Introducción a Transformers

Aprendizaje Automático

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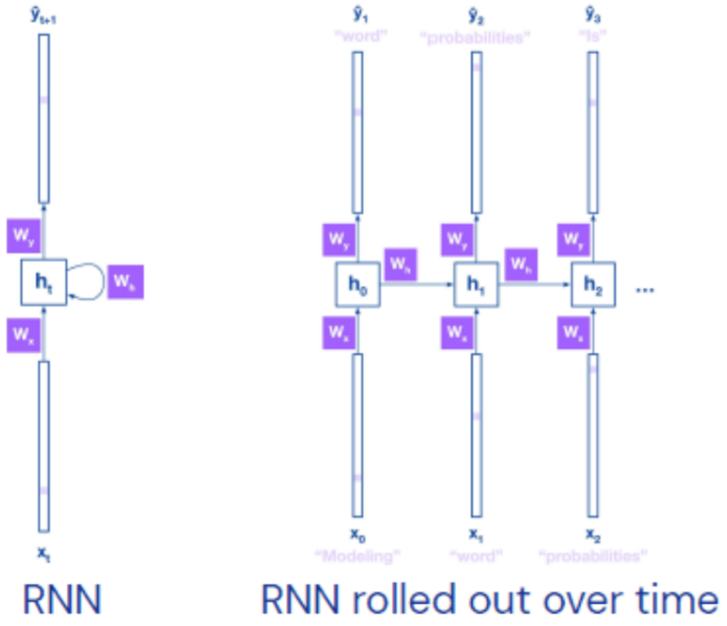
Redes recurrentes

Weights are shared over time steps



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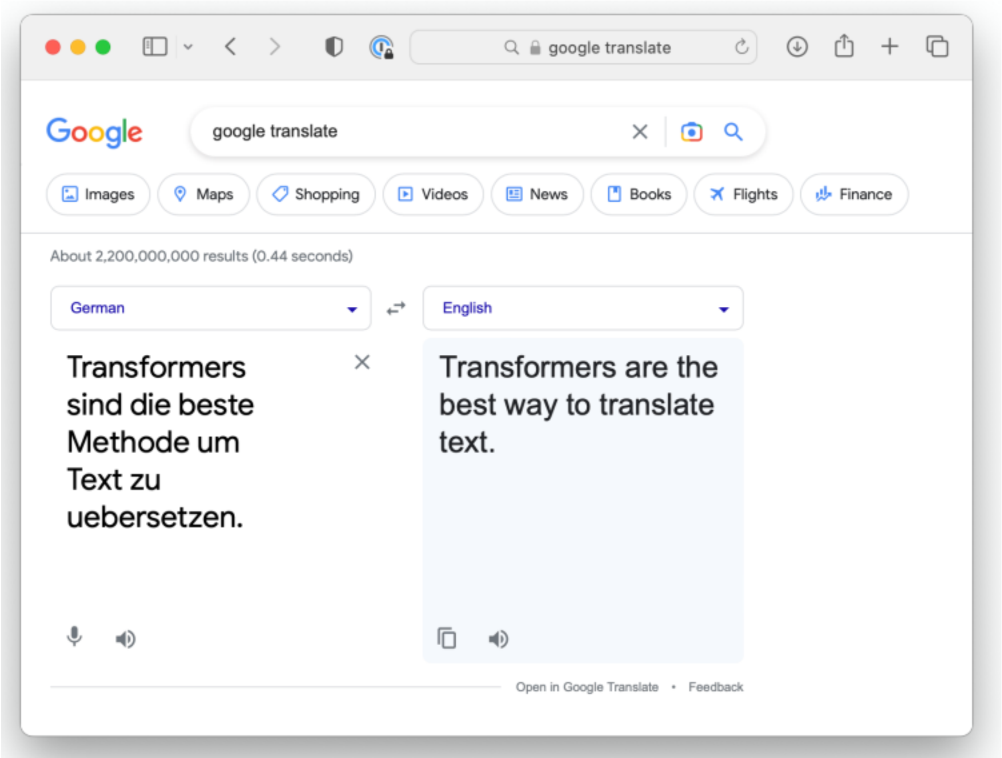

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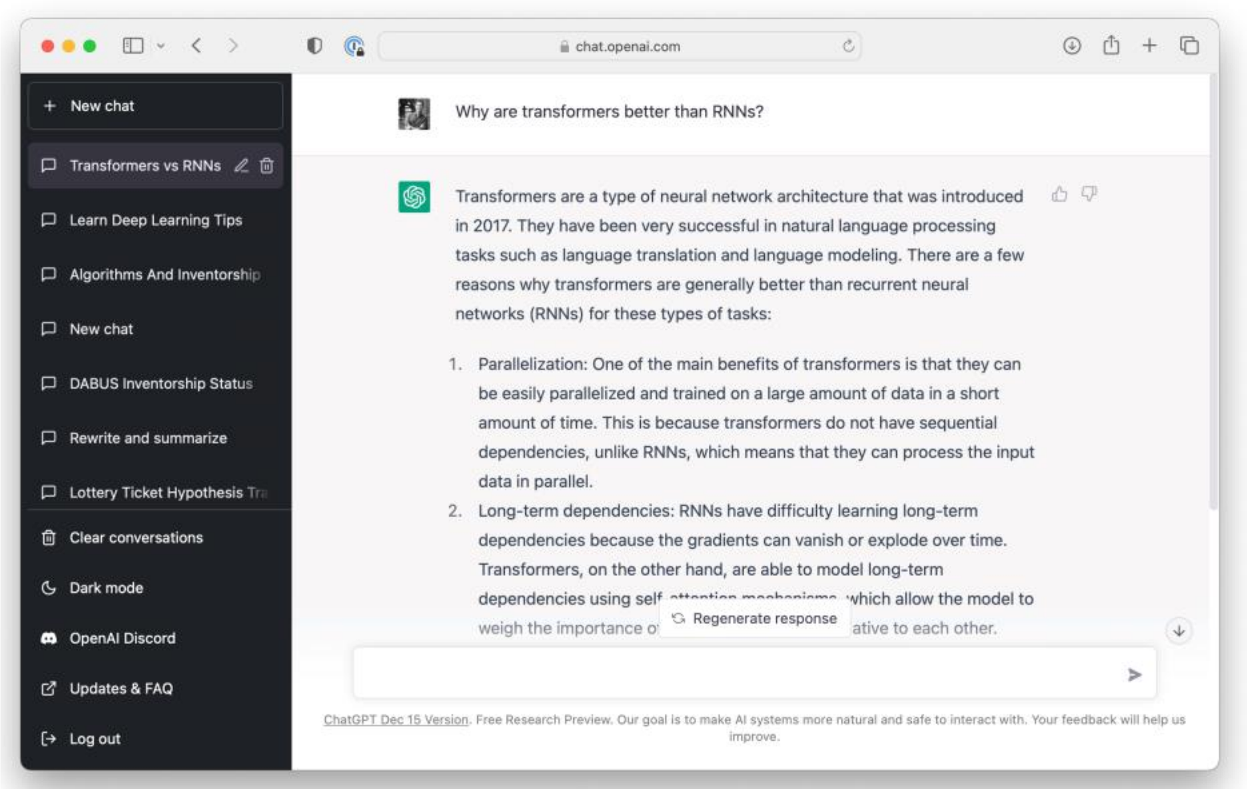

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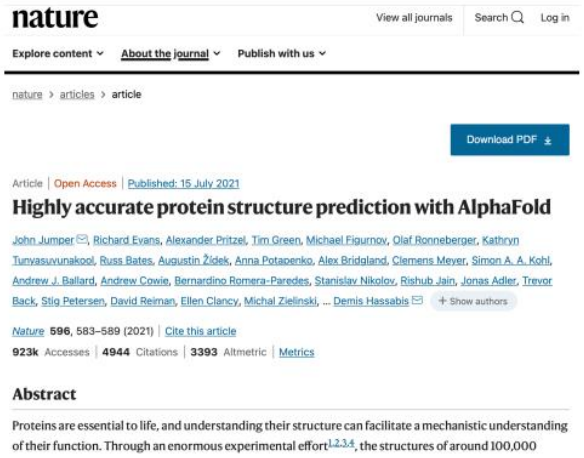

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Highly accurate protein structure prediction with AlphaFold

John Jumper, Richard Evans, Alexander Pritzel, Tim Green, Michael Figurnov, Olaf Ronneberger, Kathryn Tunyasuvunakool, Russ Bates, Augustin Žídek, Anna Potapenko, Alex Bridgland, Clemens Meyer, Simon A. A. Kohl, Andrew J. Ballard, Andrew Cowie, Bernardino Romera-Paredes, Stanislav Nikolov, Rishub Jain, Jonas Adler, Trevor Back, Stig Petersen, David Reiman, Ellen Clancy, Michal Zielinski, ... Demis Hassabis + Show authors

Nature **596**, 583–589 (2021) | Cite this article

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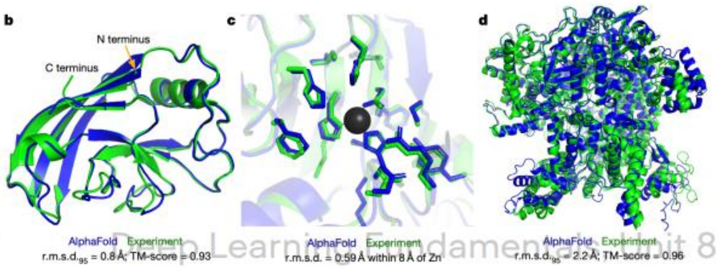
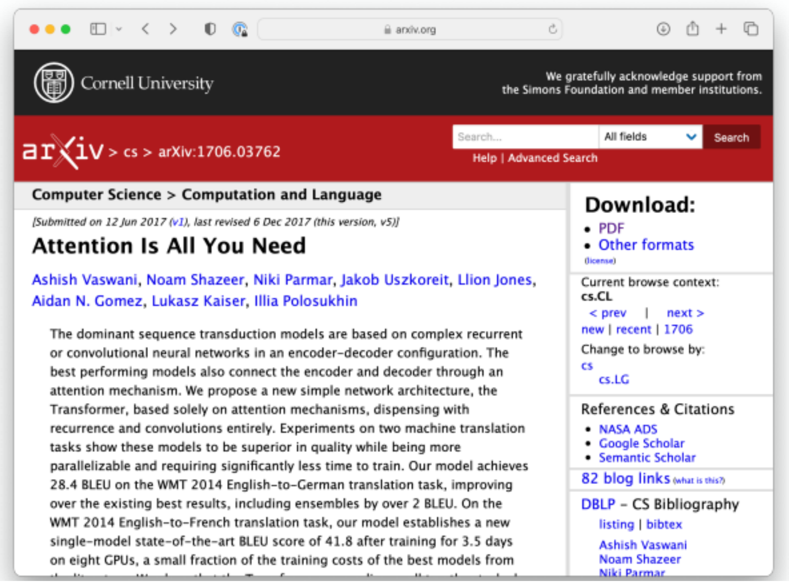
Abstract

Proteins are essential to life, and understanding their structure can facilitate a mechanistic understanding of their function. Through an enormous experimental effort[1,2,3,4], the structures of around 100,000



Artículo original



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Computer Science > Computation and Language

[Submitted on 12 Jun 2017 (v1), last revised 6 Dec 2017 (this version, v5)]

Attention Is All You Need

Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N. Gomez, Lukasz Kaiser, Illia Polosukhin

The dominant sequence transduction models are based on complex recurrent or convolutional neural networks in an encoder-decoder configuration. The best performing models also connect the encoder and decoder through an attention mechanism. We propose a new simple network architecture, the Transformer, based solely on attention mechanisms, dispensing with recurrence and convolutions entirely. Experiments on two machine translation tasks show these models to be superior in quality while being more parallelizable and requiring significantly less time to train. Our model achieves 28.4 BLEU on the WMT 2014 English-to-German translation task, improving over the existing best results, including ensembles by over 2 BLEU. On the WMT 2014 English-to-French translation task, our model establishes a new single-model state-of-the-art BLEU score of 41.8 after training for 3.5 days on eight GPUs, a small fraction of the training costs of the best models from

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Ashish Vaswani
Noam Shazeer
Niki Parmar

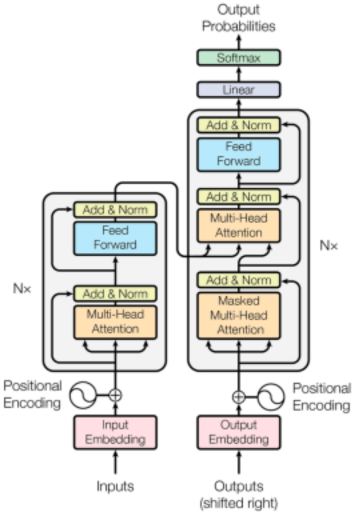
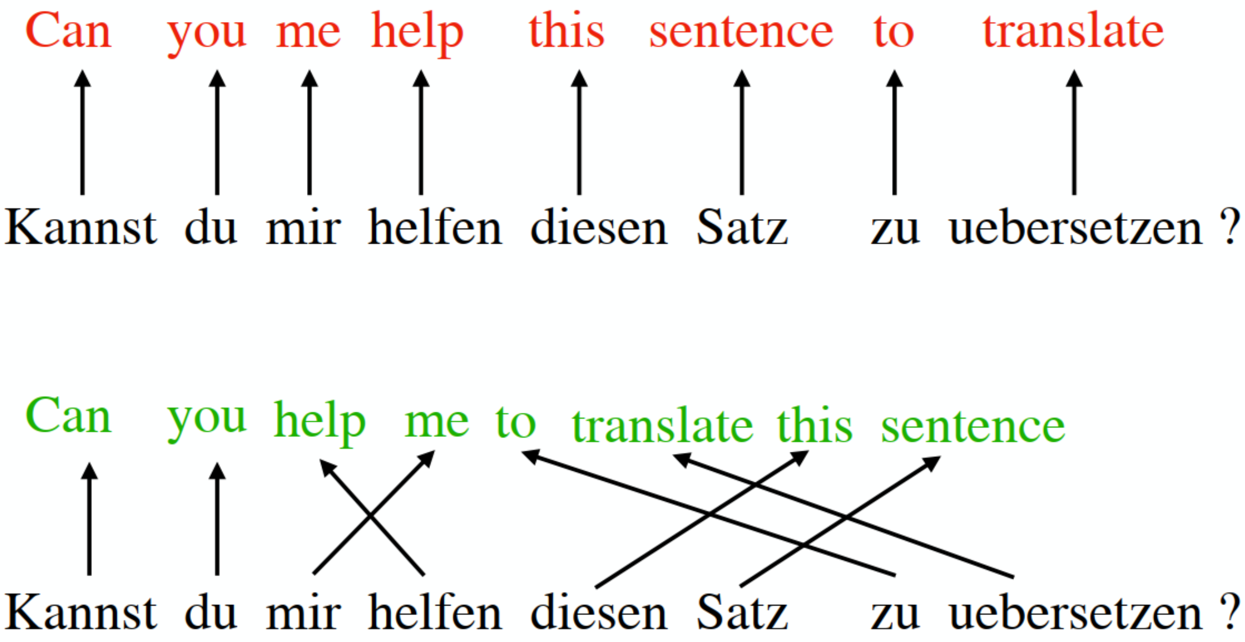


Figure 1: The Transformer - model architecture.

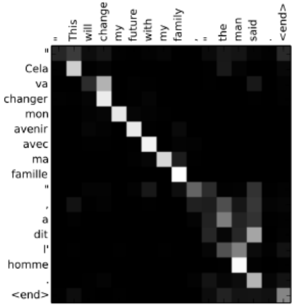
Atención

Nosotros no traducimos documentos palabra por palabra



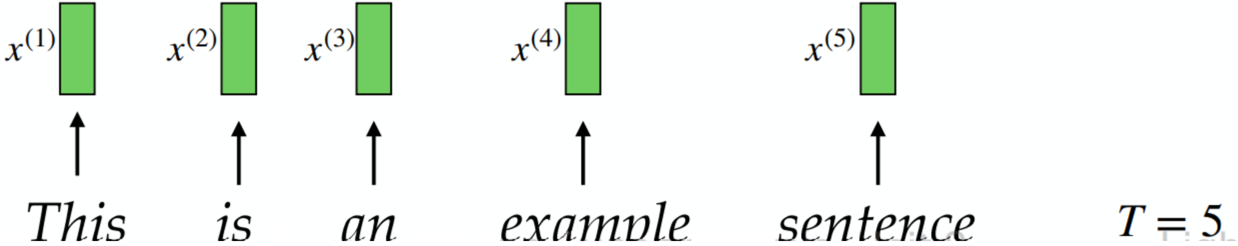
Atención

Idea: Crear vectores de contexto que contengan información acerca de la secuencia completa. Utilizar **scores de atención** para ponderar la importancia de cada palabra



$$z^{(i)} = \sum_{j=1}^{T} \alpha_{ij} \cdot x^{(j)}$$

Ejemplo: $i = 2$



Self-attention

$$z^{(i)} = \sum_{j=1}^{T} \boxed{\alpha_{ij}} \cdot x^{(j)}$$

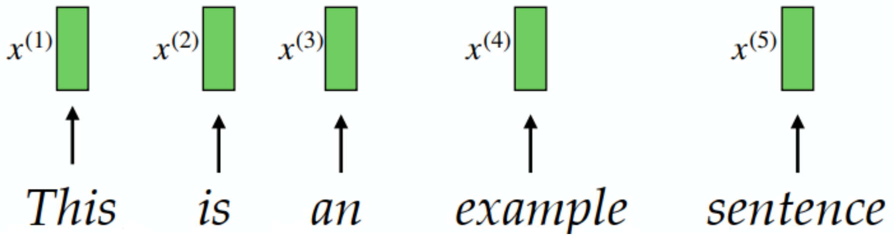
1. **Similarity** between i-th element all inputs $j = 1 \ldots T$

$$\omega_{ij} = x^{(i)\top} \cdot x^{(j)}$$

2. **Normalize** ω values to obtain attention scores α

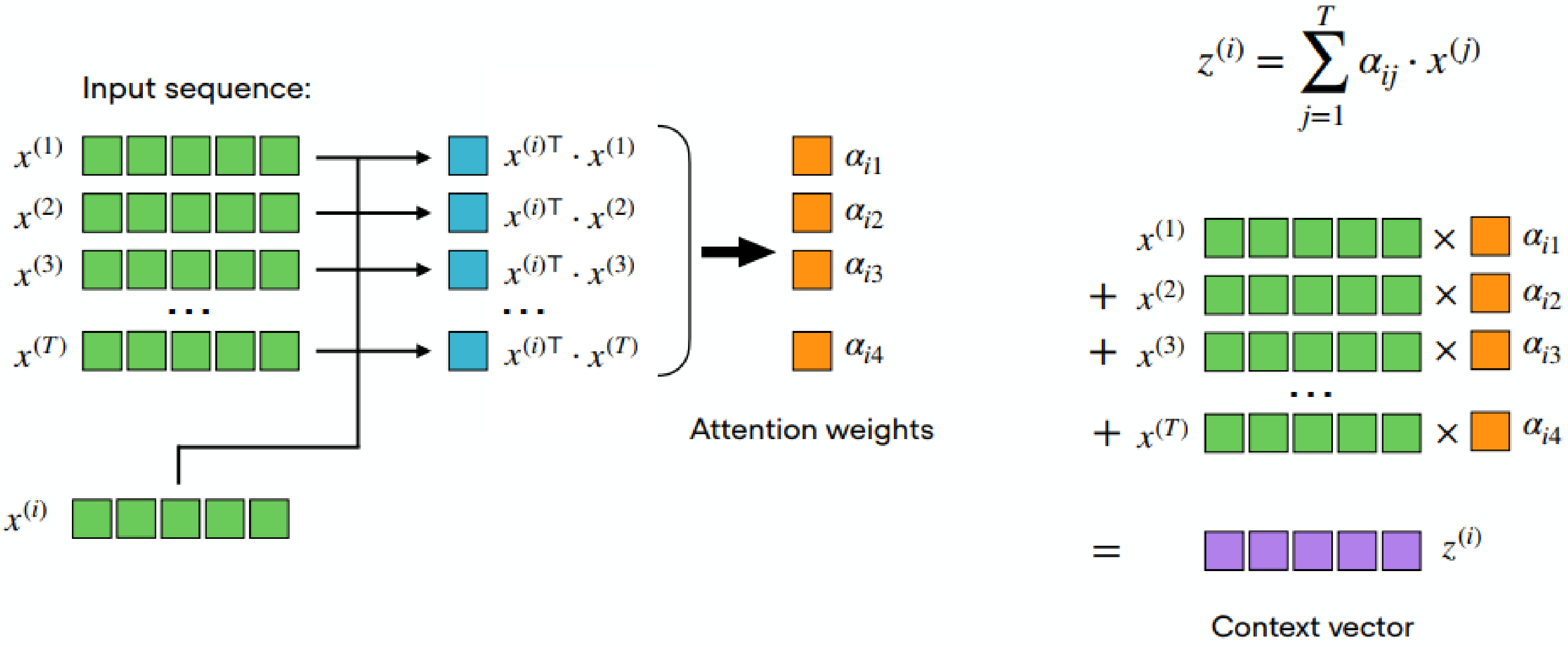
$$\alpha_{ij} = \frac{\exp\left(\omega_{ij}\right)}{\sum_{j=1}^{T} \exp\left(\omega_{ij}\right)} = \operatorname{softmax}\left(\left[\omega_{ij}\right]_{j=1\ldots T}\right)$$

So that attention value sum to 1 $\quad \sum_{j=1}^{T} \alpha_{ij} = 1$



$T = 5$

Self-attention



Self-attention with learneable weights

Idea: El modelo aprende qué tan importante es cada palabra. Modelo de atención más utilizado y propuesto en el paper original

query sequence: $q^{(i)} = U_q x^{(i)} \quad \text{for } i \in [1,...,T]$

key sequence: $k^{(i)} = U_k x^{(i)} \quad \text{for } i \in [1,...,T]$

value sequence: $v^{(i)} = U_v x^{(i)} \quad \text{for } i \in [1,...,T]$

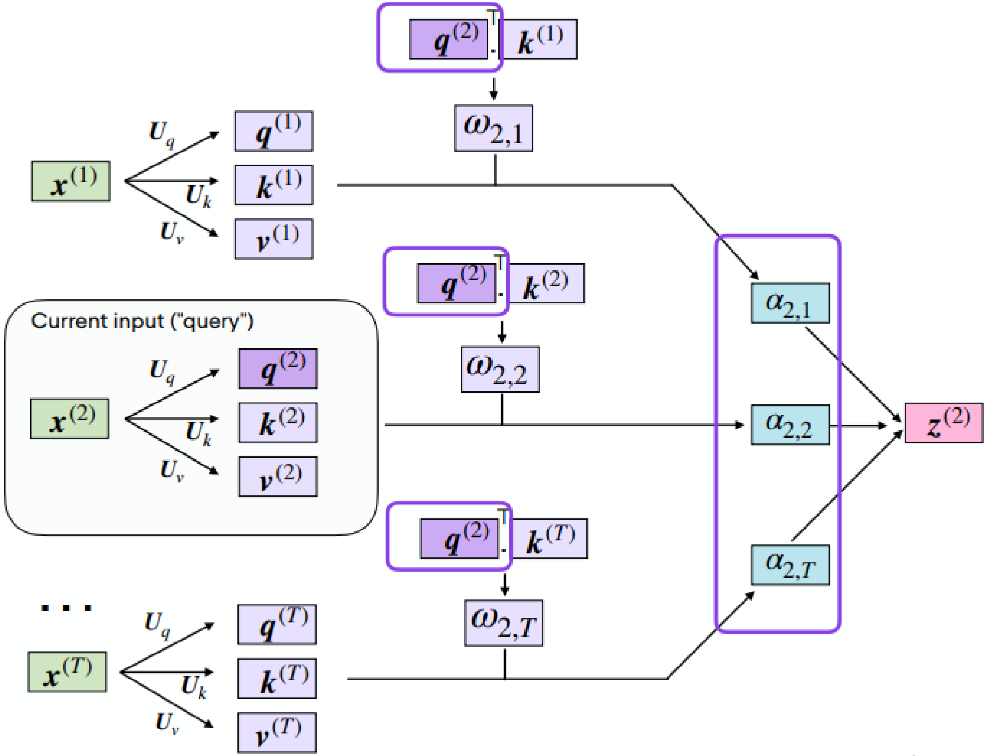
Self-attention with learneable weights

Query, key y value se inspiran en sistemas de recuperación de información.

query se compara con **key** para devolver un **value.**

Al igual al módulo básico de self-attention, debemos calcular un **vector de contexto**

Self-attention with learneable weights



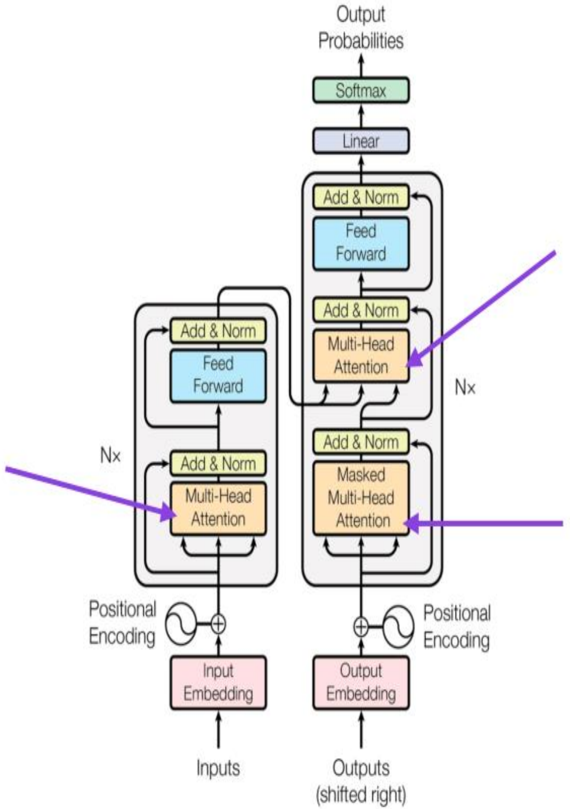
where $z^{(2)} = \sum_{j=1}^{T} \boxed{\alpha_{2,j}}\, v^{(j)}$

Self-attention with learneable weights

Resumen

Para cada token, el mecanismo de self-attention:

- Compara el query de cada palabra con los keys de todas las palabras en la secuencia de entrada
- Calcula el score de atención a partir de los valores obtenidos en la comparación
- Calcula el promedio ponderado de todas las entradas
- Metodología sequence-to-sequence
  - Toma T entradas
  - Devuelve T salidas



Multi-head attention

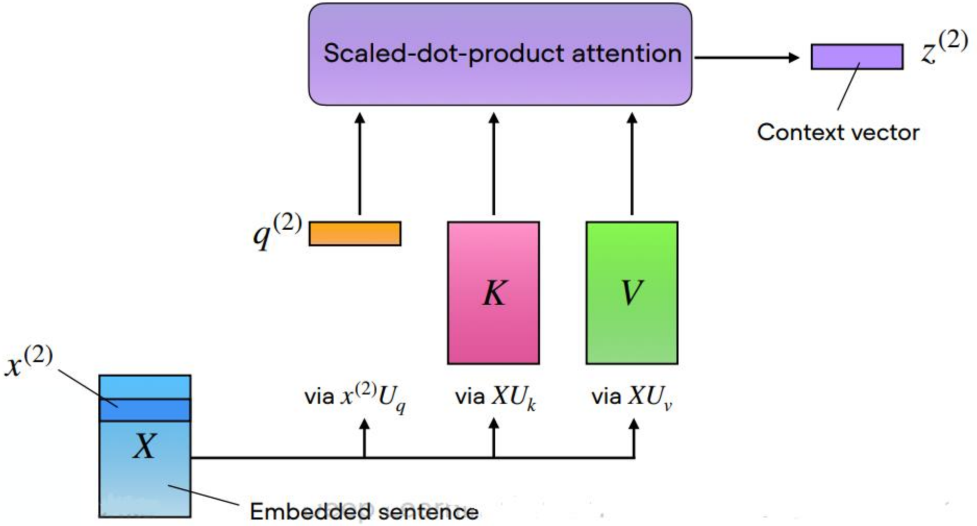
Anteriormente se usaron tres matrices de parámetros. Agreguemos un índice adicional

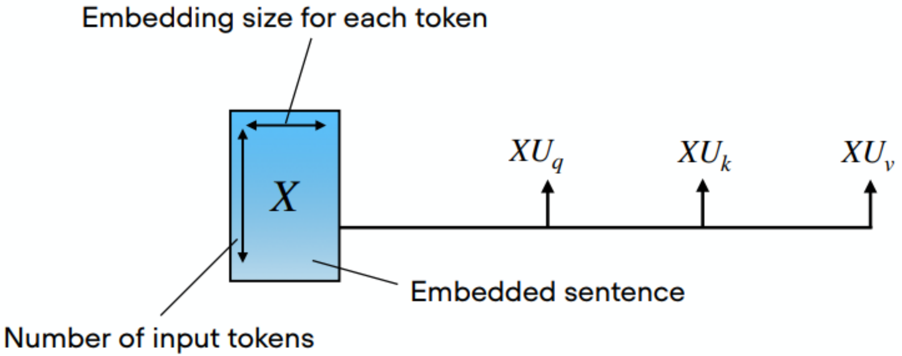
$$U_{q_1} \quad U_{k_1} \quad U_{v_1}$$

En multi-head attention tenemos un conjunto de matrices

$$U_{q_2} \quad U_{k_2} \quad U_{v_2}$$
$$U_{q_3} \quad U_{k_3} \quad U_{v_3}$$
$$\ldots$$

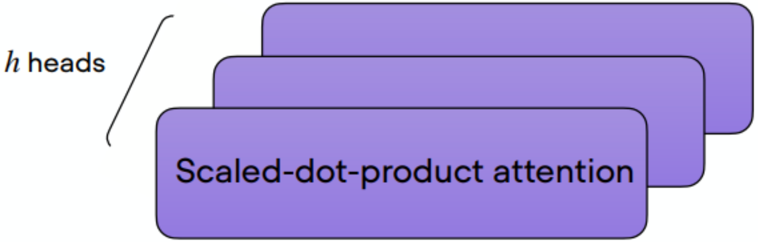
Multi-head attention



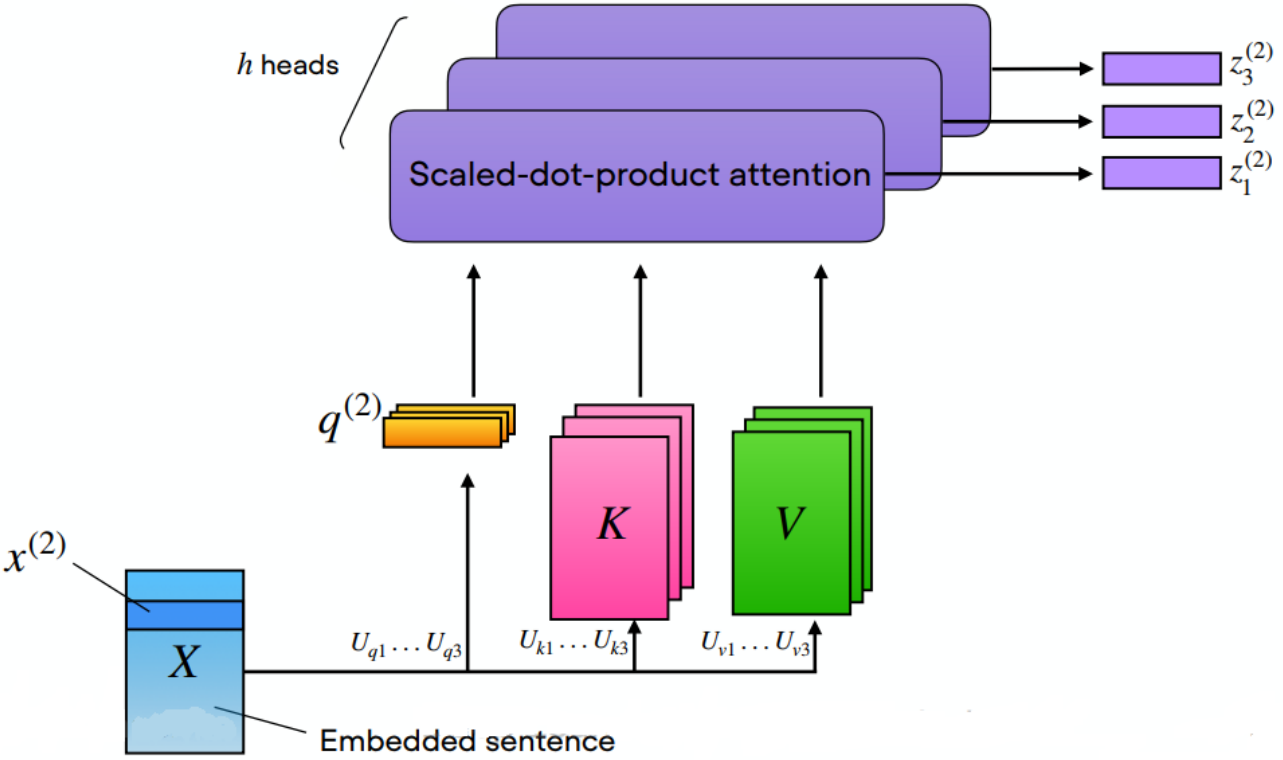


Multi-head attention

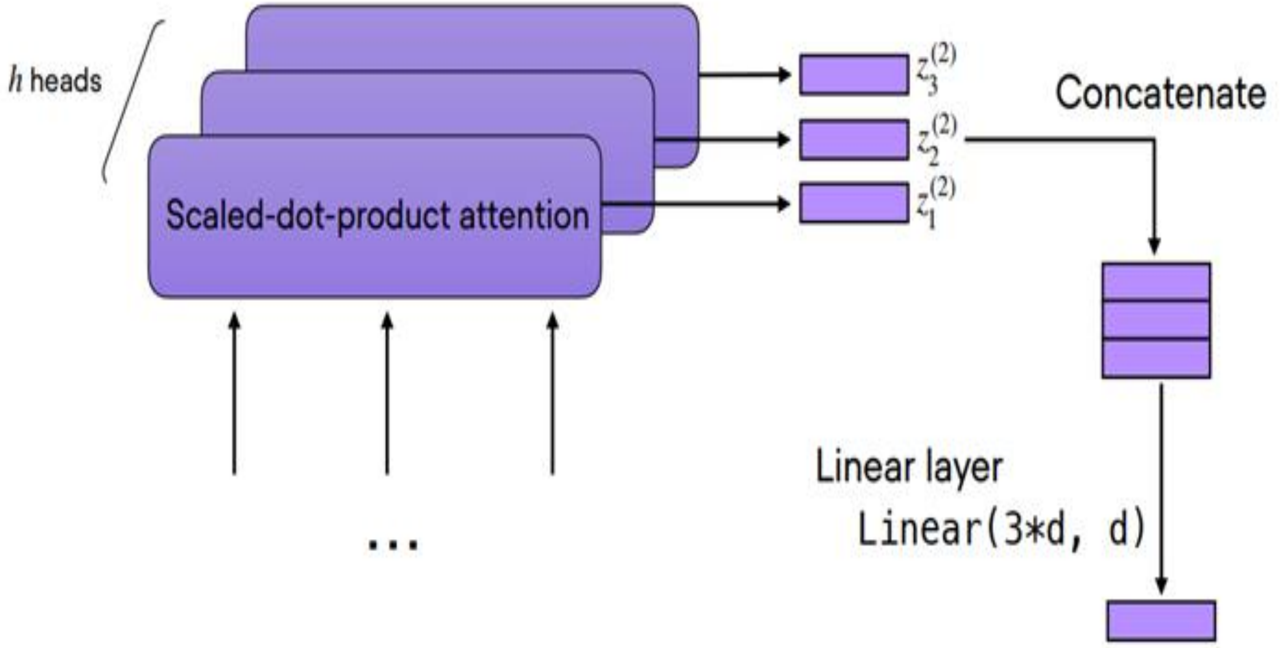
Similar a tener varios filtros convolucionales



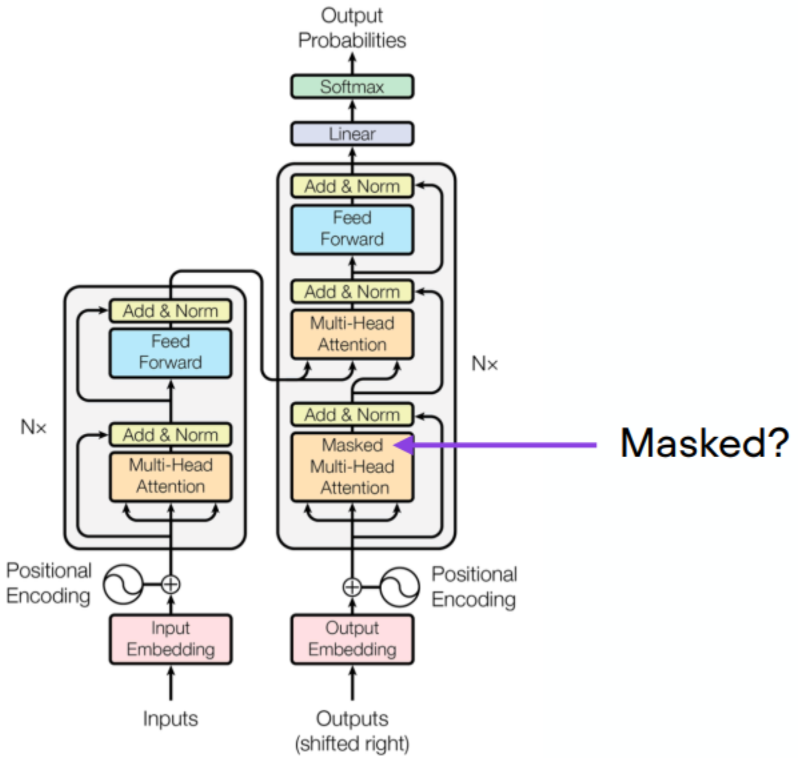
Multi-head attention



Multi-head attention



Masked Multi-head attention



Masked Multi-head attention

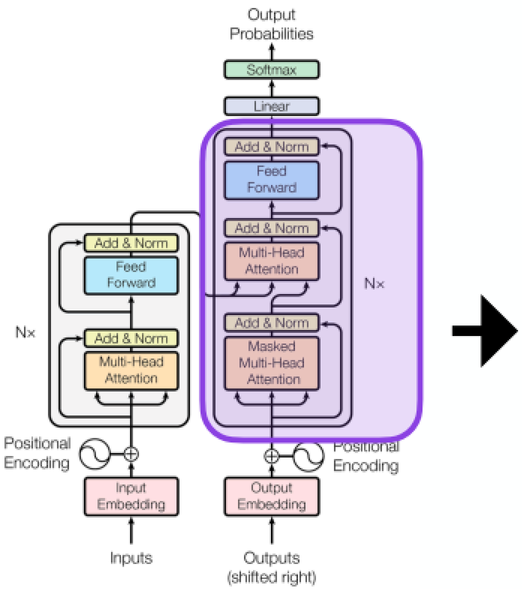
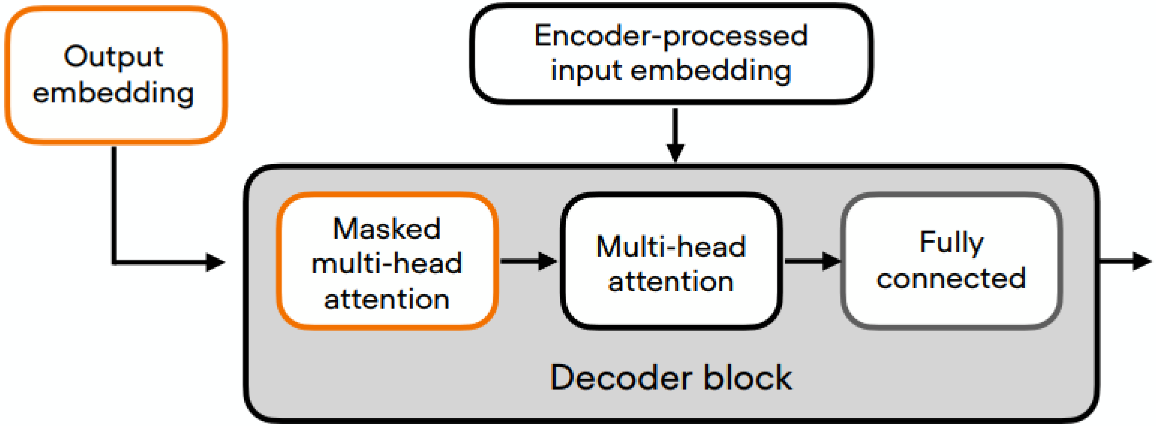


Figure 1: The Transformer - model architecture.



(A concise sketch of the decoder block)

Masked Multi-head attention

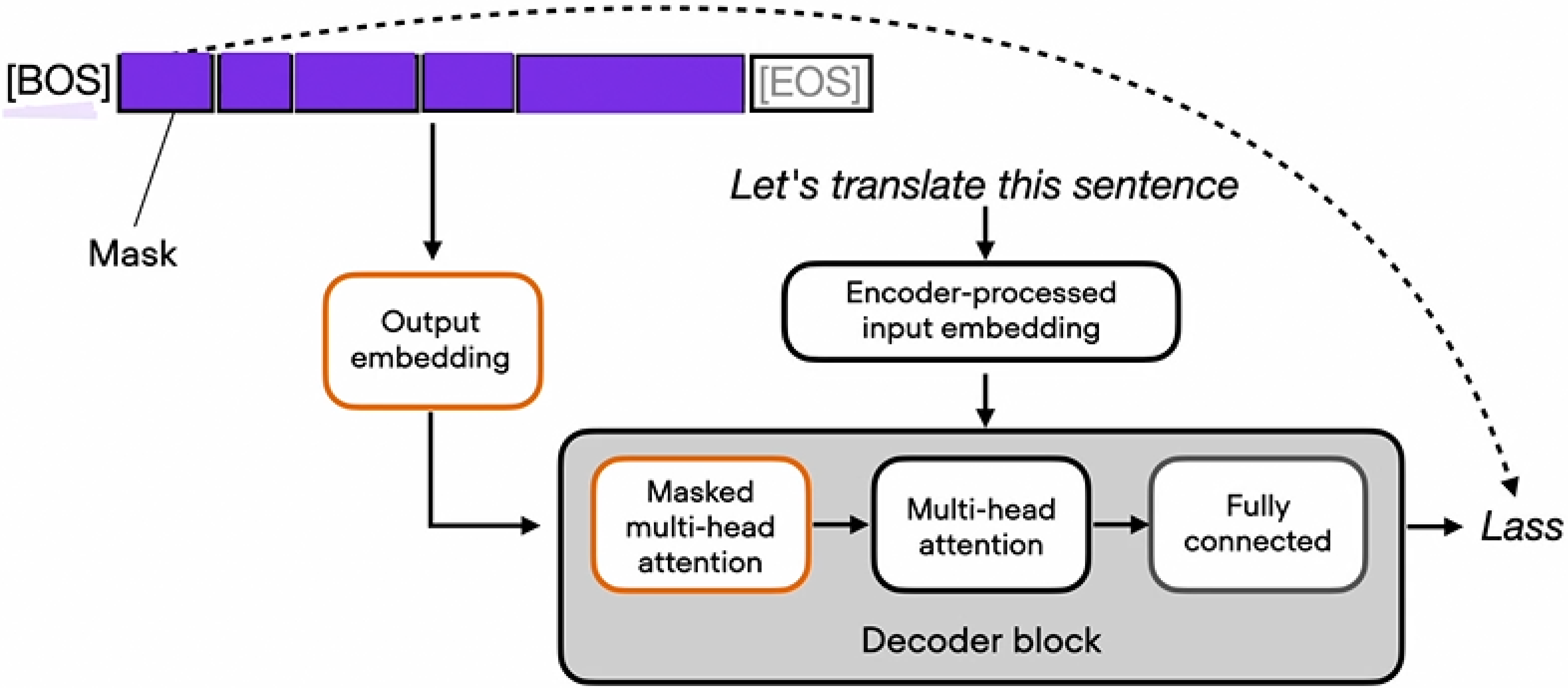
English → German Translation

Input: *Let's translate this sentence*

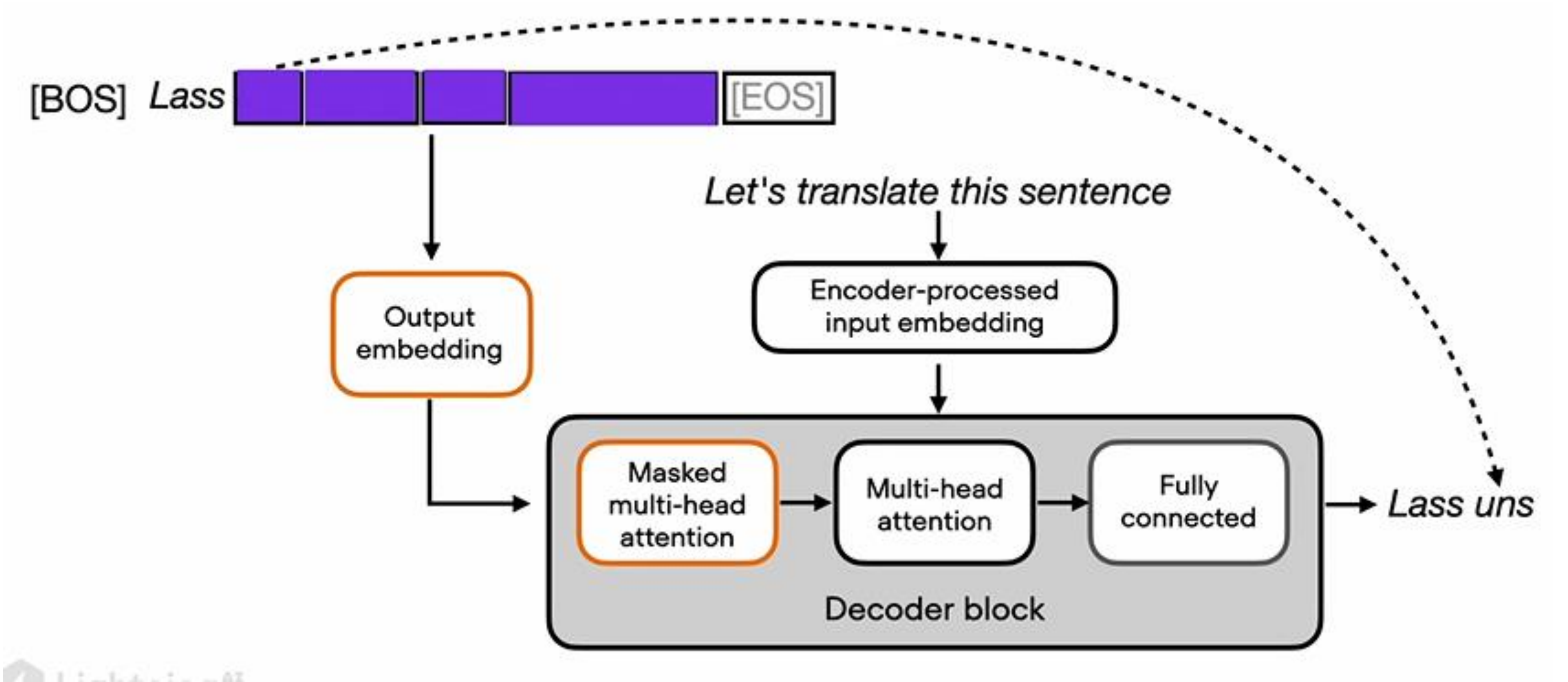
Target: *Lass uns diesen Satz uebersetzen*

Masked Multi-head attention

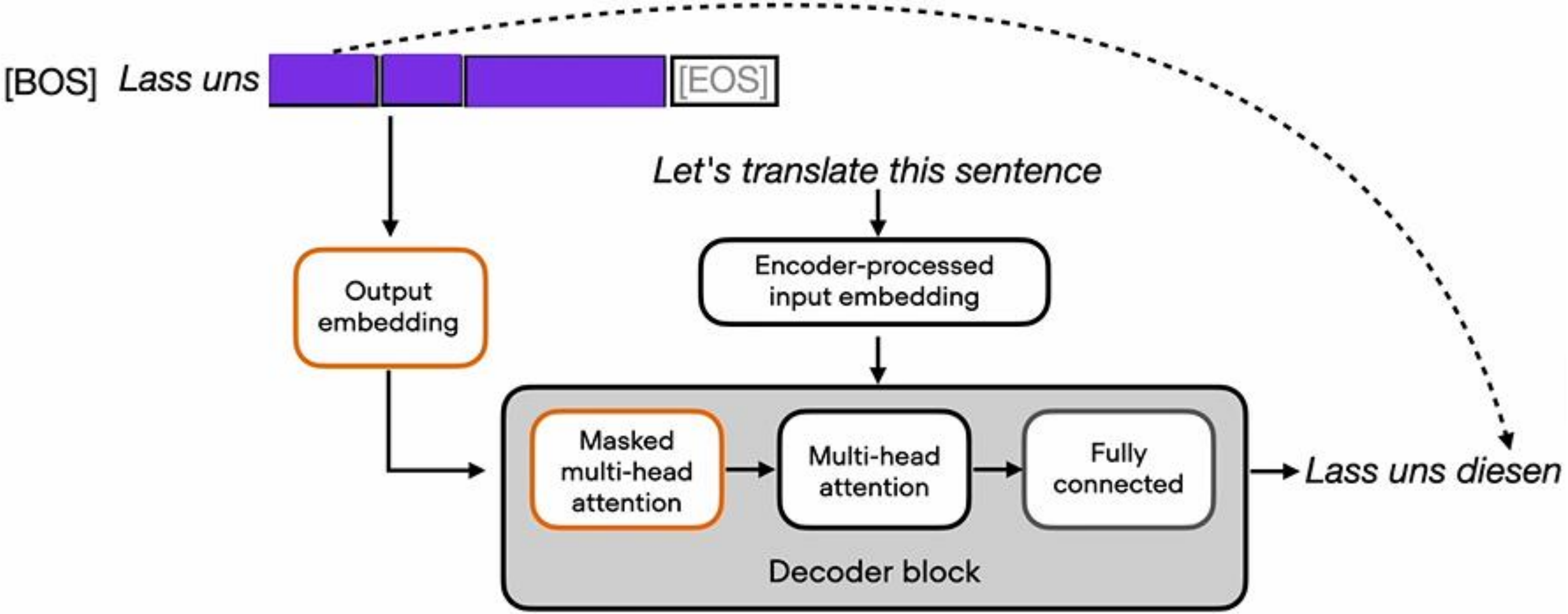
Masked attention enmascara los tokens que el modelo no ha visto.
Acá visualizamos en las entradas en lugar de los tokens por facilidad



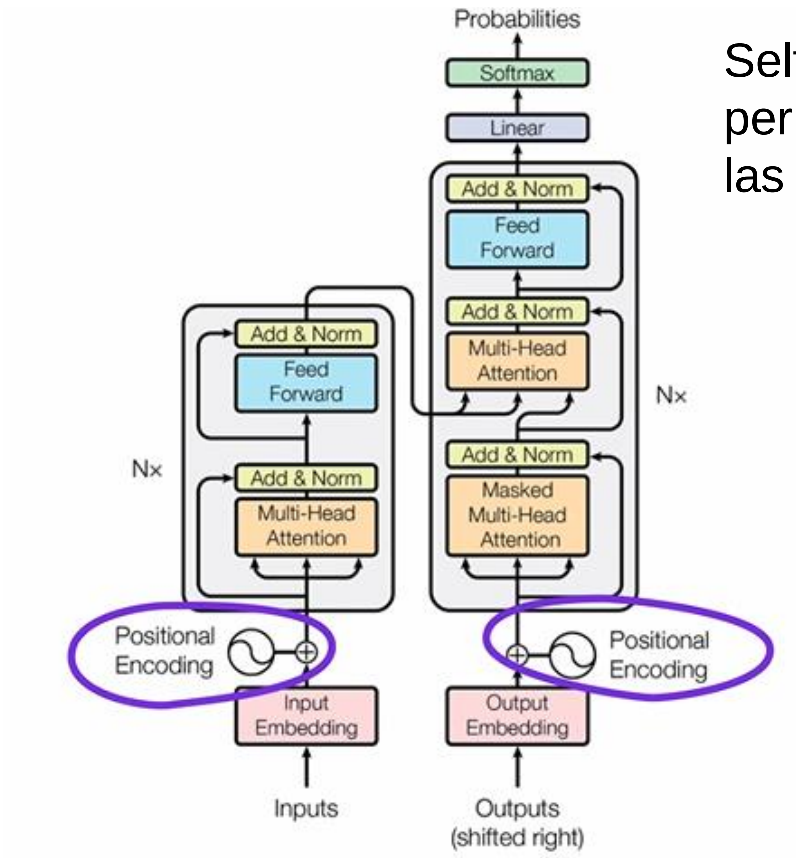
Masked Multi-head attention



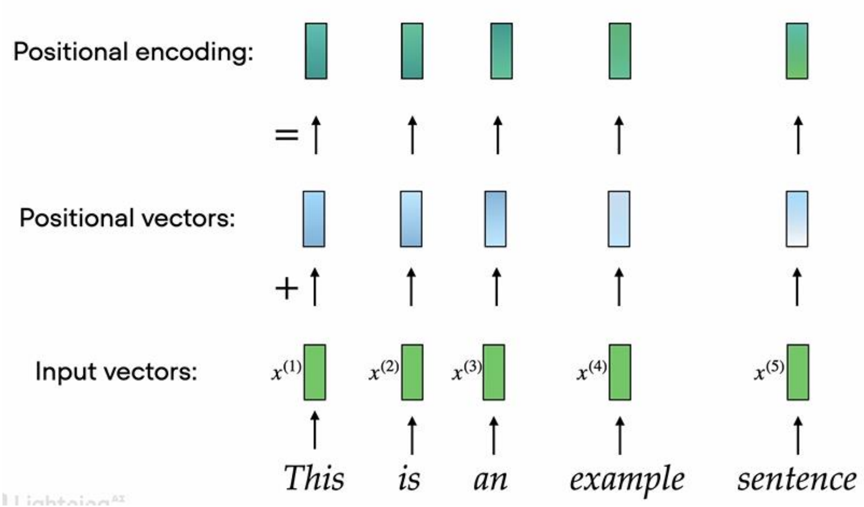
Masked Multi-head attention



Positional encoding



Self-attention y Fully Connected son invariantes a la permutación, i.e., no tienen en cuenta el orden de las palabras en la entrada



Generative Pretrained Transformers - GPT

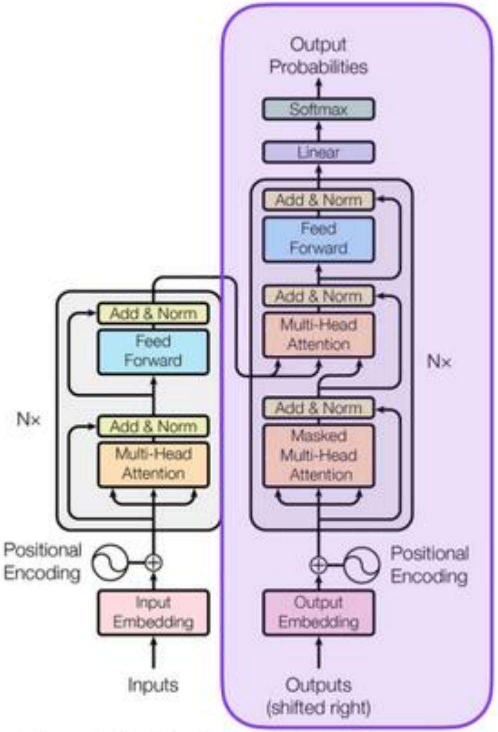
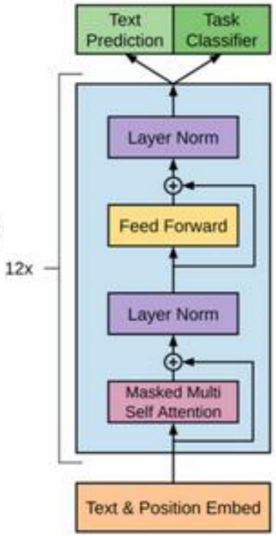


Figure 1: The Transformer - model architecture.

GPT Recap

GPT is essentially the decoder part of the original transformer



https://s3-us-west-2.amazonaws.com/openai-assets/research-covers/language-unsupervised/language_understanding_paper.pdf

Generative Pretrained Transformers - GPT

GPT ingresa el texto de izquierda a derecha de forma que el modelo aprende a predecir la palabra siguiente

Self-supervised pre-training

1. Pre-entrenar: Predecir la palabra siguiente (self-atenttion unidireccional)
2. Fine-tune

BERT

Self-supervised pre-training

1. Pre-entrenar:
    a. Predecir palabras aleatoriamente enmascaradas (bi-direccional/no direccional)
    b. Predecir el orden de las oraciones
2. Fine-tune

BERT

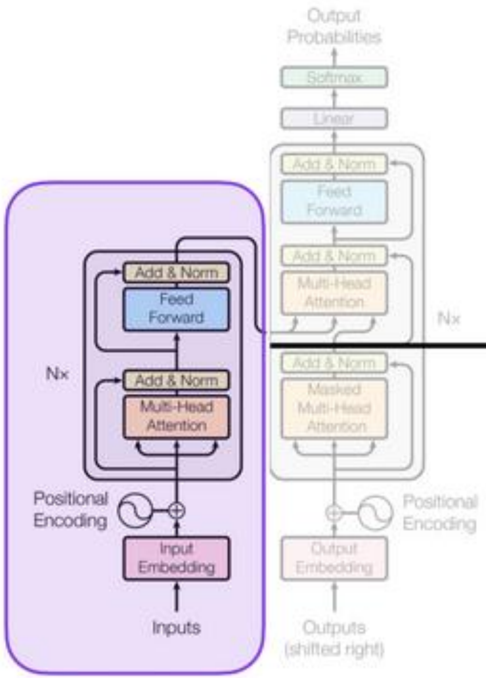
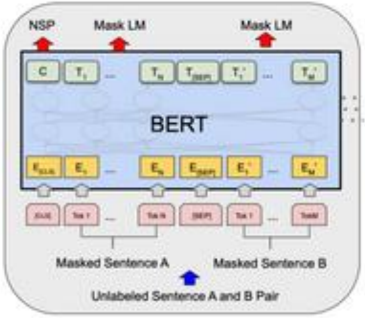


Figure 1: The Transformer - model architecture.

BERT is essentially the encoder part of the original transformer



BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding,
https://arxiv.org/abs/1810.04805

BERT

1. Pre-entrenar en un conjunto de datos no etiquetado (aprender un modelo de lenguaje general)
    a. Predecir palabras aleatoriamente enmascaradas (bi-direccional/no direccional)

Input sentence: *The curious kitten deftly climbed the bookshelf*

↓

Pick 15% of the words randomly

The curious kitten deftly ***climbed*** *the bookshelf*

↓

- 80% of the time, replace with [MASK] token
- 10% of the time, replace with random token (e.g. ate)
- 10% of the time, keep unchanged

BERT

1. Pre-entrenar en un conjunto de datos no etiquetado (aprender un modelo de lenguaje general)

    b. Predecir el orden de las oraciones

[CLS] Sentence A [SEP] Sentence B

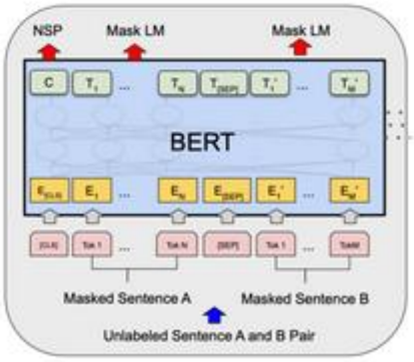
Placeholder for the IsNext=True / False label in the decoder output

[CLS] Toast is a simple yet delicious food [SEP] It's often served with butter, jam, or honey.

IsNext = True

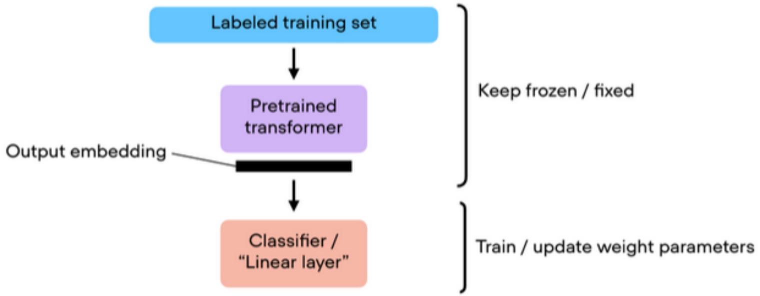
[CLS] It's often served with butter, jam, or honey. [SEP] Toast is a simple yet delicious food.

IsNext = False

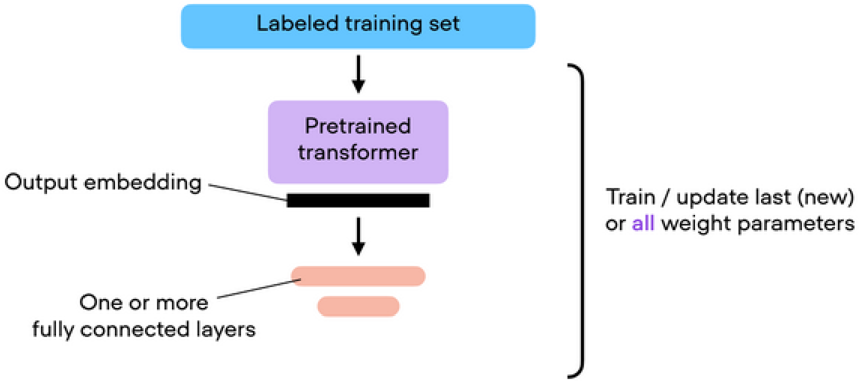


Utilización de Transformers pre-entrenados

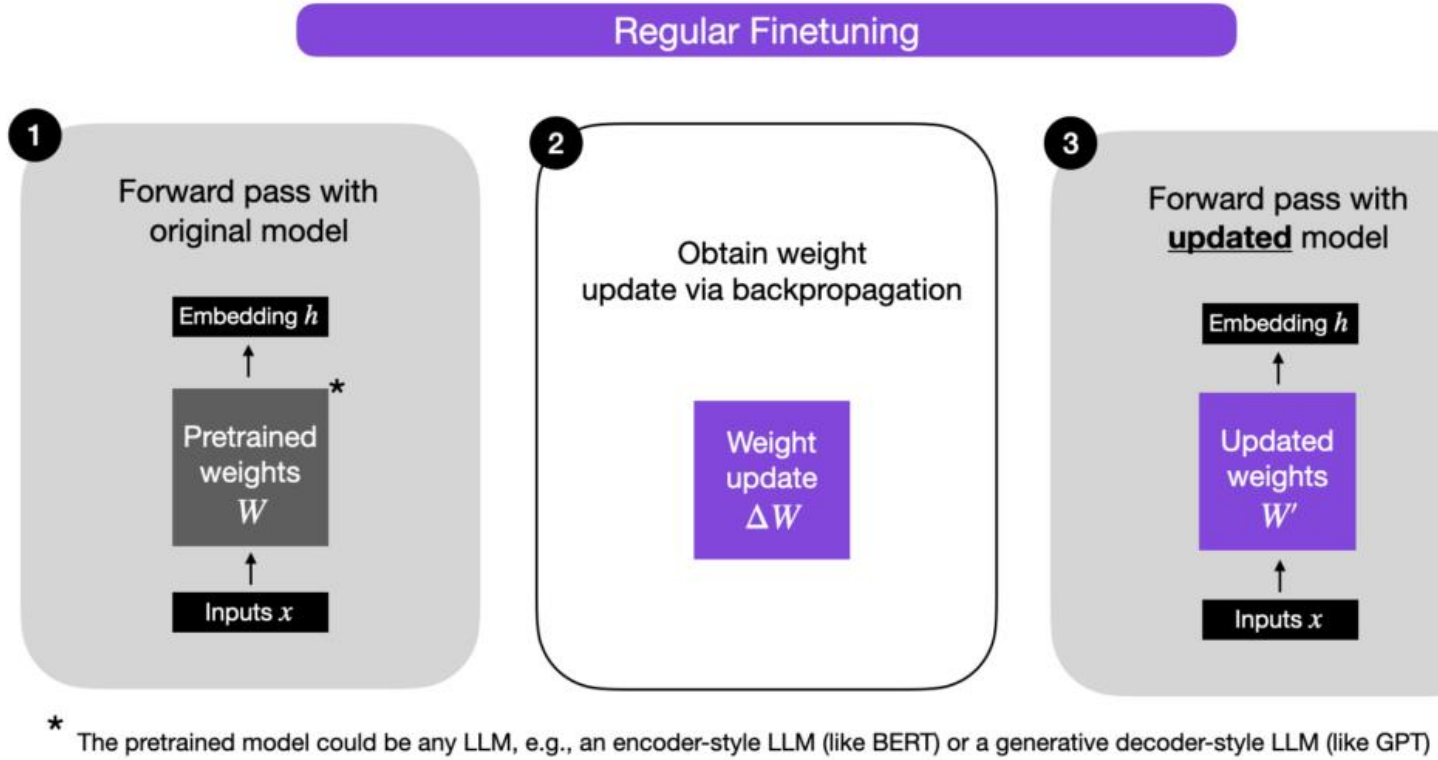
1. Feature-based approach



2. Fine-tuning approach



Parameter Efficient Fine Tuning - PEFT



LoRA: Low-Rank Adaptation of LLMs

Computer Science > Computation and Language

[Submitted on 17 Jun 2021 (v1), last revised 16 Oct 2021 (this version, v2)]

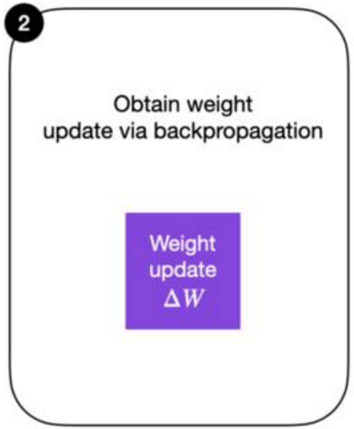
LoRA: Low-Rank Adaptation of Large Language Models

Edward J. Hu, Yelong Shen, Phillip Wallis, Zeyuan Allen-Zhu, Yuanzhi Li, Shean Wang, Lu Wang, Weizhu Chen

An important paradigm of natural language processing consists of large-scale pre-training on general domain data and adaptation to particular tasks or domains. As we pre-train larger models, full fine-tuning, which retrains all model parameters, becomes less feasible. Using GPT-3 175B as an example -- deploying independent instances of fine-tuned models, each with 175B parameters, is prohibitively expensive. We propose Low-Rank Adaptation, or LoRA, which freezes the pre-trained model weights and injects trainable rank decomposition matrices into each layer of the Transformer architecture, greatly reducing the number of trainable parameters for downstream tasks. Compared to GPT-3 175B fine-tuned with Adam, LoRA can reduce the number of trainable parameters by 10,000 times and the GPU memory requirement by 3 times. LoRA performs on-par or better than fine-tuning in model quality on RoBERTa, DeBERTa, GPT-2, and GPT-3, despite having fewer trainable parameters, a higher training throughput, and, unlike adapters, no additional inference latency. We also provide an empirical investigation into rank-deficiency in language model adaptation, which sheds light on the efficacy of LoRA. We release a package that facilitates the integration of LoRA with PyTorch models and provide our implementations and model checkpoints for RoBERTa, DeBERTa, and GPT-2 at this https URL.

Descomponer $\Delta \mathbf{W}$ en una representación de menor rango

Regular fine-tuning



Actualización:

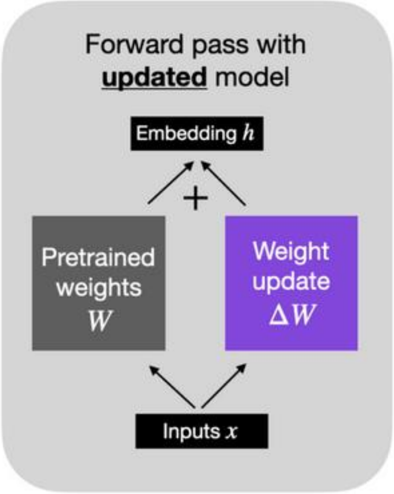
$$\Delta \mathbf{W} = -\alpha \frac{\partial \mathcal{L}}{\partial \mathbf{W}}$$

$$\mathbf{W} = \mathbf{W} + \Delta \mathbf{W}$$

$$\mathbf{h} = \mathbf{W}\mathbf{x} + \color{red}{\mathbf{b}}$$

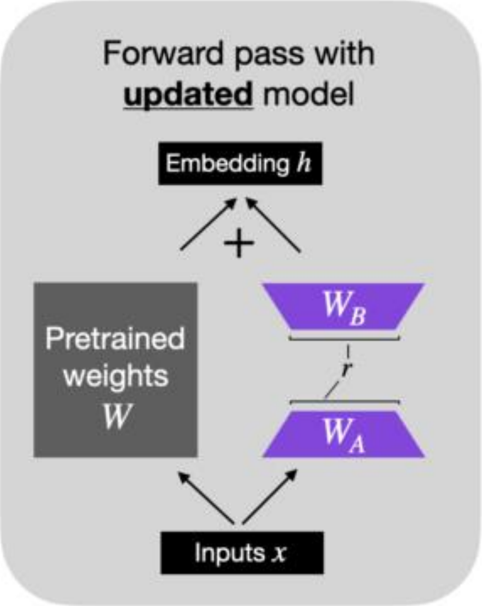
Alternativa:

$$\mathbf{h} = \mathbf{W}\mathbf{x} + \Delta \mathbf{W}\mathbf{x} + \color{red}{\mathbf{b}}$$



LoRA: Low-Rank Adaptation of LLMs

LoRA weights, W_A and W_B, represent ΔW



$$\Delta \mathbf{W} = \mathbf{W}_A \mathbf{W}_B$$
$$\mathbf{W}_A \in \Re^{A \times r}$$
$$\mathbf{W}_B \in \Re^{r \times B}$$
$$\mathbf{W} \in \Re^{A \times B}$$

Mantener "congelado" $\mathbf{W}$ y actualizar $\mathbf{W}_{AB}$

Si $r << \{A, B\}$ se actualizan muchos menos parámetros