d_{ff}$, Output size: $d_{model}$.

$$\text{FFN}(x) = \max(0, xW_1 + b_1)W_2 + b_2$$

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### 6. Add Dropout and Regularization

- **Dropout**:
  - Applied to embeddings, attention outputs, and feedforward layers to prevent overfitting.
- **Gradient Clipping**:
  - Cap gradients during backpropagation to avoid exploding gradients.

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### 7. Combine and Stack Layers

- Stack $N$ identical encoder layers (or decoder layers if using the full Transformer).
- Each layer contains:
  1. **Multi-Head Attention**.
  2. **Feedforward Network**.
  3. Residual connections and layer normalization for both components.

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### 8. Initialize the Output Layer

- **Language Modeling Tasks**:
  - Use a linear layer mapping $d_{model}$ to $V$ (vocabulary size).
  - Apply a softmax function to get probabilities over tokens.
- **Classification Tasks**:
  - Add a classification head (e.g., linear layer with `num_classes` output size).

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### 9. Define the Loss Function

- **Common Losses**:
  - **Cross-Entropy Loss**: For language modeling or classification.
  - **Mean Squared Error (MSE)**: For regression tasks.
  - **Custom Losses**: Depending on the task.

Would you like an example code snippet for initializing a Transformer?

explain multihead self attention mechanism clearly

## Multi-Head Self-Attention Mechanism: Step-by-Step Explanation

The multi-head self-attention mechanism is a core component of Transformer models. It allows the model to focus on different parts of the input sequence simultaneously, capturing various relationships (e.g., syntactic or semantic).

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### Key Concepts

1. **Attention Mechanism**:
   - Computes how strongly one token relates to others in the sequence.
   - Assigns weights to other tokens based on their relevance to the current token.
2. **Self-Attention**:
   - Attention is computed within the same sequence (e.g., a sentence).
   - Helps understand dependencies between tokens.
3. **Multi-Head**:
   - Uses multiple attention "heads" to focus on different parts of the sequence.
   - Combines their outputs to create a richer representation.

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### Inputs to Multi-Head Self-Attention

- **Query (Q)**: Represents the current token for which attention is being calculated.
- **Key (K)**: Represents all tokens in the sequence.
- **Value (V)**: Represents the information of all tokens, weighted by attention.

For a sequence of $n$ tokens with an embedding size of $d_{model}$:

- $Q, K, V$ are $n \times d_{model}$ matrices.

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### Step-by-Step Process

1. **Linear Transformations**:
   - Learnable weight matrices $W_Q, W_K, W_V$ project $Q, K, V$ into smaller subspaces.
   - Dimension of each projection: $d_{head} = d_{model}/h$ (where $h$ is the number of attention heads).
   - New $Q', K', V'$:

$$Q' = QW_Q, \quad K' = KW_K, \quad V' = VW_V$$

2. **Scaled Dot-Product Attention**:
   - Compute attention scores by taking the dot product of $Q'$ and $K'^T$ for all token pairs: \text{Score}(i, j) = Q'_i \cdot K'_j^T
   - Scale the scores to stabilize gradients:

$$\text{Scaled Score}(i, j) = \frac{\text{Score}(i, j)}{\sqrt{d_{head}}}$$

   - Apply softmax to normalize scores across all tokens:

$$\text{Attention Weights}(i, j) = \text{softmax}(\text{Scaled Score}(i, j))$$

- Multiply weights with $V'$ to get the weighted sum:

$$\text{Output}(i) = \sum_j \text{Attention Weights}(i,j) \cdot V'_j$$

3. **Multi-Head Computation**:
   - Repeat the above process for $h$ attention heads, using separate $W_Q, W_K, W_V$ for each head.
   - This produces $h$ different output matrices, each of size $n \times d_{head}$.
4. **Concatenation and Linear Projection**:
   - Concatenate outputs from all attention heads into a single matrix of size $n \times d_{model}$:

$$\text{Concat} = [\text{Head}_1, \text{Head}_2, \ldots, \text{Head}_h]$$

   - Apply a final linear transformation with weight matrix $W_O$ to project back to $n \times d_{model}$.

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## Key Equations

1. **Attention Weights**:

$$\text{Attention}(Q', K', V') = \text{softmax}\left(\frac{Q'K'^T}{\sqrt{d_{head}}}\right)V'$$

2. **Multi-Head Attention**:

$$\text{MultiHead}(Q, K, V) = \text{Concat}(\text{Head}_1, \ldots, \text{Head}_h)W_O$$

   where:

$$\text{Head}_i = \text{Attention}(QW_{Q_i}, KW_{K_i}, VW_{V_i})$$

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## Advantages of Multi-Head Attention

1. **Parallel Processing**: Each head learns different types of relationships in parallel.
2. **Rich Representations**: Captures diverse dependencies (e.g., long-range, local) between tokens.
3. **Improved Expressiveness**: Each head explores unique patterns in the input data.

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## Visualization of Multi-Head Attention

1. Input embeddings for all tokens go through linear layers to produce $Q, K, V$.
2. Scaled dot-product attention is computed for each head.
3. Outputs from all heads are concatenated and projected to match the original embedding size.

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Would you like additional examples, illustrations, or Python code for this?

explain multi head self attention with a example

## Explaining Multi-Head Self-Attention with an Example

Let's walk through an example of **multi-head self-attention** with simplified numbers to illustrate the process.

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## Example Setup

**Input:**

We have a sequence of 3 tokens:

- Token 1: "The"
- Token 2: "cat"
- Token 3: "sat"

**Embedding Dimensions:**

- Embedding size ($d_{model}$): 6
- Number of heads ($h$): 2
- Size per head ($d_{head} = d_{model}/h$): 3

**Initial Embeddings:**

Suppose each token is represented by a 6-dimensional embedding:

$$\text{Embeddings (E)} = \begin{bmatrix} 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix}$$

---

## Step-by-Step Process

**1. Linear Transformations**

We compute the $Q, K, V$ matrices by applying learnable weight matrices $W_Q, W_K, W_V$. For simplicity, assume:

$$W_Q = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \\ 1 & 1 & 0 \end{bmatrix}, W_K = W_Q, W_V = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 1 \end{bmatrix}$$

- Compute $Q, K, V$ for each token:

$$Q = E \cdot W_Q, \quad K = E \cdot W_K, \quad V = E \cdot W_V$$

**Resulting Matrices:**

$$Q = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 2 & 2 & 2 \end{bmatrix}, \quad K = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 2 & 2 & 2 \end{bmatrix}, \quad V = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 2 \\ 3 & 3 & 3 \end{bmatrix}$$

---

**2. Scaled Dot-Product Attention**

For each head, compute attention scores, scale, and normalize:

- Compute $Q \cdot K^T$:

$$\text{Scores} = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 2 & 2 & 2 \end{bmatrix} \cdot \begin{bmatrix} 1 & 0 & 2 \\ 0 & 1 & 2 \\ 1 & 1 & 2 \end{bmatrix} = \begin{bmatrix} 2 & 1 & 4 \\ 1 & 2 & 4 \\ 4 & 4 & 12 \end{bmatrix}$$

- Scale by $\sqrt{d_{head}} = \sqrt{3}$:

$$\text{Scaled Scores} = \frac{1}{\sqrt{3}} \begin{bmatrix} 2 & 1 & 4 \\ 1 & 2 & 4 \\ 4 & 4 & 12 \end{bmatrix}$$

- Apply softmax row-wise:

$$\text{Attention Weights} = \text{softmax}(\text{Scaled Scores}) = \begin{bmatrix} 0.2 & 0.1 & 0.7 \\ 0.1 & 0.2 & 0.7 \\ 0.1 & 0.1 & 0.8 \end{bmatrix}$$

- Compute attention output $\text{Output} = \text{Weights} \cdot V$:

$$\text{Output} = \begin{bmatrix} 0.2 & 0.1 & 0.7 \\ 0.1 & 0.2 & 0.7 \\ 0.1 & 0.1 & 0.8 \end{bmatrix} \cdot \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 2 \\ 3 & 3 & 3 \end{bmatrix} = \begin{bmatrix} 2.6 & 2.6 & 2.8 \\ 2.5 & 2.5 & 2.7 \\ 3.1 & 3.1 & 3.4 \end{bmatrix}$$

---

**3. Multi-Head Attention**

- Repeat the above for another head with different $W_Q, W_K, W_V$.
- Concatenate the outputs from all heads:

$$\text{Concatenated Output} = [\text{Output from Head 1}; \text{Output from Head 2}]$$

- Apply a final linear transformation using $W_O$ to combine the outputs:

$$\text{Final Output} = \text{Concatenated Output} \cdot W_O$$

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## Advantages of Multi-Head Self-Attention

- Each head learns to focus on different parts of the sequence (e.g., syntactic dependencies, semantic meanings).
- The concatenation captures diverse relationships, making the model powerful for capturing global and local context.

Would you like to explore a specific part in more detail?

explain it fully with 2 heads

## Explaining Multi-Head Self-Attention with Two Heads

We will break down the **multi-head self-attention** mechanism step-by-step with **two attention heads** for simplicity.

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## Setup

**Input:**

We have a sequence of **3 tokens**:

- Token 1: "The"
- Token 2: "cat"
- Token 3: "sat"

**Parameters:**

- **Embedding size** ($d_{model}$): 6
- **Number of heads** ($h$): 2
- **Size per head** ($d_{head} = d_{model}/h = 6/2 = 3$)

**Initial Embeddings:**

The tokens are represented as embeddings:

$$\text{Embeddings (E)} = \begin{bmatrix} 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix}$$

---

## Step-by-Step Explanation

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#### 1. Linear Transformations

We create separate learnable weight matrices for **each head** for $Q, K, V$. Assume the following matrices:

**Head 1**:

$$W_Q^1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \\ 1 & 1 & 0 \end{bmatrix}, \quad W_K^1 = W_Q^1, \quad W_V^1 = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 1 \end{bmatrix}$$

**Head 2**:

$$W_Q^2 = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 1 & 1 \end{bmatrix}, \quad W_K^2 = W_Q^2, \quad W_V^2 = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 1 & 1 \end{bmatrix}$$

We compute $Q, K, V$ for **each head** by multiplying embeddings ($E$) with the weight matrices.

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**For Head 1:**

$$Q^1 = E \cdot W_Q^1, \quad K^1 = E \cdot W_K^1, \quad V^1 = E \cdot W_V^1$$

$$Q^1 = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 2 & 2 & 2 \end{bmatrix}, \quad K^1 = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 2 & 2 & 2 \end{bmatrix}, \quad V^1 = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 2 \\ 3 & 3 & 3 \end{bmatrix}$$

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**For Head 2:**

$$Q^2 = E \cdot W_Q^2, \quad K^2 = E \cdot W_K^2, \quad V^2 = E \cdot W_V^2$$

$$Q^2 = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 3 & 2 & 3 \end{bmatrix}, \quad K^2 = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 3 & 2 & 3 \end{bmatrix}, \quad V^2 = \begin{bmatrix} 2 & 2 & 2 \\ 1 & 1 & 1 \\ 4 & 4 & 4 \end{bmatrix}$$

---

#### 2. Scaled Dot-Product Attention

For each head, we compute:

1. **Attention Scores**: $\text{Scores} = Q \cdot K^T$
2. **Scaling**: Divide by $\sqrt{d_{head}}$.

3. **Softmax**: Normalize scores across tokens.
4. **Weighted Sum**: Multiply attention weights by $V$.

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**For Head 1**:

$$\text{Scores}^1 = \begin{bmatrix} 2 & 1 & 3 \\ 1 & 2 & 4 \\ 3 & 4 & 12 \end{bmatrix}, \quad \text{Scaled Scores}^1 = \frac{\text{Scores}^1}{\sqrt{3}}$$

Apply softmax and compute attention outputs.

**For Head 2**:

$$\text{Scores}^2 = \begin{bmatrix} 3 & 3 & 9 \\ 3 & 3 & 9 \\ 9 & 9 & 27 \end{bmatrix}, \quad \text{Scaled Scores}^2 = \frac{\text{Scores}^2}{\sqrt{3}}$$

Apply softmax and compute attention outputs.

---

**3. Combine Heads**

Concatenate the outputs of Head 1 and Head 2 into a single matrix:

$$\text{Output of Multi-Head Attention} = \begin{bmatrix} \text{Head 1 Output} \\ \text{Head 2 Output} \end{bmatrix}$$

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**4. Final Linear Projection**

Pass the concatenated matrix through a final linear layer with learnable weights $W_O$ to produce the final output of the multi-head self-attention mechanism.

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This process is repeated for every layer in the Transformer. Let me know if you want numerical details for scaling, softmax, or further clarification!

after combining heads explain clearly

## Combining Heads in Multi-Head Self-Attention

Once the attention calculations for all heads are completed, the outputs of the heads are combined and processed further. Let's continue the explanation assuming we've completed attention computations for two heads.

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## Step 5: Combine the Outputs of All Heads

**Output of Each Head:**

Each head produces an output matrix ($O_1$ and $O_2$), which has the size $n \times d_{head}$, where:

- $n$: Number of tokens in the sequence.
- $d_{head}$: Dimensionality of each head's output.

Let's assume:

$$O_1 = \begin{bmatrix} 2 & 1 & 3 \\ 3 & 2 & 1 \\ 1 & 0 & 4 \end{bmatrix}, \quad O_2 = \begin{bmatrix} 1 & 4 & 0 \\ 2 & 3 & 1 \\ 3 & 5 & 2 \end{bmatrix}$$

**Concatenate Outputs:**

We concatenate the outputs from all heads along the feature dimension to form a single matrix:

$$O = [O_1; O_2]$$

Result:

$$O = \begin{bmatrix} 2 & 1 & 3 & 1 & 4 & 0 \\ 3 & 2 & 1 & 2 & 3 & 1 \\ 1 & 0 & 4 & 3 & 5 & 2 \end{bmatrix}$$

Size of $O$: $n \times d_{model}$ (3 tokens $\times$ 6 dimensions).

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## Step 6: Final Linear Transformation

After concatenating the outputs from all heads, a final **linear layer** is applied to mix the features from all heads and project the output back to the original embedding size ($d_{model}$).

- **Weight Matrix for Projection** ($W_O$): A learnable weight matrix of size $d_{model} \times d_{model}$.

  Assume:

$$W_O = \begin{bmatrix} 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 1 \end{bmatrix}$$

- **Final Output**: Multiply $O$ by $W_O$:

$$Final\ Output = O \cdot W_O$$

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## Step 7: Residual Connection and Layer Normalization

- Add a **residual connection** by adding the input embeddings ($E$) back to the transformed output:

$$Residual\ Output = Final\ Output + E$$

- Apply **layer normalization** to stabilize the training process:

$$Normalized\ Output = LayerNorm(Residual\ Output)$$

This normalized output becomes the input to the next Transformer layer or is used for downstream tasks.

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## Summary

1. Each head focuses on different relationships between tokens by computing self-attention independently.
2. The outputs from all heads are concatenated to combine diverse representations.
3. A linear layer projects the combined output back to the original embedding size.
4. Residual connections and normalization ensure stability and gradient flow.

This process ensures the model learns complex dependencies in the sequence while preserving rich contextual information.

in multi head we are using different weight matrices and full embedding vector of sequence

Yes, you're correct! In multi-head self-attention, we use **different weight matrices** for each head, and the entire embedding vector of the sequence is used for computation. Here's a clear explanation:

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## Key Points About Multi-Head Self-Attention

1. **Different Weight Matrices for Each Head**:
   - Each attention head has its own set of learnable weight matrices for $Q$, $K$, and $V$.
   - For $h$ heads, we have $3h$ separate matrices:
   $$W_Q^1, W_Q^2, \ldots, W_Q^h; \quad W_K^1, W_K^2, \ldots, W_K^h; \quad W_V^1, W_V^2, \ldots, W_V^h$$
   - These matrices allow each head to focus on different aspects of the input data.
2. **Full Embedding Vector is Used**:
   - The input to the self-attention mechanism is the **entire sequence of token embeddings**.
   - For a sequence of $n$ tokens, with each token represented by an embedding of size $d_{model}$, the input is a matrix of size $n \times d_{model}$.
3. **Splitting the Embedding Vector Across Heads**:
   - The embedding size $d_{model}$ is split across the $h$ attention heads:
   $$d_{head} = \frac{d_{model}}{h}$$
   - Each head operates on a smaller subspace of the original embeddings, making the computations more efficient.
4. **Independent Attention Calculations**:
   - Each head performs attention calculations (scaled dot-product attention) independently on its respective subspace:
   $$Q_h = X \cdot W_Q^h, \quad K_h = X \cdot W_K^h, \quad V_h = X \cdot W_V^h$$
   - $Q_h$, $K_h$, and $V_h$ have dimensions $n \times d_{head}$.
5. **Concatenating Head Outputs**:
   - After computing attention outputs for all heads, the results ($O_1, O_2, \ldots, O_h$) are concatenated:
   $$O = [O_1; O_2; \ldots; O_h]$$
   - The concatenated matrix has dimensions $n \times d_{model}$.
6. **Final Linear Transformation**:
   - The concatenated outputs are passed through a linear layer with weights $W_O$ (size $d_{model} \times d_{model}$) to combine information across all heads:
   $$Final\ Output = O \cdot W_O$$

---

## Why Use Different Weight Matrices?

Using different weight matrices for each head allows the model to capture diverse relationships and patterns within the data:

- One head might focus on local dependencies (e.g., adjacent words).
- Another head might focus on long-range dependencies (e.g., subject-verb agreement).
- The diversity improves the model's ability to understand the input sequence holistically.

---

## Summary

- The **entire embedding vector** is used as input.
- Each head uses its **own weight matrices** for $Q$, $K$, and $V$.
- Heads work on **smaller subspaces** (splitting the embedding vector) and then combine their outputs to create a richer representation of the input sequence.

dimensions of wighted matrices of heads?explain fully

### Dimensions of Weight Matrices in Multi-Head Self-Attention

In multi-head self-attention, the weight matrices for $Q$, $K$, and $V$ play a crucial role in projecting the input embeddings into different subspaces for each attention head. Let's clearly explain their dimensions step by step.

---

### Key Parameters

1. **Input Sequence**:
   - $n$: Number of tokens in the input sequence.
   - $d_{model}$: Dimensionality of the input embeddings.
2. **Multi-Head Configuration**:
   - $h$: Number of attention heads.
   - $d_{head} = \frac{d_{model}}{h}$: Dimensionality of each attention head's subspace.

---

### 1. Weight Matrices for $Q$, $K$, and $V$

**Each Attention Head:**

- For each head $i$, the weight matrices $W_Q^i, W_K^i, W_V^i$ project the input embeddings ($n \times d_{model}$) into $n \times d_{head}$.
- **Dimensions of $W_Q^i, W_K^i, W_V^i$**:

$$W_Q^i, W_K^i, W_V^i \in \mathbb{R}^{d_{model} \times d_{head}}$$

**All Attention Heads:**

- We typically concatenate all the attention heads' projections. However, the weight matrices for $Q, K, V$ across all heads are conceptually grouped:
  - For $h$ heads:

$$W_Q \in \mathbb{R}^{d_{model} \times d_{model}}, \quad W_K \in \mathbb{R}^{d_{model} \times d_{model}}, \quad W_V \in \mathbb{R}^{d_{model} \times d_{model}}$$

These are implemented as $h$ independent $d_{model} \times d_{head}$ matrices.

---

### 2. Output of Attention Heads

**For a Single Head:**

- The output of one head is:

$$O_i = \text{Attention}(Q_i, K_i, V_i)$$

  - $Q_i, K_i, V_i \in \mathbb{R}^{n \times d_{head}}$
  - $O_i \in \mathbb{R}^{n \times d_{head}}$

**For All Heads:**

- The outputs of all heads are concatenated:

$$O = [O_1; O_2; \ldots; O_h]$$

- $O \in \mathbb{R}^{n \times d_{model}}$ (since $h \cdot d_{head} = d_{model}$).

---

### 3. Final Linear Transformation

After concatenating the outputs from all heads, we apply a final linear layer to project the concatenated output back to $d_{model}$.

- Weight matrix of the final linear layer:

$$W_O \in \mathbb{R}^{d_{model} \times d_{model}}$$

---

### Summary of Weight Matrix Dimensions

| Component | Matrix | Dimensions |
|---|---|---|
| Query, Key, Value | $W_Q, W_K, W_V$ | $d_{model} \times d_{model}$ |
| Single Head | $W_Q^i, W_K^i, W_V^i$ | $d_{model} \times d_{head}$ |
| Final Linear Layer | $W_O$ | $d_{model} \times d_{model}$ |

---

### Example with Values

Let's assume:

- $d_{model} = 512$
- $h = 8$
- $d_{head} = \frac{d_{model}}{h} = 64$
- $n = 10$ (10 tokens in the input sequence)

| Component | Matrix | Dimensions |
|---|---|---|
| Query, Key, Value | $W_Q, W_K, W_V$ | $512 \times 512$ |
| Single Head | $W_Q^i, W_K^i, W_V^i$ | $512 \times 64$ |
| Final Linear Layer | $W_O$ | $512 \times 512$ |

- Inputs for each head: $Q_i, K_i, V_i \in \mathbb{R}^{10 \times 64}$
- Concatenated output: $O \in \mathbb{R}^{10 \times 512}$

explain detaidly please

### Detailed Explanation of Weight Matrices in Multi-Head Self-Attention

Let's go through the dimensions of each weight matrix in the multi-head self-attention mechanism in detail, along with how they interact with the input data.

---

### Key Definitions

1. **Input Sequence:**
   - $n$: Number of tokens in the input sequence.
   - $d_{model}$: Dimensionality of the input embeddings (e.g., 512 in Transformers).

   The input embeddings for all tokens form a matrix:

$$X \in \mathbb{R}^{n \times d_{model}}$$

2. **Multi-Head Attention:**
   - $h$: Number of attention heads (e.g., 8 or 12).
   - $d_{head}$: Dimensionality of each head, calculated as:

     $$d_{head} = \frac{d_{model}}{h}$$

     Example: If $d_{model} = 512$ and $h = 8$, then $d_{head} = 64$.

---

## 1. Weight Matrices for Query ($Q$), Key ($K$), and Value ($V$)

For each attention head, the weight matrices project the input embeddings ($X$) into subspaces for query, key, and value representations.

**For One Attention Head:**

- **Weight Matrices:**
  - $W_Q^i$: Projects input to queries for head $i$.
  - $W_K^i$: Projects input to keys for head $i$.
  - $W_V^i$: Projects input to values for head $i$.

  Each weight matrix has dimensions:

  $$W_Q^i, W_K^i, W_V^i \in \mathbb{R}^{d_{model} \times d_{head}}$$

  Why? Because:
  - Input embeddings have size $d_{model}$.
  - Each head works in a smaller $d_{head}$-dimensional subspace.

**For All Attention Heads:**

- If we group all heads together, $W_Q, W_K, W_V$ combine the projections for all heads into a single weight matrix:

  $$W_Q, W_K, W_V \in \mathbb{R}^{d_{model} \times d_{model}}$$

  These are implemented as $h$ separate $d_{model} \times d_{head}$ weight matrices stacked horizontally.

---

## 2. Input Projections for Query, Key, and Value

The input sequence $X$ is multiplied by the weight matrices to compute queries, keys, and values for all heads.

**For One Head:**

- **Query ($Q$):**

  $$Q_i = X \cdot W_Q^i \quad \text{where } Q_i \in \mathbb{R}^{n \times d_{head}}$$

- **Key ($K$):**

  $$K_i = X \cdot W_K^i \quad \text{where } K_i \in \mathbb{R}^{n \times d_{head}}$$

- **Value ($V$):**

  $$V_i = X \cdot W_V^i \quad \text{where } V_i \in \mathbb{R}^{n \times d_{head}}$$

**For All Heads:**

- $Q, K, V$ matrices for all heads are concatenated:

  $$Q, K, V \in \mathbb{R}^{n \times d_{model}}$$

Internally, these are split into $h$ separate $n \times d_{head}$ matrices.

---

### 3. Scaled Dot-Product Attention

For each head, we compute attention scores using $Q_i, K_i, V_i$:

**Attention Scores:**

$$\text{Attention}_i(Q_i, K_i, V_i) = \text{softmax}\left(\frac{Q_i K_i^T}{\sqrt{d_{head}}}\right) V_i$$

- $Q_i K_i^T$: Produces a score matrix of size $n \times n$ (token-to-token similarity).
- Softmax normalizes these scores.
- Multiplying with $V_i$ gives the weighted sum of values.

The output of each head is:

$$O_i \in \mathbb{R}^{n \times d_{head}}$$

---

### 4. Concatenating the Outputs of All Heads

The outputs from all heads are concatenated:

$$O = [O_1; O_2; \ldots; O_h] \quad \text{where } O \in \mathbb{R}^{n \times d_{model}}$$

This combines information from all heads into a single representation.

---

### 5. Final Linear Transformation

The concatenated output $O$ is passed through a linear layer to project it back to the original embedding size ($d_{model}$).

**Final Linear Layer:**

- Weight matrix:
$$W_O \in \mathbb{R}^{d_{model} \times d_{model}}$$
- Output:
$$Final\ Output = O \cdot W_O \quad \text{where } Final\ Output \in \mathbb{R}^{n \times d_{model}}$$

---

### Summary of Dimensions

| Component | Dimension | Description |
|---|---|---|
| Input Embeddings ($X$) | $n \times d_{model}$ | Sequence of token embeddings. |
| $W_Q, W_K, W_V$ | $d_{model} \times d_{head}$ | Weight matrices for each head. |
| Queries, Keys, Values ($Q, K, V$) | $n \times d_{head}$ | Projected embeddings for one head. |
| Attention Output ($O_i$) | $n \times d_{head}$ | Output of one attention head. |
| Concatenated Output ($O$) | $n \times d_{model}$ | Combined output from all heads. |
| Final Linear Layer ($W_O$) | $d_{model} \times d_{model}$ | Projects concatenated output back. |

This detailed breakdown should clarify the role and dimensions of all weight matrices in multi-head self-attention.

explain example of calculation of Q,K,V

Let's calculate $Q$, $K$, and $V$ with an example to understand how the computations work.

---

## Problem Setup

1. **Input Sequence**:
   - Assume we have 2 tokens in a sequence: `["The", "cat"]`.
   - Each token is represented by an embedding vector of size $d_{model} = 4$.
   - Input embeddings matrix ($X$) is:

$$X = \begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix}$$

   $X \in \mathbb{R}^{2\times 4}$ (2 tokens, each of size 4).
2. **Number of Heads**:
   - $h = 2$ heads.
   - Size of each head ($d_{head}$) is:

$$d_{head} = \frac{d_{model}}{h} = \frac{4}{2} = 2$$

3. **Weight Matrices**:
   - For simplicity, let's assume the weight matrices $W_Q^i, W_K^i, W_V^i$ are randomly initialized for **Head 1** and **Head 2** as follows:

$$W_Q^1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 0 \\ 0 & 1 \end{bmatrix}, W_K^1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \\ 0 & 1 \\ 1 & 0 \end{bmatrix}, W_V^1 = \begin{bmatrix} 1 & 1 \\ 0 & 1 \\ 1 & 0 \\ 0 & 0 \end{bmatrix}$$

---

## Step-by-Step Calculation for Head 1

**1. Query ($Q$) Calculation:**

$$Q = X \cdot W_Q^1$$

- Matrix multiplication:

$$\begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 1+1 & 0+0 \\ 0+0 & 1+1 \end{bmatrix} = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}$$

- $Q \in \mathbb{R}^{2\times 2}$.

**2. Key ($K$) Calculation:**

$$K = X \cdot W_K^1$$

- Matrix multiplication:

$$\begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} 0 & 1 \\ 1 & 0 \\ 0 & 1 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} 0+0 & 1+1 \\ 1+1 & 0+0 \end{bmatrix} = \begin{bmatrix} 0 & 2 \\ 2 & 0 \end{bmatrix}$$

- $K \in \mathbb{R}^{2\times 2}$.

**3. Value ($V$) Calculation:**

$$V = X \cdot W_V^1$$

- Matrix multiplication:

$$\begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} 1 & 1 \\ 0 & 1 \\ 1 & 0 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 1+1 & 1+0 \\ 0+0 & 1+0 \end{bmatrix} = \begin{bmatrix} 2 & 1 \\ 0 & 1 \end{bmatrix}$$

- $V \in \mathbb{R}^{2\times 2}$.

---

### Results for Head 1

- $Q = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}$
- $K = \begin{bmatrix} 0 & 2 \\ 2 & 0 \end{bmatrix}$
- $V = \begin{bmatrix} 2 & 1 \\ 0 & 1 \end{bmatrix}$

For **Head 2**, similar calculations are performed using $W_Q^2$, $W_K^2$, and $W_V^2$, with the results concatenated.

---

### Next Steps

These $Q, K, V$ matrices are used to compute **attention scores** and produce the final output for each head.

explain calculation of attention scores

### Step-by-Step Calculation of Attention Scores

The attention scores are calculated as part of the **scaled dot-product attention mechanism**. Here's a detailed example based on the $Q$, $K$, and $V$ matrices computed earlier.

---

### Setup

- $Q$: Query matrix ($n \times d_{head}$).
- $K$: Key matrix ($n \times d_{head}$).
- $V$: Value matrix ($n \times d_{head}$).
- $n$: Number of tokens in the input sequence.
- $d_{head}$: Dimensionality of each head.

**Matrices:**

From the previous computation for **Head 1**:

$$Q = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}, \quad K = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad V = \begin{bmatrix} 2 & 1 \\ 1 & 0 \end{bmatrix}$$

---

### Step 1: Compute the Attention Scores

**Formula:**

The attention scores are computed as:

$$\text{Scores} = Q \cdot K^\top$$

**Matrix Multiplication:**

1. Compute $K^\top$:

$$K^\top = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

2. Multiply $Q$ and $K^\top$:

$$\text{Scores} = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} \cdot \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} (2 \cdot 0) + (0 \cdot 1) & (2 \cdot 1) + (0 \cdot 0) \\ (0 \cdot 0) + (2 \cdot 1) & (0 \cdot 1) + (2 \cdot 0) \end{bmatrix} = \begin{bmatrix} 0 & 2 \\ 2 & 0 \end{bmatrix}$$

**Attention Scores:**

$$\text{Scores} = \begin{bmatrix} 0 & 2 \\ 2 & 0 \end{bmatrix}$$

---

## Step 2: Scale the Attention Scores

**Formula:**

To avoid large values affecting the softmax computation, scale the scores by $\sqrt{d_{head}}$:

$$\text{Scaled Scores} = \frac{\text{Scores}}{\sqrt{d_{head}}}$$

- Here, $d_{head} = 2$, so $\sqrt{d_{head}} = \sqrt{2} \approx 1.41$.

**Computation:**

$$\text{Scaled Scores} = \frac{\begin{bmatrix} 0 & 2 \\ 2 & 0 \end{bmatrix}}{1.41} = \begin{bmatrix} 0 & 1.41 \\ 1.41 & 0 \end{bmatrix}$$

---

## Step 3: Apply Softmax

**Formula:**

The softmax function converts scores into probabilities:

$$\text{Attention Weights}_{ij} = \frac{e^{\text{Scaled Scores}_{ij}}}{\sum_k e^{\text{Scaled Scores}_{ik}}}$$

**Computation:**

1. Compute $e^{\text{Scaled Scores}}$:

$$e^{\text{Scaled Scores}} = \begin{bmatrix} e^0 & e^{1.41} \\ e^{1.41} & e^0 \end{bmatrix} = \begin{bmatrix} 1 & 4.1 \\ 4.1 & 1 \end{bmatrix}$$

2. Row-wise sum:

$$\text{Row Sums} = \begin{bmatrix} 1 + 4.1 \\ 4.1 + 1 \end{bmatrix} = \begin{bmatrix} 5.1 \\ 5.1 \end{bmatrix}$$

3. Compute softmax:

$$\text{Attention Weights} = \begin{bmatrix} \frac{1}{5.1} & \frac{4.1}{5.1} \\ \frac{4.1}{5.1} & \frac{1}{5.1} \end{bmatrix} = \begin{bmatrix} 0.20 & 0.80 \\ 0.80 & 0.20 \end{bmatrix}$$

### Step 4: Weighted Sum of Values

**Formula:**

The output of the attention mechanism is the weighted sum of the value vectors:

$$\text{Output}_i = \sum_j \text{Attention Weights}_{ij} \cdot V_j$$

**Computation:**

For $V = \begin{bmatrix} 2 & 1 \\ 1 & 0 \end{bmatrix}$ and Attention Weights $\begin{bmatrix} 0.20 & 0.80 \\ 0.80 & 0.20 \end{bmatrix}$:

1. For Token 1:

$$\text{Output}_1 = 0.20 \cdot \begin{bmatrix} 2 \\ 1 \end{bmatrix} + 0.80 \cdot \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0.4 \\ 0.2 \end{bmatrix} + \begin{bmatrix} 0.8 \\ 0 \end{bmatrix} = \begin{bmatrix} 1.2 \\ 0.2 \end{bmatrix}$$

2. For Token 2:

$$\text{Output}_2 = 0.80 \cdot \begin{bmatrix} 2 \\ 1 \end{bmatrix} + 0.20 \cdot \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 1.6 \\ 0.8 \end{bmatrix} + \begin{bmatrix} 0.2 \\ 0 \end{bmatrix} = \begin{bmatrix} 1.8 \\ 0.8 \end{bmatrix}$$

---

### Final Attention Output

The output matrix for the attention mechanism is:

$$\text{Output} = \begin{bmatrix} 1.2 & 0.2 \\ 1.8 & 0.8 \end{bmatrix}$$

Size: $n \times d_{head} = 2 \times 2$.

This process is repeated for all heads, and the outputs are concatenated and linearly transformed in the final stage.

explain the steps with example after concatanation

Sure! Let's walk through the **final steps of multi-head self-attention** after concatenating the outputs from all attention heads. We'll use an example to explain how to compute the final output.

### Step-by-Step Explanation After Concatenation

**1. Recap of Key Matrices and Outputs**

We'll continue from the previous example, where we had two attention heads. Let's summarize the key parts:

- **Query ($Q$)**, **Key ($K$)**, and **Value ($V$)** matrices are computed for each head.
- After computing the **attention scores**, applying the **softmax function**, and getting the **attention weights**, each head computes an output $O_1$ and $O_2$.

Let's assume that after applying the attention mechanism (i.e., computing the weighted sum of values), we get the following outputs for **Head 1** and **Head 2**:

$$O_1 = \begin{bmatrix} 0.8 & 1.0 \\ 1.1 & 0.9 \end{bmatrix}, \quad O_2 = \begin{bmatrix} 0.5 & 0.7 \\ 0.9 & 0.3 \end{bmatrix}$$

Here:

- $O_1$ is the output of **Head 1** after performing attention, and
- $O_2$ is the output of **Head 2** after performing attention.
- Both matrices are of shape $n \times d_{head}$, where $n = 2$ (number of tokens) and $d_{head} = 2$ (dimension of each attention head).

---

**2. Concatenate the Outputs of All Heads**

Once we have the output of all attention heads, we concatenate them along the feature dimension (i.e., horizontally). In our case, we have **Head 1** and **Head 2**.

- **Output of Head 1**: $O_1 \in \mathbb{R}^{2\times 2}$
- **Output of Head 2**: $O_2 \in \mathbb{R}^{2\times 2}$

The concatenation of outputs from **Head 1** and **Head 2** results in:

$$O = [O_1; O_2] = \begin{bmatrix} 0.8 & 1.0 & 0.5 & 0.7 \\ 1.1 & 0.9 & 0.9 & 0.3 \end{bmatrix}$$

Here, the concatenated output matrix $O$ has shape $2 \times 4$, where $n = 2$ (number of tokens) and $d_{model} = 4$ (total dimension after concatenating the two heads, i.e., $2 \times 2$).

---

**3. Linear Transformation (Final Projection)**

After concatenating the outputs from all attention heads, we apply a linear transformation (i.e., a fully connected layer) to project the concatenated output back to the original dimensionality $d_{model}$.

- The **weight matrix** for this linear transformation is $W_O$, which has dimensions $d_{model} \times d_{model}$. For our example, $d_{model} = 4$, so $W_O$ will have shape $4 \times 4$.

Assume the **weight matrix** $W_O$ is:

$$W_O = \begin{bmatrix} 0.1 & 0.2 & 0.3 & 0.4 \\ 0.5 & 0.6 & 0.7 & 0.8 \\ 0.9 & 1.0 & 1.1 & 1.2 \\ 1.3 & 1.4 & 1.5 & 1.6 \end{bmatrix}$$

- **Output after Linear Transformation**:

$$\text{Final Output} = O \cdot W_O$$

Perform the matrix multiplication:

$$\begin{bmatrix} 0.8 & 1.0 & 0.5 & 0.7 \\ 1.1 & 0.9 & 0.9 & 0.3 \end{bmatrix} \cdot \begin{bmatrix} 0.1 & 0.2 & 0.3 & 0.4 \\ 0.5 & 0.6 & 0.7 & 0.8 \\ 0.9 & 1.0 & 1.1 & 1.2 \\ 1.3 & 1.4 & 1.5 & 1.6 \end{bmatrix} = \begin{bmatrix} (0.8 \cdot 0.1 + 1.0 \cdot 0.5 + 0.5 \cdot 0.9 + 0.7 \cdot 1.3) & (0.8 \cdot 0.2 + 1.0 \cdot 0.6 + 0.5 \cdot 1.0 + 0.7 \cdot 1.4) & \dots \\ (1.1 \cdot 0.1 + 0.9 \cdot 0.5 + 0.9 \cdot 0.9 + 0.3 \cdot 1.3) & (1.1 \cdot 0.2 + 0.9 \cdot 0.6 + 0.9 \cdot 1.0 + 0.3 \cdot 1.4) & \dots \end{bmatrix}$$

Performing the arithmetic for each element:

$$\text{Final Output} = \begin{bmatrix} 2.3 & 2.7 & \dots \\ 1.9 & 2.2 & \dots \end{bmatrix}$$

---

**4. Resulting Final Output**

After the linear transformation, we have the final output, which is a projection of the concatenated attention head outputs back into the original embedding space. This output is used as the input for the next layer in the transformer model (such as the feed-forward neural network).

In summary:

- **Concatenate the outputs** from each attention head.
- **Apply a linear transformation** (using $W_O$) to get the final output.

This is how the attention mechanism processes the input, gathers context from each token, and outputs a contextually enriched representation of each token.

what is BERT

## BERT: Bidirectional Encoder Representations from Transformers

**BERT** (Bidirectional Encoder Representations from Transformers) is a transformer-based model for natural language understanding (NLU), introduced by Google in 2018. BERT is designed to pre-train deep bidirectional representations by jointly conditioning on both left and right context in all layers. This means that BERT is capable of understanding the full context of a word in a sentence by looking at the words before and after it, which was not possible with earlier models like GPT (which only considered the left context).

---

### Key Features of BERT:

1. **Bidirectional Contextual Understanding**:
   - Unlike traditional models like GPT that read text input from left to right, BERT reads the text **both left-to-right and right-to-left**, allowing it to capture the context from both directions simultaneously.
   - This bidirectional approach helps BERT understand the deeper meaning of words in the context of a sentence, especially for polysemy (words with multiple meanings based on context).
2. **Pre-training and Fine-tuning Paradigm**:
   - **Pre-training**: BERT is pre-trained on a large corpus of text (e.g., Wikipedia, BookCorpus) using two tasks:
     1. **Masked Language Model (MLM)**: Random words in the sentence are replaced with a special token [MASK], and the model must predict the original words.
     2. **Next Sentence Prediction (NSP)**: BERT is trained to predict whether two sentences appear consecutively in the text.
   - **Fine-tuning**: After pre-training, BERT can be fine-tuned for specific downstream tasks like question answering, sentiment analysis, or named entity recognition (NER) by adding a small task-specific layer on top and training on labeled data.
3. **Transformer Architecture**:
   - BERT is based on the **transformer encoder architecture**, which is effective in capturing the relationships between words in a sentence.
   - It uses **self-attention** to understand the relationships between all words in a sequence, and positional encoding to account for the order of words.
4. **Handling Long-Term Dependencies**:
   - Since BERT uses the transformer architecture, it can model long-term dependencies in text. This is different from older RNN and LSTM-based models, which struggled with long-range dependencies.
5. **Bidirectional Attention**:
   - BERT's attention mechanism allows it to consider the relationships between all words in the sentence at once, enabling a more holistic understanding of the sentence structure and meaning.

---

### BERT Architecture Overview:

BERT uses a stack of **transformer encoder layers**. The architecture can be described as follows:

- **Input**: The input to BERT is tokenized text with additional information, like [CLS] (classification token) at the beginning of the sequence and [SEP] (separator token) between sentences.
- **Embedding Layer**: The model uses **WordPiece embeddings** to represent each word as a vector.
- **Encoder Layers**: BERT stacks multiple transformer encoder layers to capture the relationships between tokens. BERT-base has 12 layers, while BERT-large has 24 layers.
- **Output**: The output is a contextually rich representation for each token in the input sequence, which can be used for downstream tasks.

---

### How BERT Works:

1. **Masked Language Model (MLM)**:
   - During pre-training, random words in the input text are replaced with a special [MASK] token, and the model is trained to predict the original word.
   - For example, in the sentence "The cat sat on the [MASK]", BERT would try to predict the word “mat” based on the context from both sides.
2. **Next Sentence Prediction (NSP)**:
   - BERT is also trained on pairs of sentences. The model receives two sentences as input, and the goal is to predict if the second sentence follows the first one in the original text.
   - For example, given the sentence pair:
     - "The man went to the store."
     - "He bought some milk."
   - BERT will predict whether the second sentence logically follows the first one.

---

### Applications of BERT:

BERT can be used for a variety of natural language understanding tasks by fine-tuning on specific datasets. Some common applications include:

- **Question Answering**: BERT can be fine-tuned to answer questions based on context from a paragraph.
- **Sentiment Analysis**: Fine-tuning BERT to classify text into positive, negative, or neutral sentiments.
- **Named Entity Recognition (NER)**: Identifying proper nouns like names, places, or dates in text.
- **Text Classification**: Classifying text into categories like spam detection, topic categorization, etc.
- **Textual Entailment**: Predicting whether one sentence logically follows from another.

---

### Example of BERT's Effectiveness:

Consider the sentence:

- **"I can’t eat the sandwich because it’s too salty."**
- In a traditional left-to-right or right-to-left model, "it" could refer to either the sandwich or the salt. But with BERT's bidirectional nature, it can understand that "it" refers to the sandwich because of the context in the sentence.

---

### BERT Variants:

There are several variants of BERT that have been developed to improve performance, reduce the model size, or make the model more efficient:

- **DistilBERT**: A smaller, distilled version of BERT that retains most of its performance but is faster and more memory-efficient.
- **RoBERTa**: A variant that improves on BERT by training with more data and removing the NSP task.
- **ALBERT**: A lighter version of BERT that reduces the number of parameters and increases efficiency.
- **TinyBERT**: A smaller version of BERT optimized for mobile and embedded devices.

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### Conclusion:

BERT represents a major advancement in NLP by leveraging bidirectional attention and a pre-training and fine-tuning approach. It has set new records on several NLP benchmarks and has been the foundation for many state-of-the-art models that followed. Its ability to understand context from both directions makes it more powerful than previous models.

explain BERT architecture

## BERT Architecture Explained

BERT (Bidirectional Encoder Representations from Transformers) is a transformer-based model designed to generate contextualized representations of words by using the **transformer encoder architecture**. Here's a detailed breakdown of its architecture:

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### 1. Overview of BERT

- BERT is **based on the transformer encoder** architecture.
- It processes the input text in a **bidirectional manner**, unlike models like GPT, which process text in a unidirectional (left-to-right) manner.
- BERT has two main configurations:
  - **BERT-Base**: 12 transformer layers (or encoder blocks), 768 hidden units, 12 attention heads, 110M parameters.
  - **BERT-Large**: 24 transformer layers, 1024 hidden units, 16 attention heads, 340M parameters.

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### 2. Input Representation

BERT's input combines three types of embeddings:

1. **Token Embeddings**: Each word is mapped to a vector using the WordPiece tokenization technique.
   - Example: "unaffable" → ["un", "##aff", "##able"]
2. **Segment Embeddings**: Used to distinguish between different sentences (e.g., Sentence A and Sentence B) in tasks like Next Sentence Prediction (NSP).
   - $E_A$: For tokens in Sentence A.
   - $E_B$: For tokens in Sentence B.
3. **Positional Embeddings**: Adds positional information to the tokens since transformers don't inherently encode sequence order.

**Final Input Representation**:

$$\text{Input Embedding} = \text{Token Embedding} + \text{Segment Embedding} + \text{Positional Embedding}$$

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### 3. Transformer Encoder Architecture

BERT stacks multiple **transformer encoder blocks** (12 for BERT-Base, 24 for BERT-Large).

**Components of a Transformer Encoder Block:**

1. **Multi-Head Self-Attention**:
   - Captures the relationships between all tokens in the sequence by attending to every other token.
   - Outputs a context-aware representation of each token.

   **Key Steps**:
   - Compute queries ($Q$), keys ($K$), and values ($V$) using learned weight matrices.
   - Calculate attention scores: $\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^\top}{\sqrt{d_{head}}}\right)V$.
   - Perform this computation independently across multiple heads, then concatenate and project the results.
2. **Add & Norm**:
   - Adds the input of the self-attention module to its output (residual connection).
   - Applies layer normalization.

$$\text{Output} = \text{LayerNorm}(\text{Input} + \text{Self-Attention Output})$$

3. **Feed-Forward Neural Network (FFN)**:
   - Applies two linear transformations with a ReLU activation in between:
   $$\text{FFN}(x) = \text{ReLU}(xW_1 + b_1)W_2 + b_2$$
   - This module is applied independently to each token.
4. **Add & Norm** (again):
   - Adds the input to the FFN module's output and applies layer normalization.
   $$\text{Output} = \text{LayerNorm}(\text{Input} + \text{FFN Output})$$

---

## 4. Special Tokens in Input

- **[CLS]**: A classification token added at the beginning of every sequence. Its final hidden state is used for classification tasks.
- **[SEP]**: A separator token used to distinguish between Sentence A and Sentence B in tasks like NSP.

Example Input:

$$[\text{CLS}, \text{Token}_1, \text{Token}_2, \ldots, \text{Token}_n, \text{SEP}]$$

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## 5. Output Representations

1. **Per-Token Output**:
   - Each token's final representation captures its meaning in the context of the entire sequence.
   - Used for token-level tasks like Named Entity Recognition (NER) or Question Answering (QA).
2. **[CLS] Token Output**:
   - The hidden state of the [CLS] token is used for sentence-level tasks like sentiment analysis or NSP.

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## 6. Pretraining Tasks

1. **Masked Language Modeling (MLM)**:
   - Randomly masks some tokens in the input and trains BERT to predict the masked tokens.
   - Example: Input: "The [MASK] is on the table." Output: Predict "cat".
2. **Next Sentence Prediction (NSP)**:
   - Given two sentences, predict if the second sentence follows the first in the original text.
   - Example:
     - Sentence A: "The cat is on the table."
     - Sentence B: "It is drinking milk." → Label: True

---

## 7. Fine-Tuning BERT

- After pretraining, BERT can be fine-tuned on specific downstream tasks by adding a task-specific output layer (e.g., softmax for classification).
- Examples of tasks:
  - Sentiment Analysis (classification).

- Question Answering (QA) tasks like SQuAD.
- Named Entity Recognition (NER).

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## Summary

- **Input Embedding**: Combines token, positional, and segment embeddings.
- **Transformer Layers**: Multiple layers of attention and feed-forward networks process the input.
- **Output Representations**: Contextual embeddings for tokens and sequences are produced.
- **Pretraining Tasks**: MLM and NSP prepare BERT for understanding language.
- **Fine-Tuning**: BERT is adapted to a variety of downstream tasks.

This combination of bidirectional attention and deep contextual understanding has made BERT a state-of-the-art model for many NLP tasks.

example of training

Let's walk through a simplified example of **training BERT** on a **Masked Language Model (MLM)** task. We'll break it into clear steps.

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## Step-by-Step Training Example

**Task: Masked Language Model (MLM)**

The MLM task involves predicting masked tokens in a sentence. During pre-training:

1. Randomly mask 15% of the tokens in the input sequence.
2. Train the model to predict these masked tokens based on the surrounding context.

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## Example Setup

1. **Input Sentence**:

   ```arduino
   "The cat sat on the mat."
   ```

2. **Tokenized Input**:

   ```css
   ["[CLS]", "The", "cat", "sat", "on", "the", "mat", "[SEP]"]
   ```

   BERT uses special tokens:

   - `[CLS]` : Marks the start of the sequence.
   - `[SEP]` : Marks the end or separates two sentences.

3. **Masked Sentence**: Randomly mask one of the tokens (e.g., "cat"):

   ```css
   ["[CLS]", "The", "[MASK]", "sat", "on", "the", "mat", "[SEP]"]
   ```

---

### Step 1: Embedding Layer

BERT converts each token into a vector using:

1. **Token Embedding**: Maps words to vectors using WordPiece embeddings.
2. **Segment Embedding**: Distinguishes sentences (e.g., Sentence A vs. Sentence B).
3. **Positional Embedding**: Adds sequence order information.

**Example:**

Let's assume:

- "The" → [0.1, 0.2, 0.3, 0.4]
- "[MASK]" → [0.5, 0.6, 0.7, 0.8]
- ... and so on.

---

### Step 2: Transformer Encoder Layers

The token embeddings pass through multiple transformer encoder layers, which include:

- **Multi-Head Self-Attention**: Captures relationships between tokens (e.g., "[MASK]" attends to "The" and "sat").
- **Feed-Forward Neural Network (FFN)**: Processes the tokens independently.

**Output:**

Each token is now represented by a **contextualized embedding** (e.g., "[MASK]" considers the context of "The" and "sat").

---

### Step 3: Predict Masked Token

The final embedding of the masked token ("[MASK]") is passed through a **softmax classifier** to predict the missing word:

1. **Classifier Input**: Contextualized embedding of "[MASK]".
2. **Classifier Output**: Probability distribution over the vocabulary.

**Example:**

For the word "cat":

- Probability of "cat" = 0.85
- Probability of "dog" = 0.10
- Probability of "hat" = 0.05

---

### Step 4: Loss Calculation

The model uses a **cross-entropy loss** to compare the predicted word ("cat") with the ground truth.

**Example:**

If the model predicts "cat" with 85% probability and the ground truth is "cat", the loss will be small. If it predicts another word (e.g., "dog"), the loss will be higher.

---

### Step 5: Backpropagation and Weight Update

- Gradients are computed using backpropagation.

- The weights of the transformer layers are updated using an optimization algorithm like Adam.

---

### Step 6: Repeat for Next Batch

The training continues on new batches of data, iteratively updating the model weights.

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### Fine-Tuning on Downstream Tasks

After pre-training, BERT can be fine-tuned on specific tasks like:

1. **Question Answering**: Identify the span of the answer in a paragraph.
2. **Text Classification**: Predict sentiment or other classes.
3. **Named Entity Recognition (NER)**: Label words with entity types (e.g., names, dates).

In fine-tuning, a task-specific layer is added, and BERT is trained on labeled data.

explain GPT architecture

### GPT Architecture: Generative Pre-trained Transformer

**GPT** (Generative Pre-trained Transformer) is a unidirectional transformer-based language model primarily designed for **text generation tasks**. Unlike **BERT**, which uses a bidirectional encoder, GPT focuses on **left-to-right text generation** by predicting the next word given a sequence of previous words.

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### Key Components of GPT Architecture

**1. Input Representation**

- GPT accepts a sequence of tokens as input, where each token represents a word or subword.
- Tokens are converted into embeddings using:
  1. **Token Embedding**: Maps tokens to dense vectors.
  2. **Positional Embedding**: Adds positional information to each token embedding, since transformers don't inherently capture sequence order.

**Input Representation**:

$$\text{Input Embedding} = \text{Token Embedding} + \text{Positional Embedding}$$

---

**2. Transformer Decoder Blocks**

GPT is built using stacks of **transformer decoder blocks** (12 layers in GPT-2 small, 24 in GPT-3 medium, etc.).

Each block consists of the following:

**a. Masked Multi-Head Self-Attention**

- GPT uses a **causal attention mask** to ensure the model can only attend to tokens **before the current token**.
- This mask prevents "cheating" by allowing the model to only use context from the past and not future tokens.

**Key Steps**:

1. Compute **queries ($Q$)**, **keys ($K$)**, and **values ($V$)**:

$$Q = XW_Q, \quad K = XW_K, \quad V = XW_V$$

where $X$ is the input sequence and $W_Q, W_K, W_V$ are learned weight matrices.

2. Compute the attention scores:

$$\text{Scores} = \frac{QK^\top}{\sqrt{d_{head}}}$$

3. Apply the causal mask:
   - Mask out future tokens by setting their attention scores to $-\infty$, ensuring the model only considers past tokens.
4. Apply softmax and compute the output:

$$\text{Attention}(Q, K, V) = \text{softmax}(\text{Scores})V$$

**b. Add & Norm**

- Adds the input of the self-attention module to its output (residual connection).
- Applies **layer normalization**:

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

**c. Feed-Forward Neural Network (FFN)**

- Processes each token independently using a two-layer fully connected network:

$$\text{FFN}(x) = \text{ReLU}(xW_1 + b_1)W_2 + b_2$$

**d. Add & Norm (again)**

- Adds the FFN's output to its input (residual connection) and normalizes.

---

**3. Output Layer**

- After passing through the stacked decoder layers, the model produces contextual embeddings for each token.
- These embeddings are fed into a **softmax layer** over the vocabulary to predict the next token.

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## GPT vs. BERT

| Feature | GPT | BERT |
|---|---|---|
| Architecture | Decoder (causal, unidirectional) | Encoder (bidirectional) |
| Training Objective | Language Modeling (predict next token) | Masked Language Model (MLM) |
| Context | Left-to-right | Both directions (bidirectional) |
| Main Use | Text generation | Text understanding |

---

## Example of GPT in Action

**Input Sequence:**

```arduino
"The cat sat on the"
```

**Processing:**

1. The input is tokenized and converted into embeddings.

2. Each token passes through the transformer decoder layers, attending only to previous tokens.
3. The output of the final layer predicts the next token:

```arduino
Predicted Token: "mat"
```

---

### GPT Variants

- **GPT-1**: Introduced the basic architecture with 12 layers and 110M parameters.
- **GPT-2**: Improved model with larger datasets and multiple variants (117M to 1.5B parameters).
- **GPT-3**: A massive model with 175B parameters, capable of performing complex tasks with minimal fine-tuning.

GPT's architecture demonstrates the power of self-attention and pre-training for generative tasks.