

Self-Attention, Transformers, BERT

Pavlos Protopapas



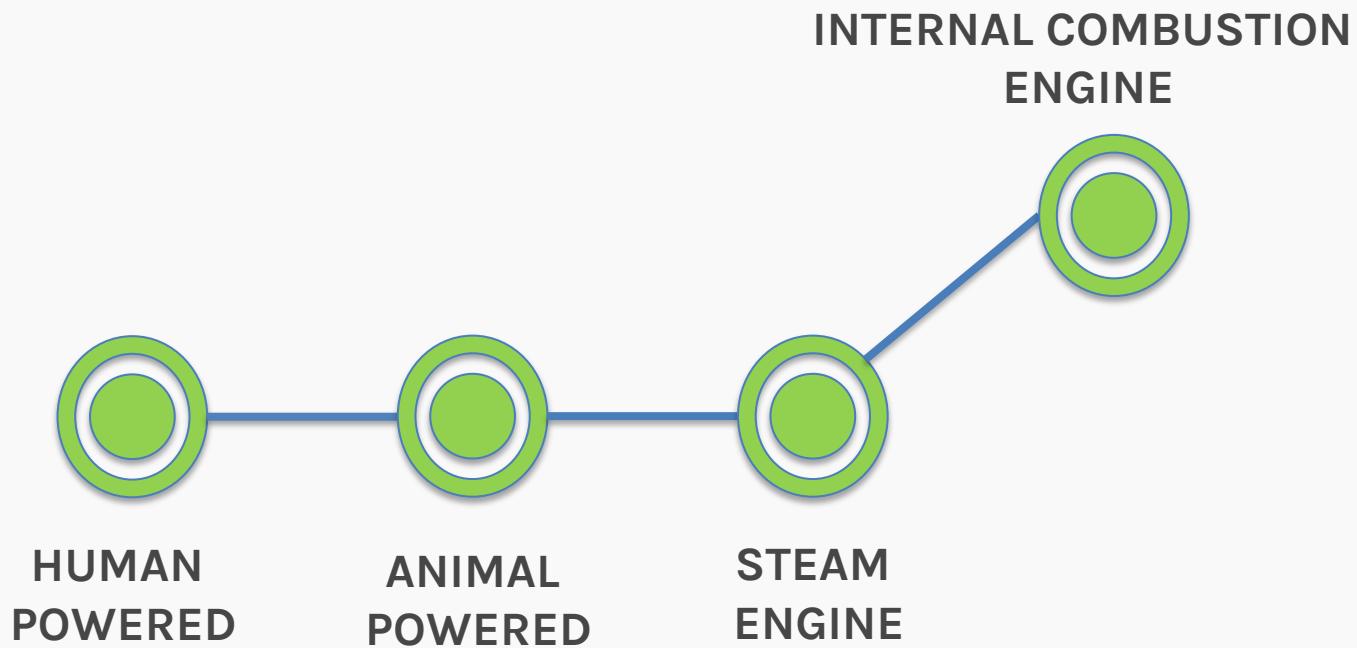
# Outline

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- Motivation for Attention
  - Recap Seq2Seq
  - Limitations of RNNs
- Attention Basics
  - Issues with spatial attention models
  - Using cosine similarity as a tool for contextual relations
  - Self-Attention
- Building blocks of Transformers and BERT
  - Multi-head attention block
  - Positional Encoding
  - Bringing it all together



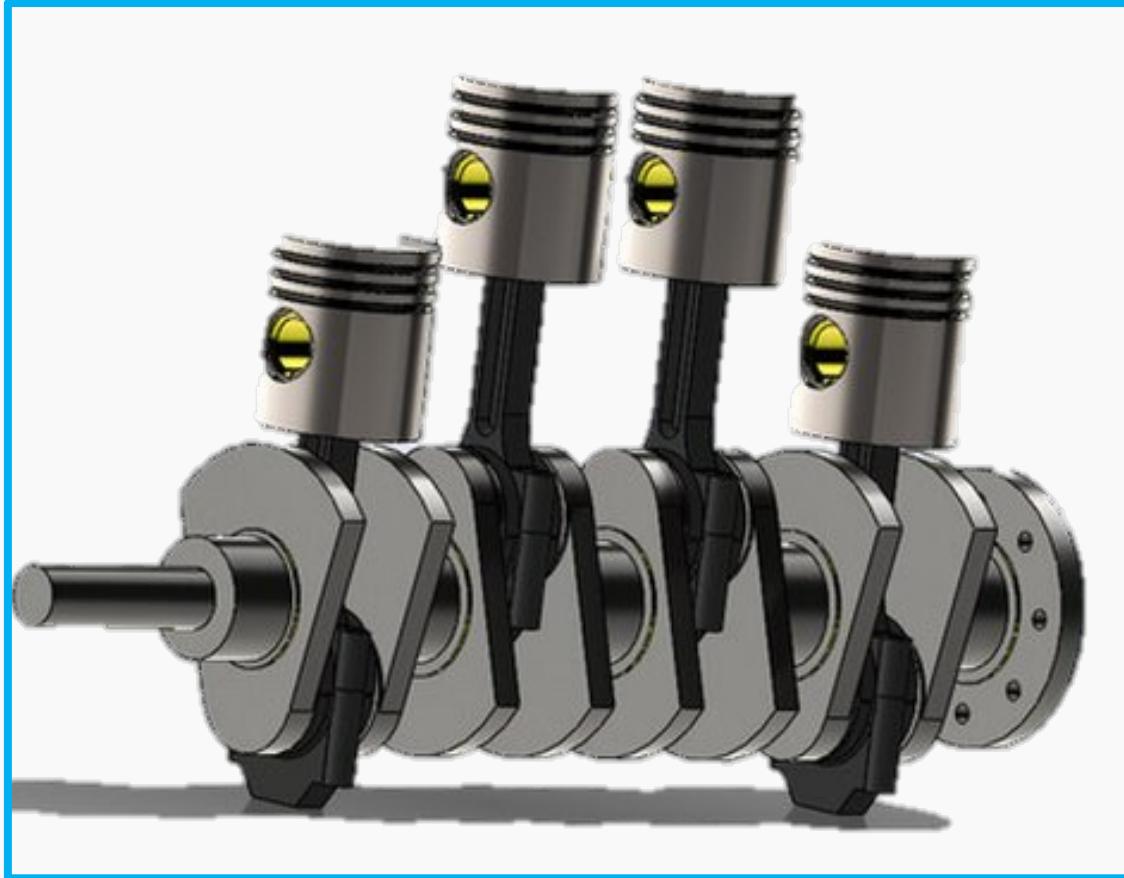
# Electricity is all you need



# A brief history of engines



FLYWHEEL



IC COMBUSTION ENGINE

PROTOPAPAS

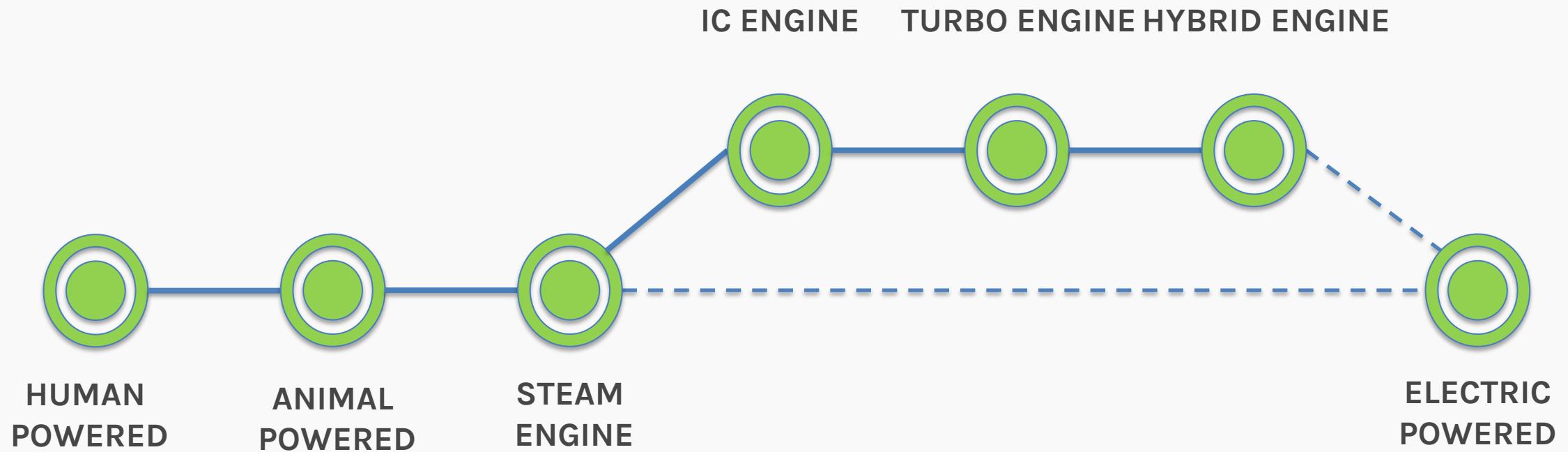
DC MOTOR



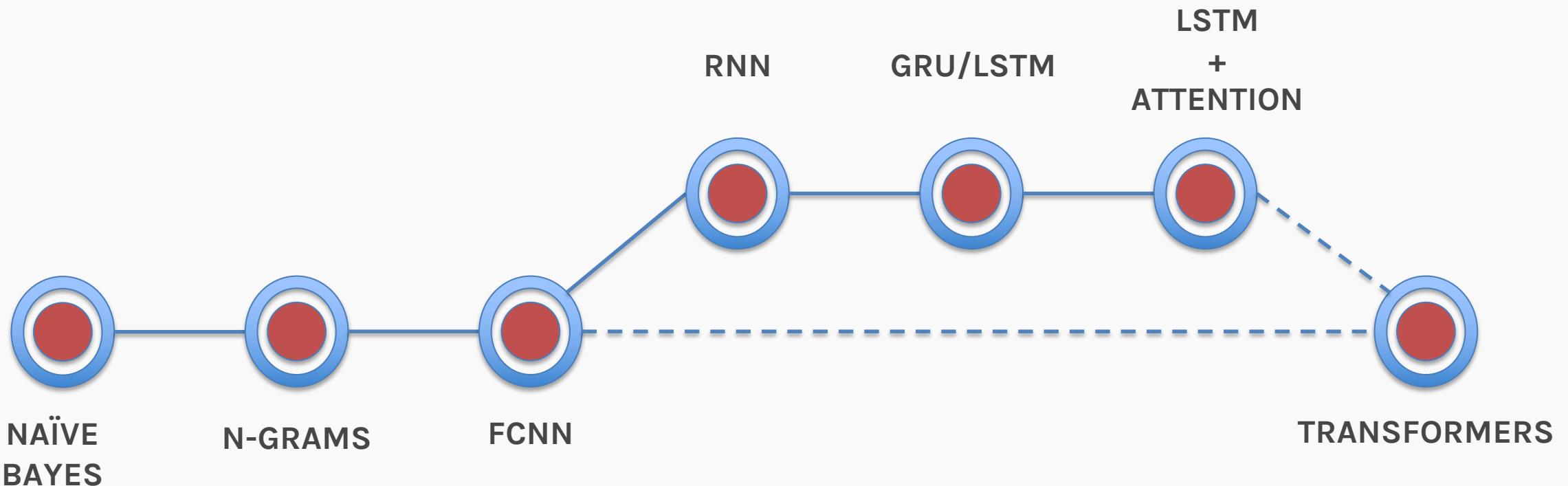
ALTERNATOR



# Electricity is all you need



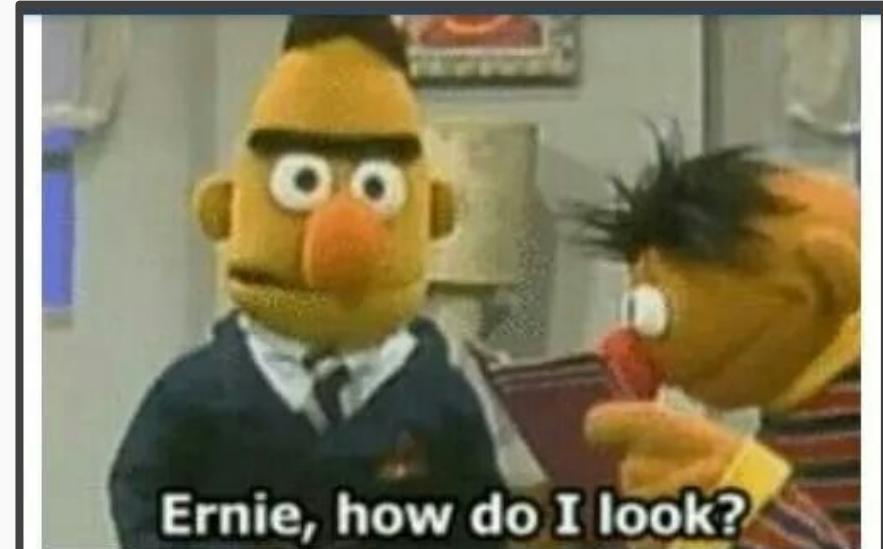
# Language modeling



# What we want

## Language Model Wishlist?

- We want to have strong contextual relations between words
- We want words to have sequential information
- We need an architecture that can be trained in parallel (non-Markovian property)



**Ernie, how do I look?**



**With your eyes, Bert.**



We've already seen an approach of relative importance  
**Attention**



# Attention: Example sentence

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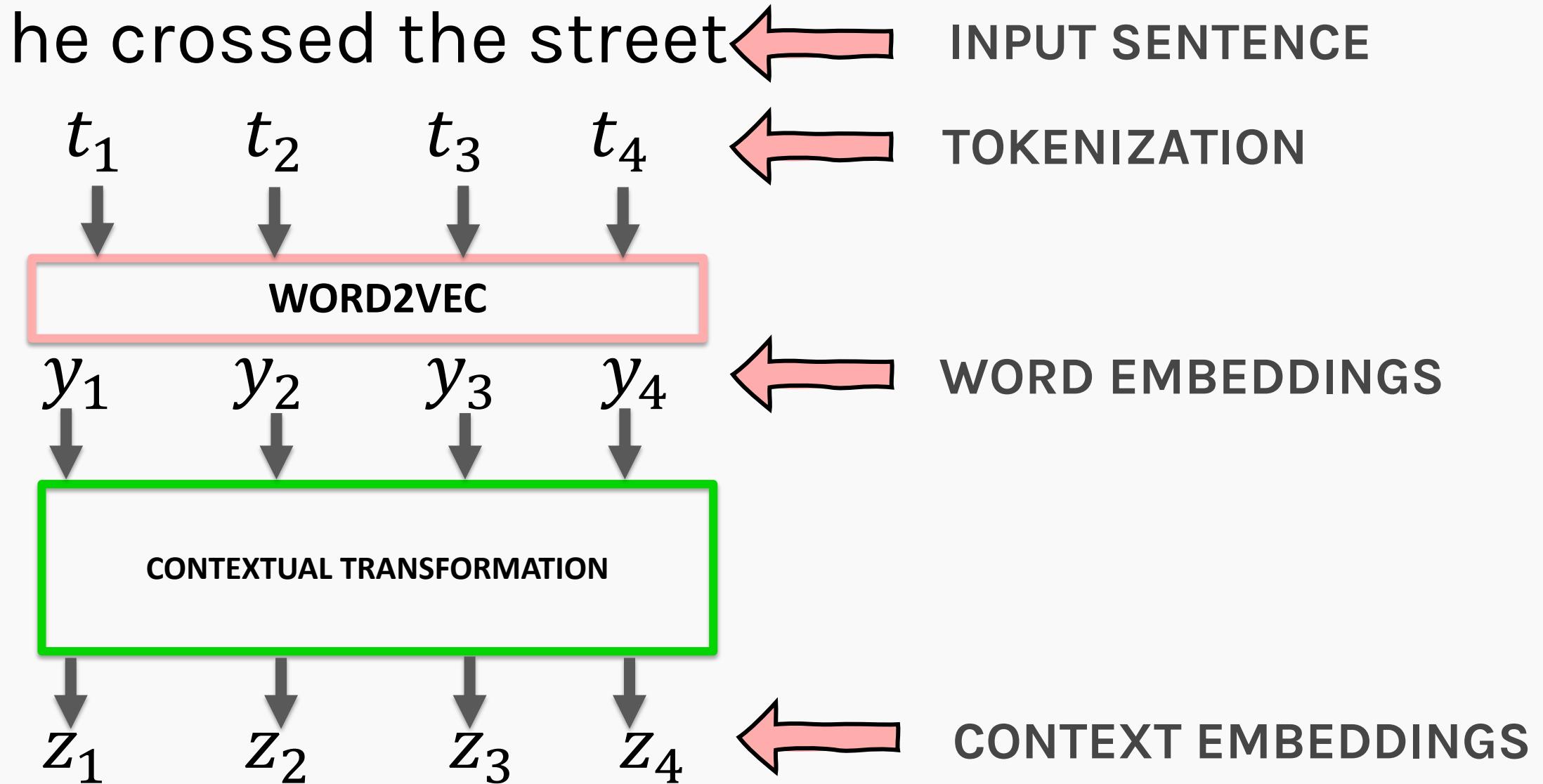
How do we find the context of the word ‘he’ in the sentence below?



Shivas was hit by a bus because **he** crossed the street



# Attention – Where to add weights?



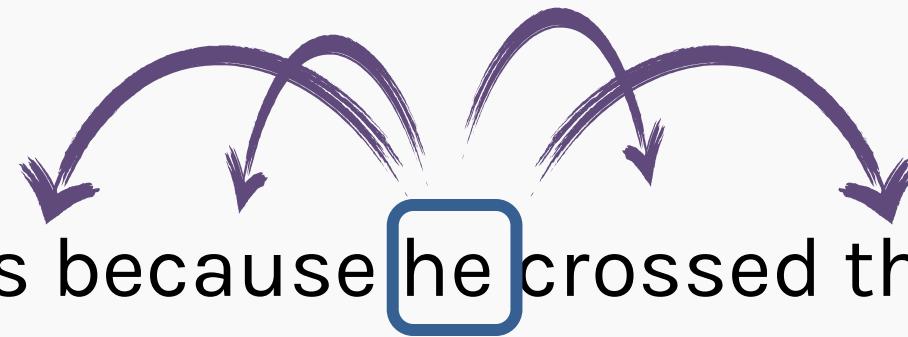
## Attention: Example sentence



### IDEA #1: Positional relationship



Shivas was hit by a bus because he crossed the street



## Attention: Example sentence



### IDEA #1: Positional transformation



Shivas was hit by a bus because he crossed the street



True context

✖ This idea does not work because context can be **unevenly** spread out in a sentence



# Attention – The basics

- We can still use the idea of transforming the word embeddings to get more context
- However, the transformation matrix A must place some importance to the relative importance of words

$$y = [y_1, y_2, y_3, \dots, y_n]$$
$$z = A y^T$$

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & \dots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \dots & a_{2n} \\ \dots & \dots & \dots & a_{ij} & \dots & a_{in} \\ a_{n1} & a_{n2} & a_{n3} & \dots & a_{nn} \end{bmatrix}$$



$a_{ij}$  must account for relative importance between word  $i$  &  $j$

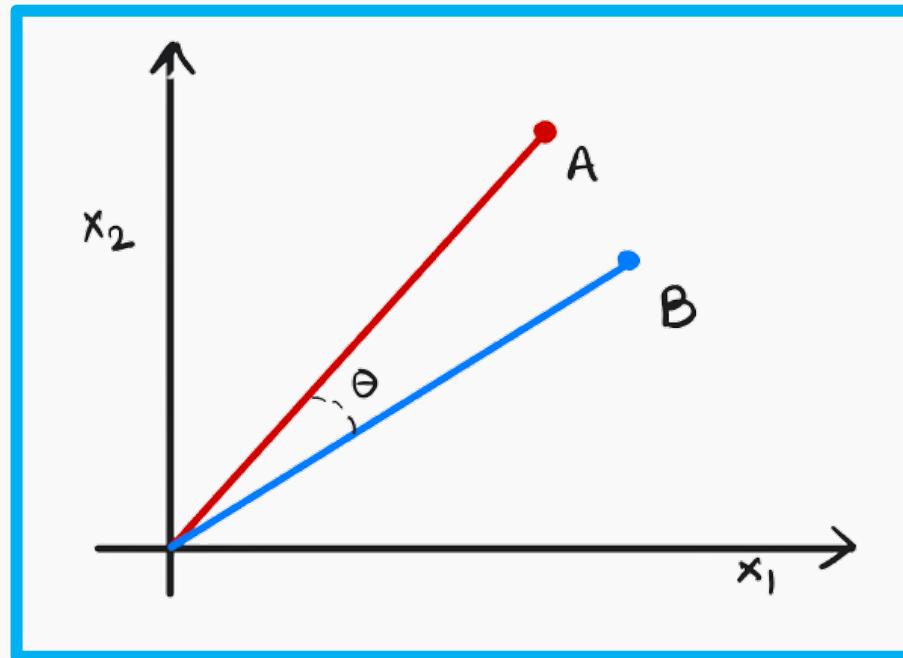


# Attention – Text Data



But how can we do it?

Yes! Let's use cosine similarity between words

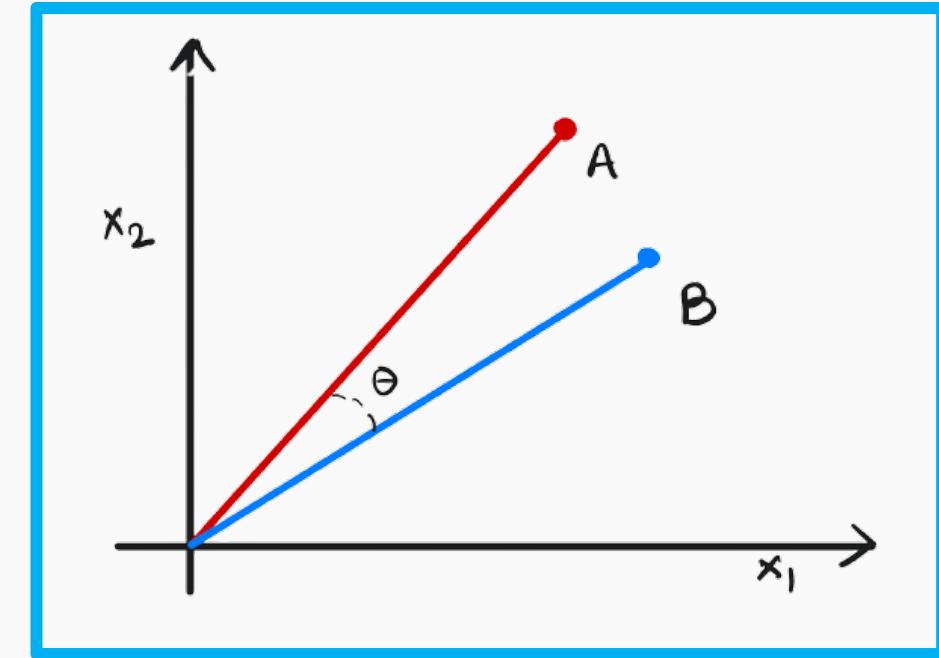
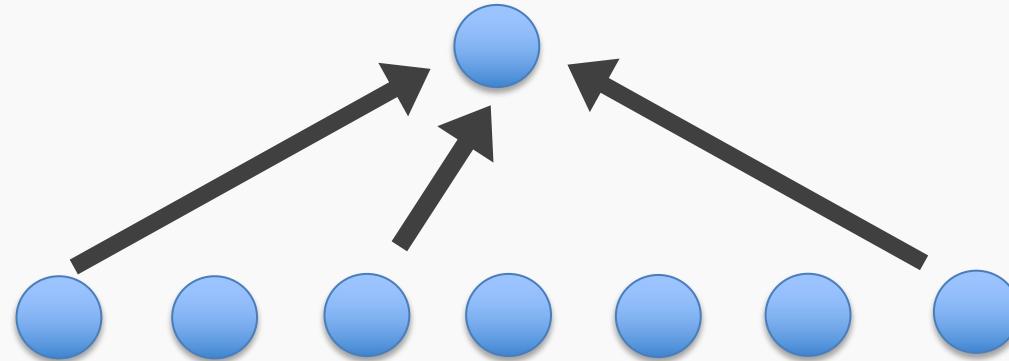


$$\cos(\theta) = \frac{\mathbf{A} \cdot \mathbf{B}}{\|\mathbf{A}\| \|\mathbf{B}\|}$$



## RECAP: Cosine Similarity

For context, we could just take the cosine similarity of the target word with respect to every other word in the sentence



$$\text{similarity} = \cos(\theta) = \frac{\mathbf{A} \cdot \mathbf{B}}{\|\mathbf{A}\| \|\mathbf{B}\|} = \frac{\sum_{i=1}^n A_i B_i}{\sqrt{\sum_{i=1}^n A_i^2} \sqrt{\sum_{i=1}^n B_i^2}}$$

Where  $A_i$  &  $B_i$  are components of vector  $A$  &  $B$  respectively



# How do we do it?



## Attention: Example sentence #2



Ignacio was standing next to the bank of the river



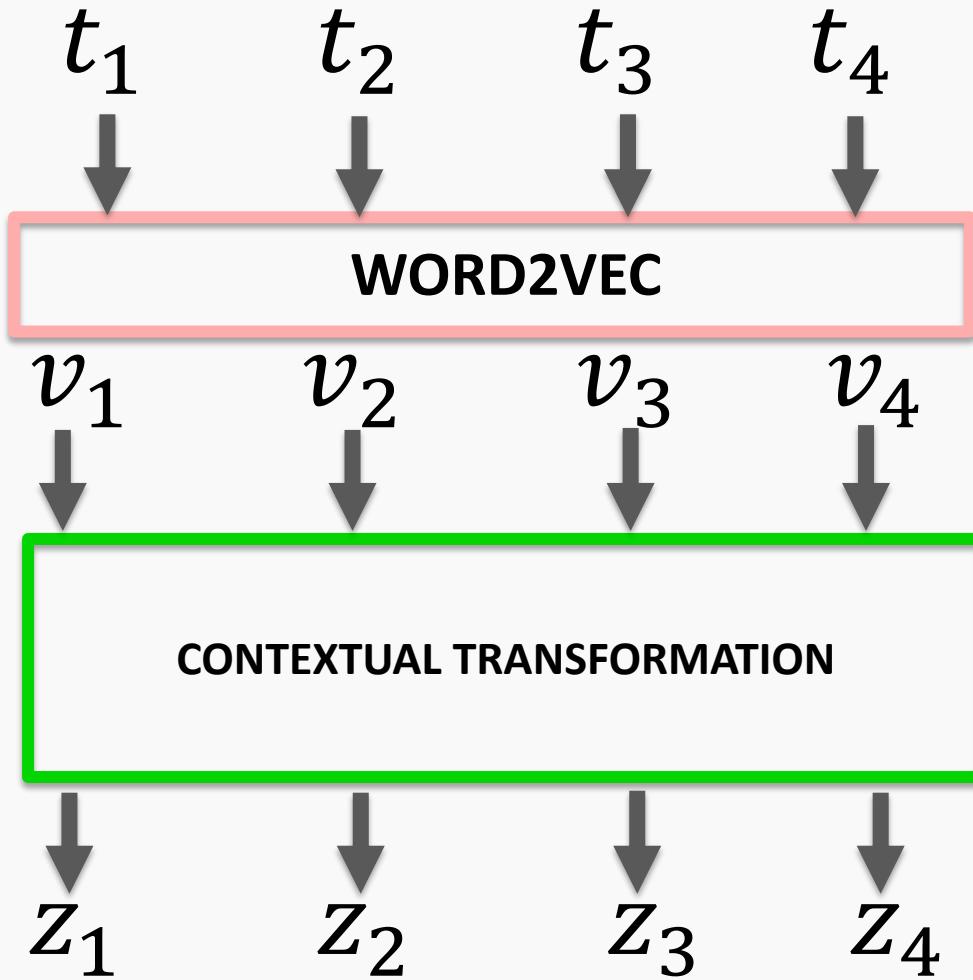
## Attention: Example sentence #2

**bank of the river**

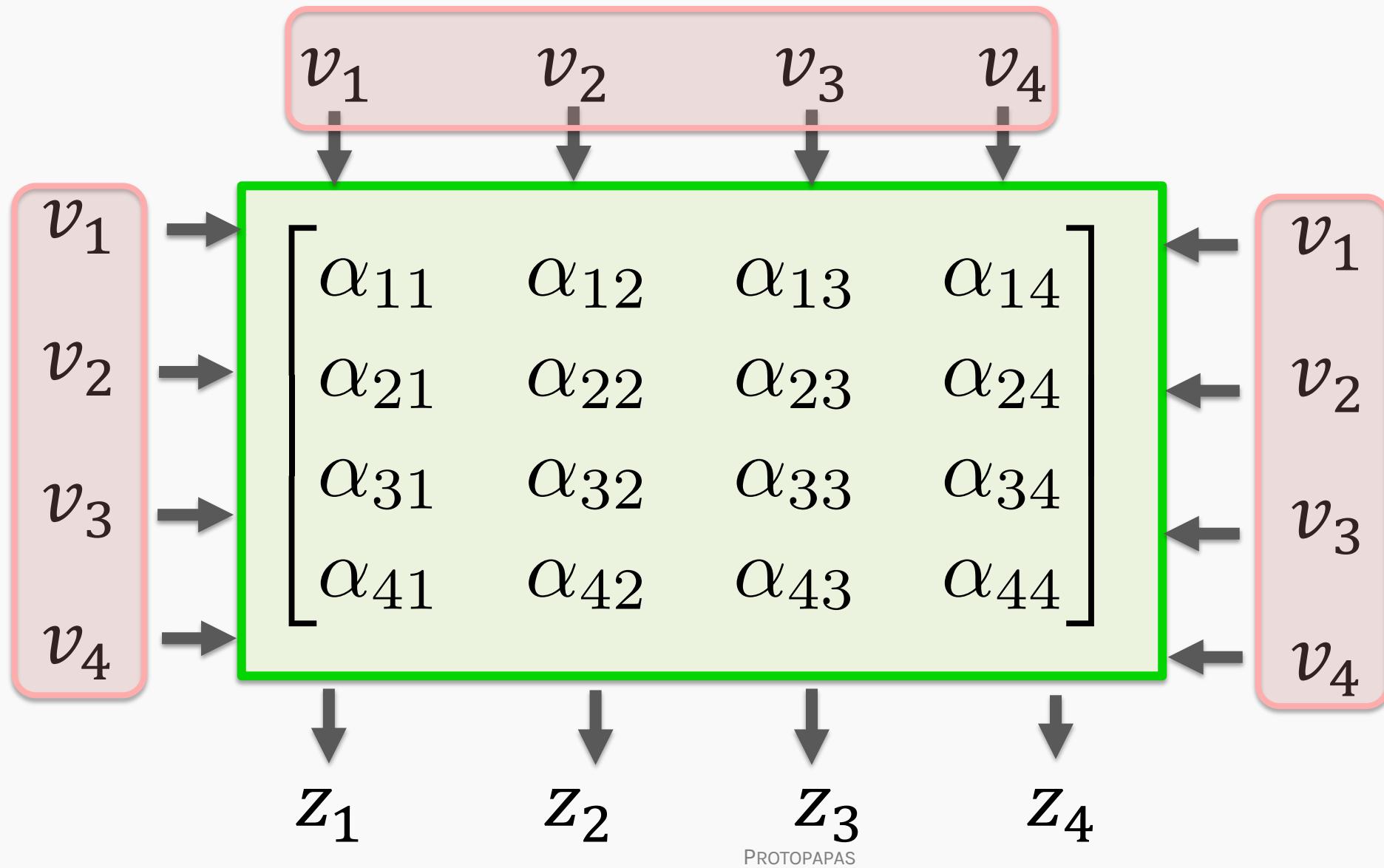


# Attention - Cosine Similarity

bank of the river



# Attention - Cosine Similarity



## Attention: Example sentence #2

$$v_1 \circ v_1 = a_{11}$$

$$v_1 \circ v_2 = a_{12}$$

$$v_1 \circ v_3 = a_{13}$$

$$v_1 \circ v_4 = a_{14}$$

WEIGHTS  
NORMALIZATION

$$\alpha_{11}$$

$$\alpha_{12}$$

$$\alpha_{13}$$

$$\alpha_{14}$$

$$\sum \alpha_{1l} = 1$$



## Attention: Example sentence #2

$$\sum \alpha_{1i} = 1$$

$$z_1 = v_1\alpha_{11} + v_2\alpha_{12} + v_3\alpha_{13} + v_4\alpha_{14}$$

New contextual  
word embedding



## Attention: Example sentence #2

Similarly...

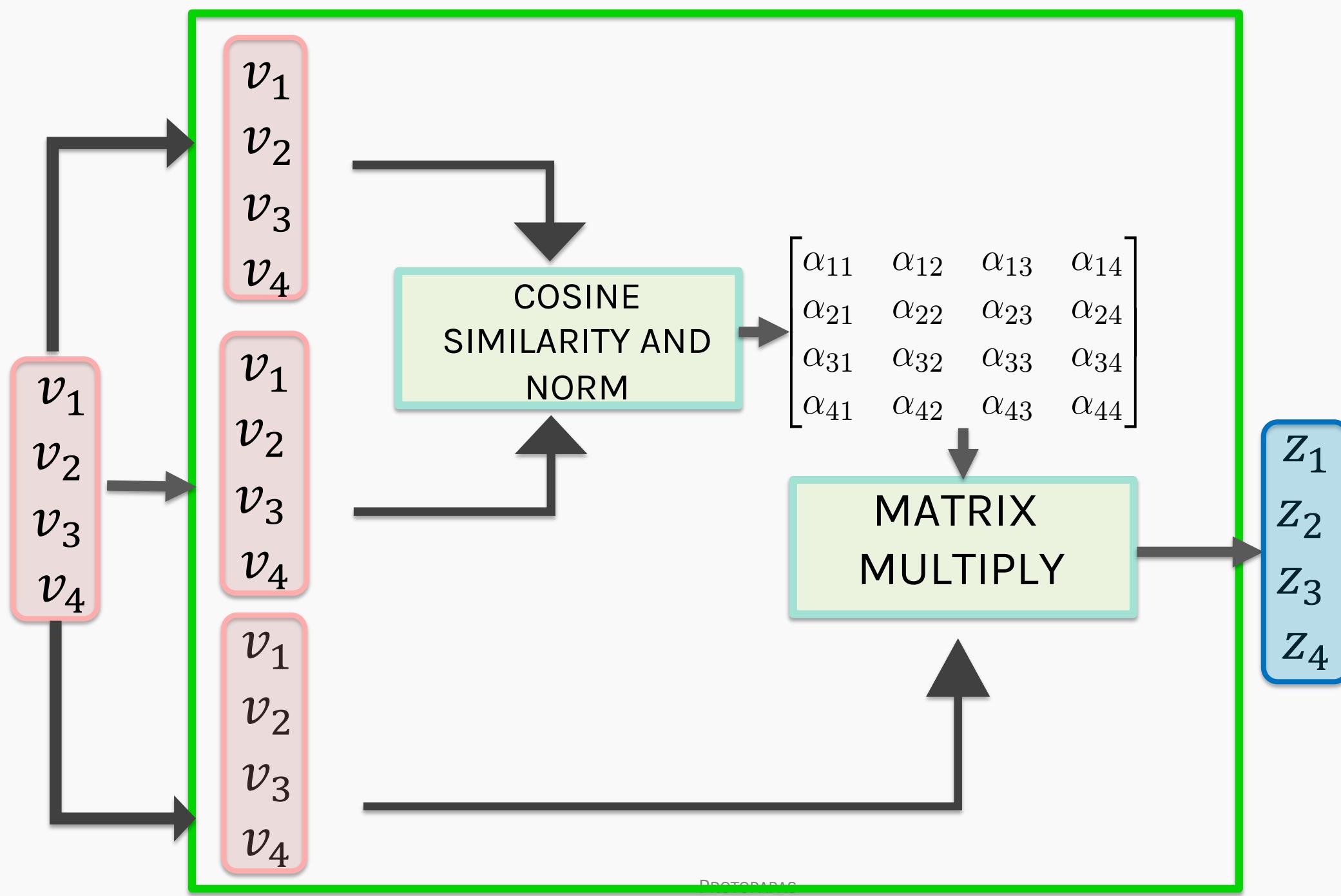
$$z_1 = v_1 \alpha_{11} + v_2 \alpha_{12} + v_3 \alpha_{13} + v_4 \alpha_{14}$$

$$z_2 = v_1 \alpha_{21} + v_2 \alpha_{22} + v_3 \alpha_{23} + v_4 \alpha_{24}$$

$$z_3 = v_1 \alpha_{31} + v_2 \alpha_{32} + v_3 \alpha_{33} + v_4 \alpha_{34}$$

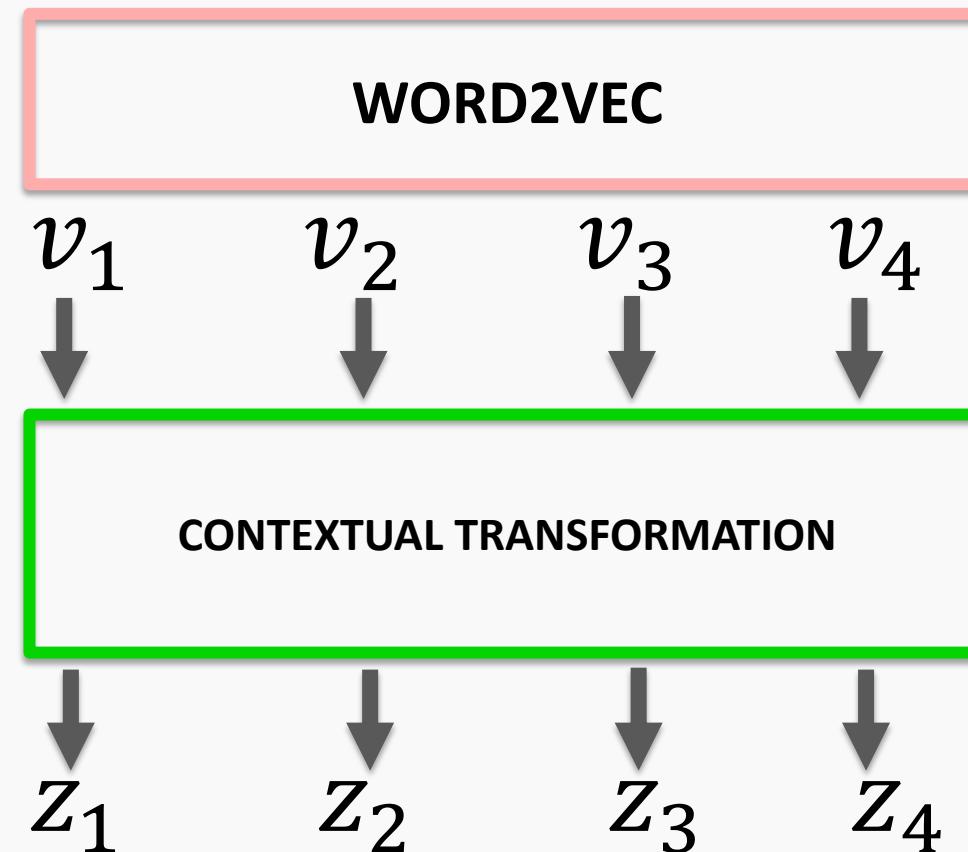
$$z_4 = v_1 \alpha_{41} + v_2 \alpha_{42} + v_3 \alpha_{43} + v_4 \alpha_{44}$$





## Attention: Example sentence #2

bank of the river



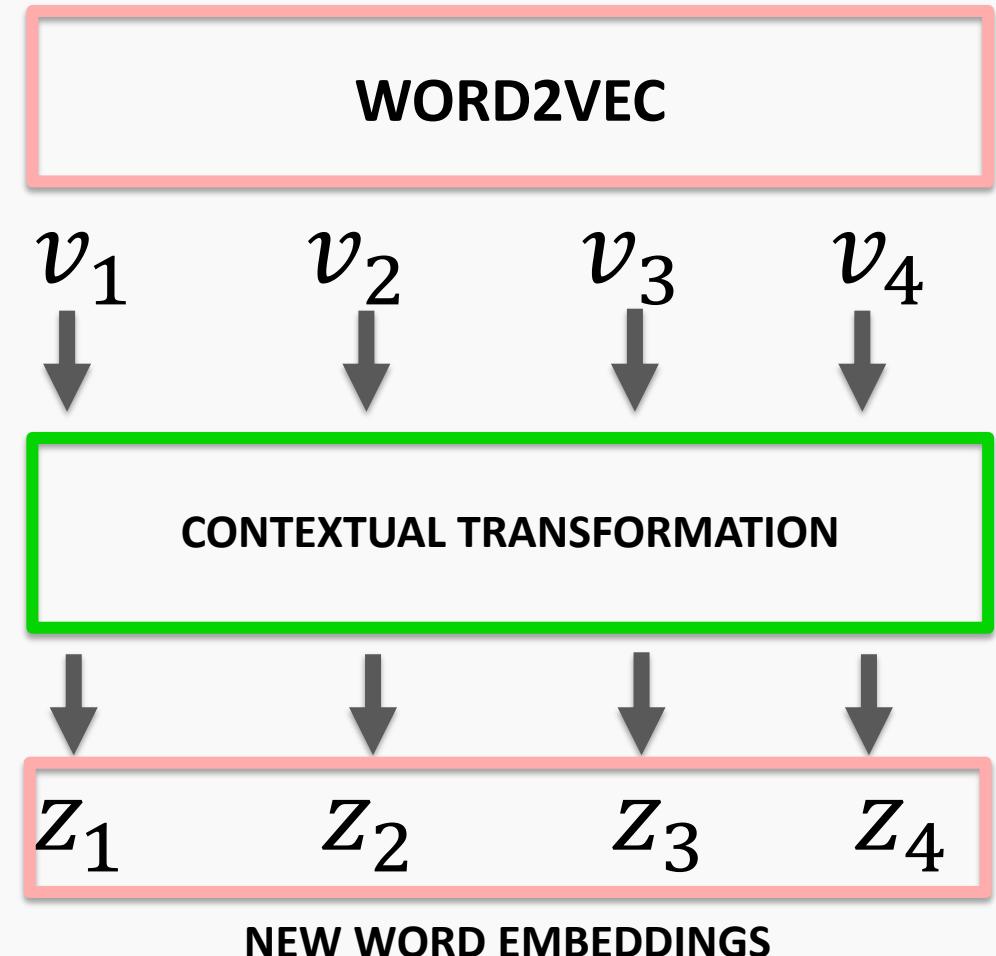
# Attention

## ATTENTION ISSUES?

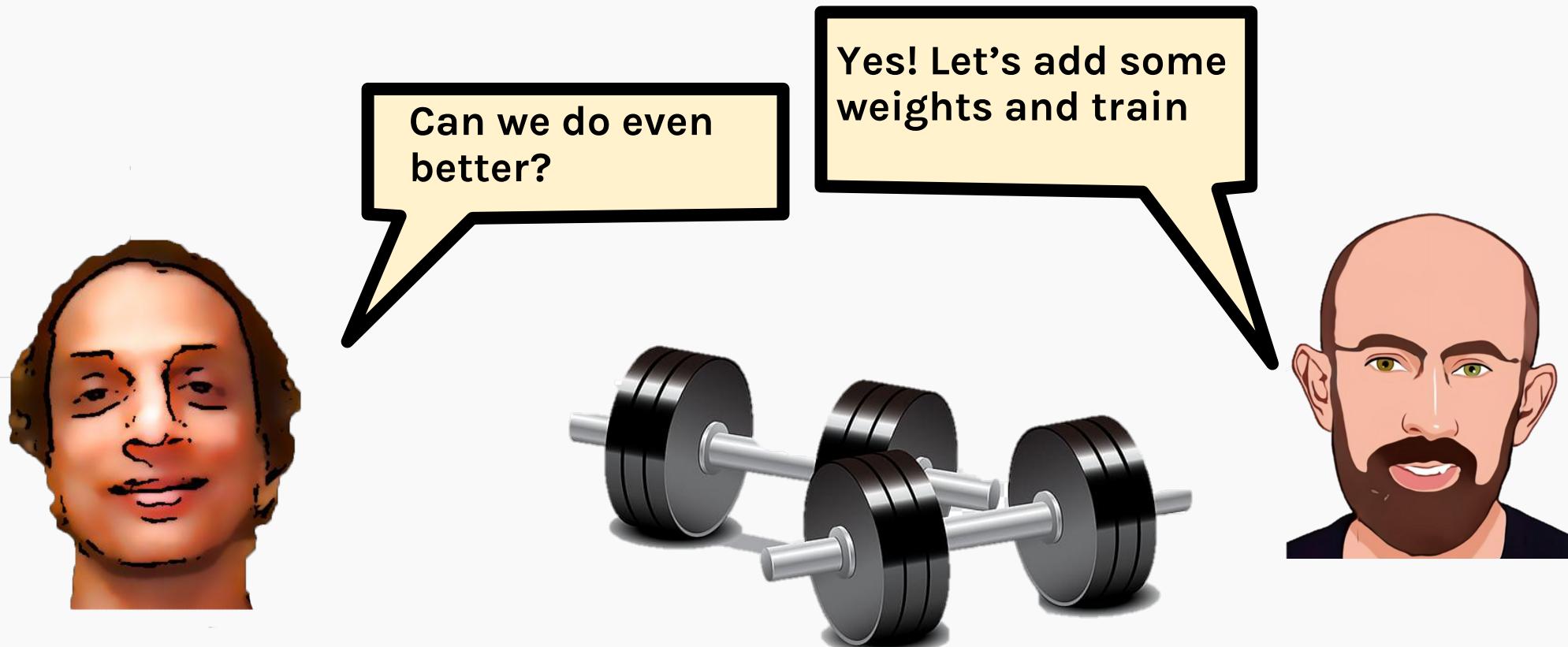
This process gives us new embeddings with some context. However, we still have the following issues:

- No weights are trained in the process
- Attention as defined to be cosine similarity leads to fixed contextual mapping (two words will always have the same cosine similarity irrespective of the context)
- There is no positional information encoded

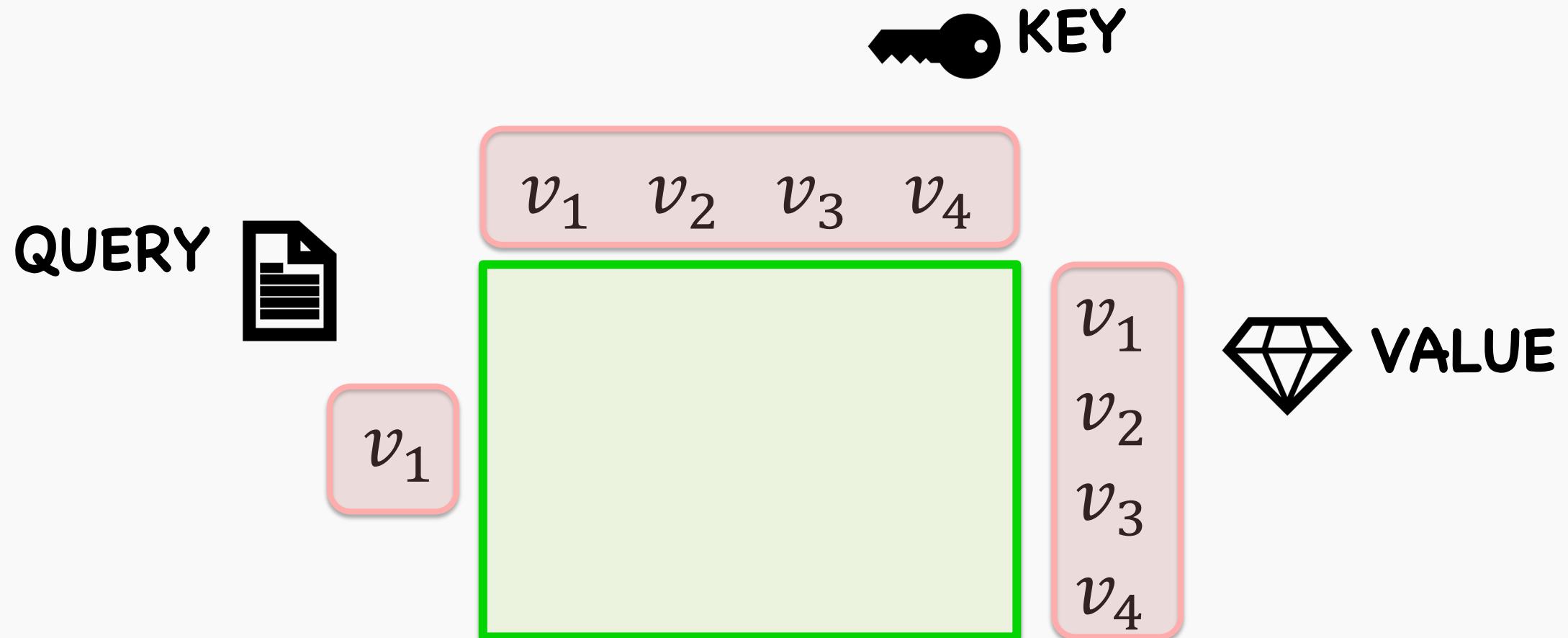
# bank of the river



# Attention – Text Data

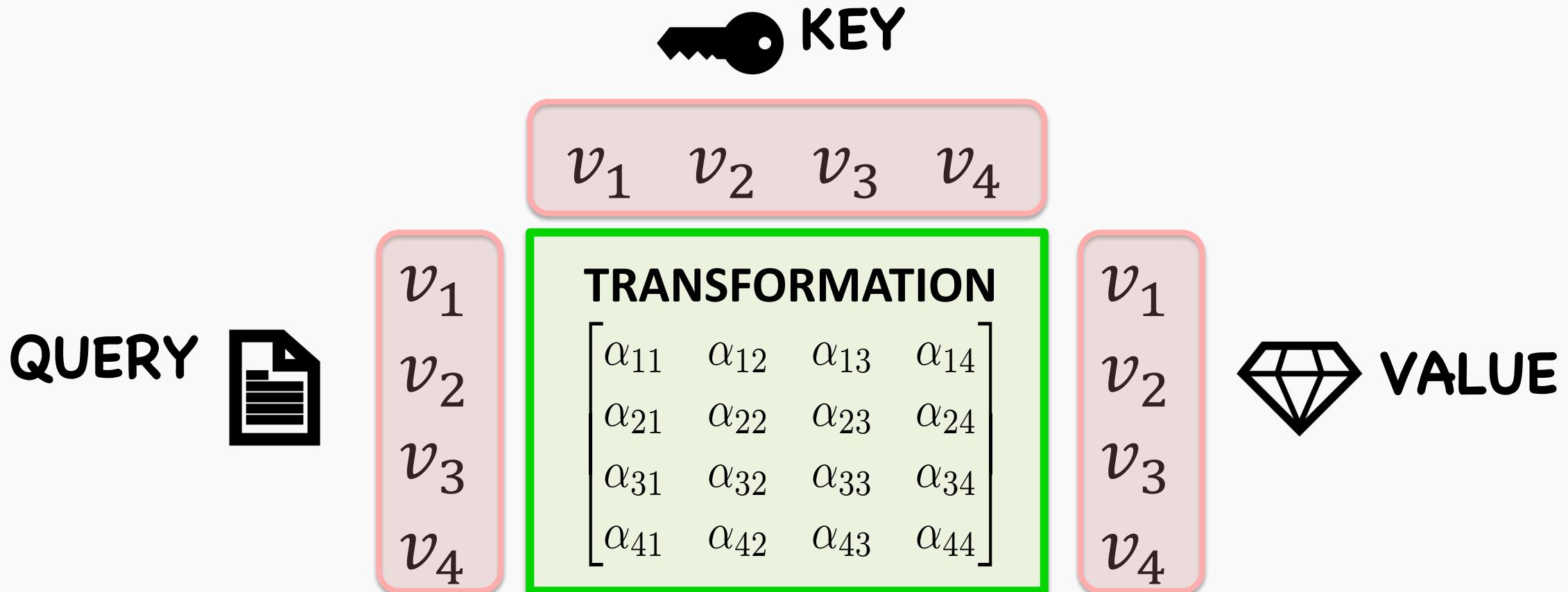


# Database Analogy

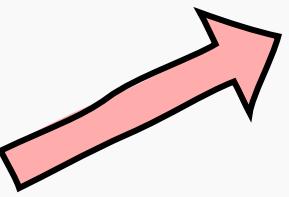


# Database Analogy

For simplicity, we stick to our database analogy of **QUERY**, **KEY** & **VALUE**



TRAINABLE WEIGHTS



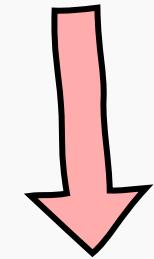
$W_K$

KEY WEIGHTS

$v_1 \ v_2 \ v_3 \ v_4$

$k_1 \ k_2 \ k_3 \ k_4$

TRAINABLE WEIGHTS



$W_Q$

QUERY WEIGHTS

$v_1 \ v_2 \ v_3 \ v_4$

$q_1 \ q_2 \ q_3 \ q_4$

TRANSFORMATION

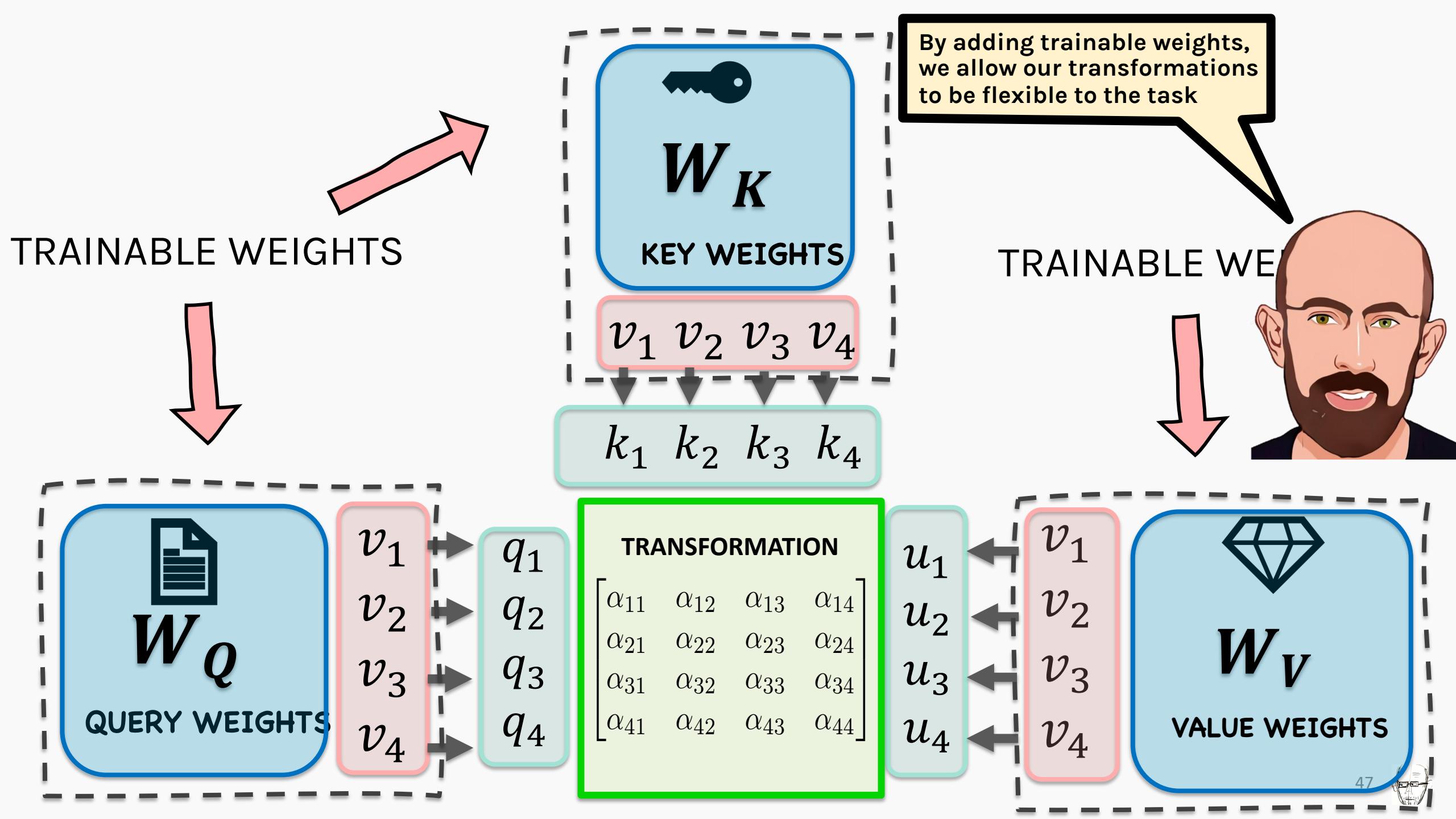
$$\begin{bmatrix} \alpha_{11} & \alpha_{12} & \alpha_{13} & \alpha_{14} \\ \alpha_{21} & \alpha_{22} & \alpha_{23} & \alpha_{24} \\ \alpha_{31} & \alpha_{32} & \alpha_{33} & \alpha_{34} \\ \alpha_{41} & \alpha_{42} & \alpha_{43} & \alpha_{44} \end{bmatrix}$$

$u_1 \ u_2 \ u_3 \ u_4$

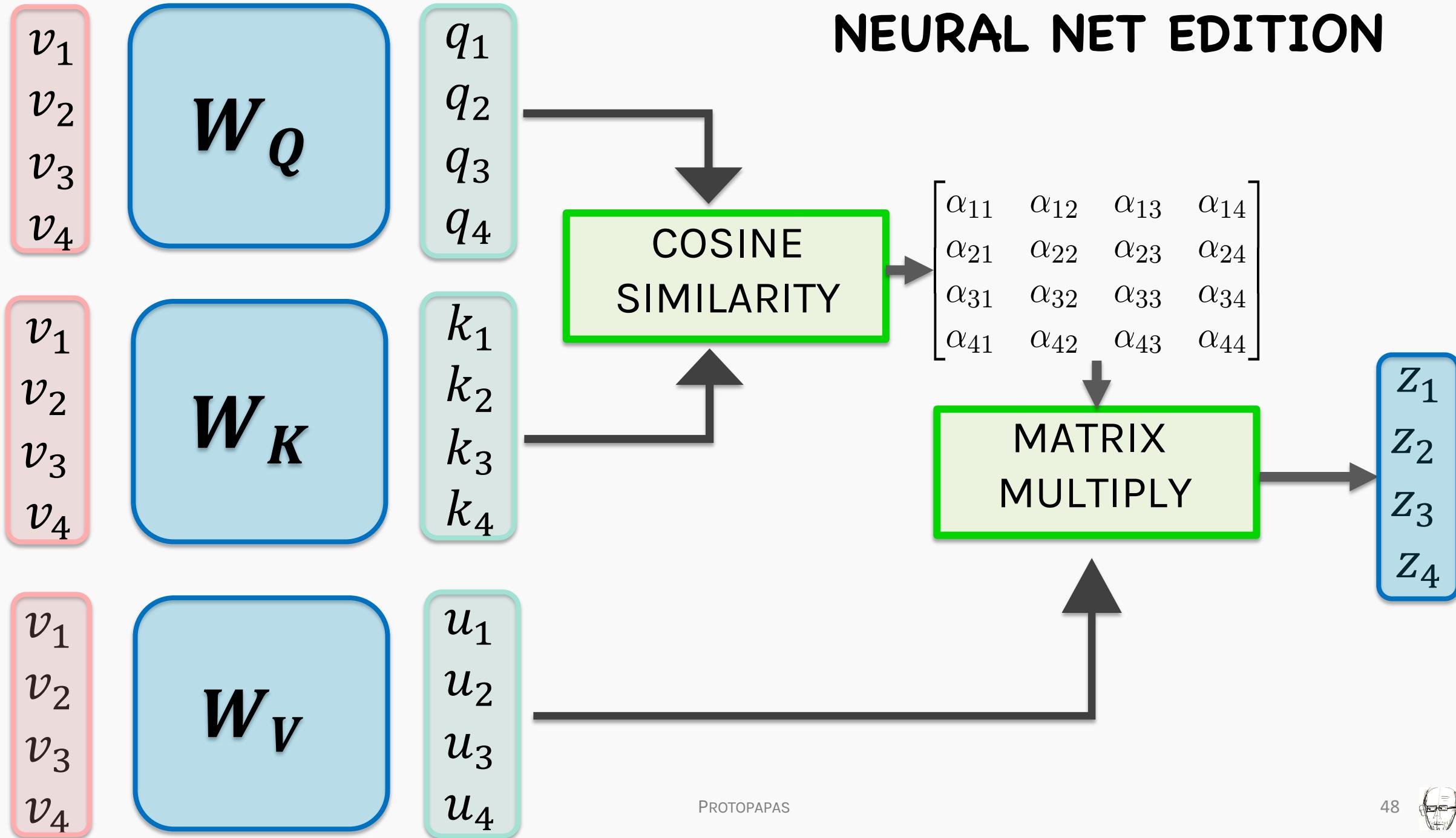


$W_V$

VALUE WEIGHTS



# NEURAL NET EDITION



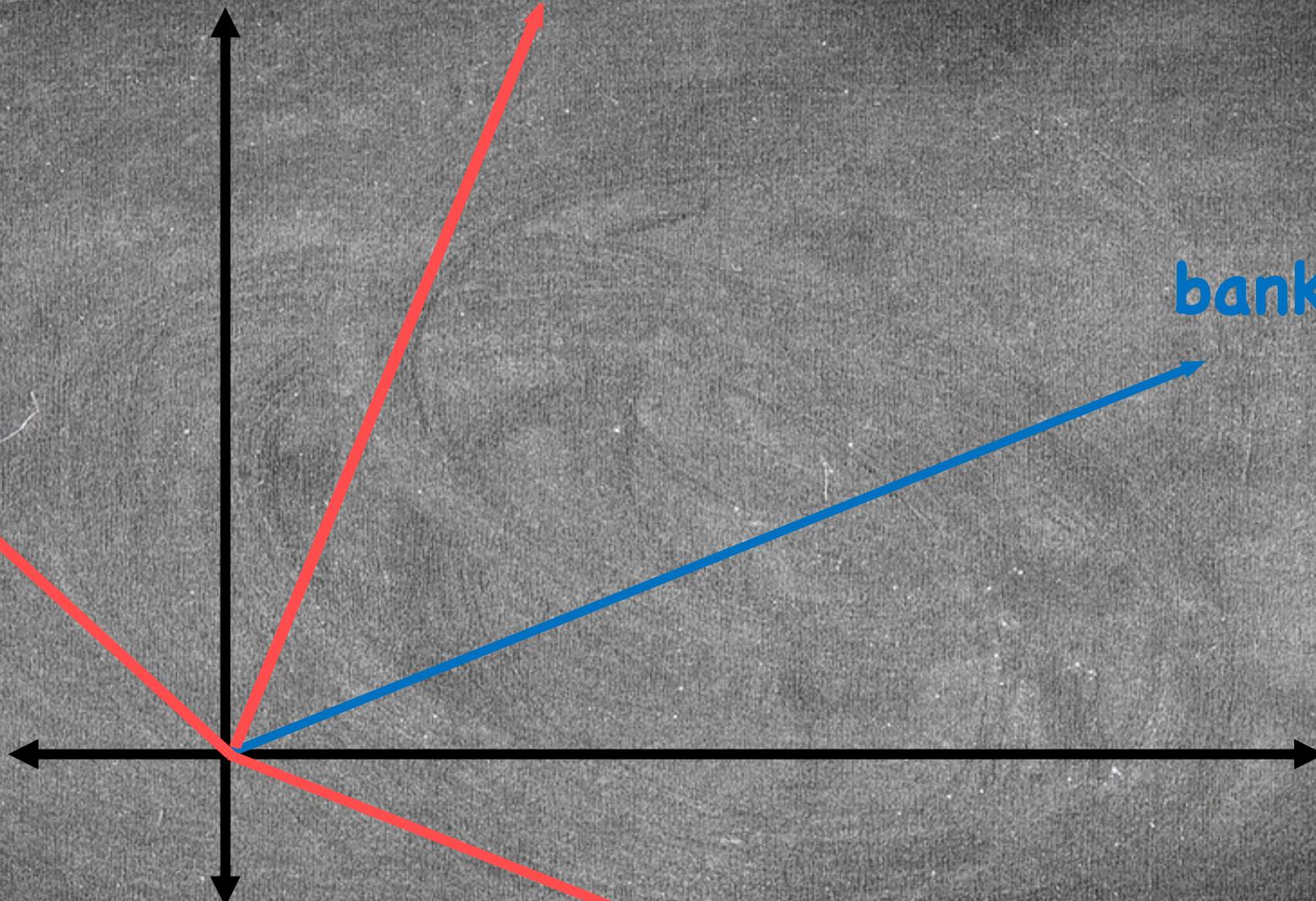
# Transformations

near

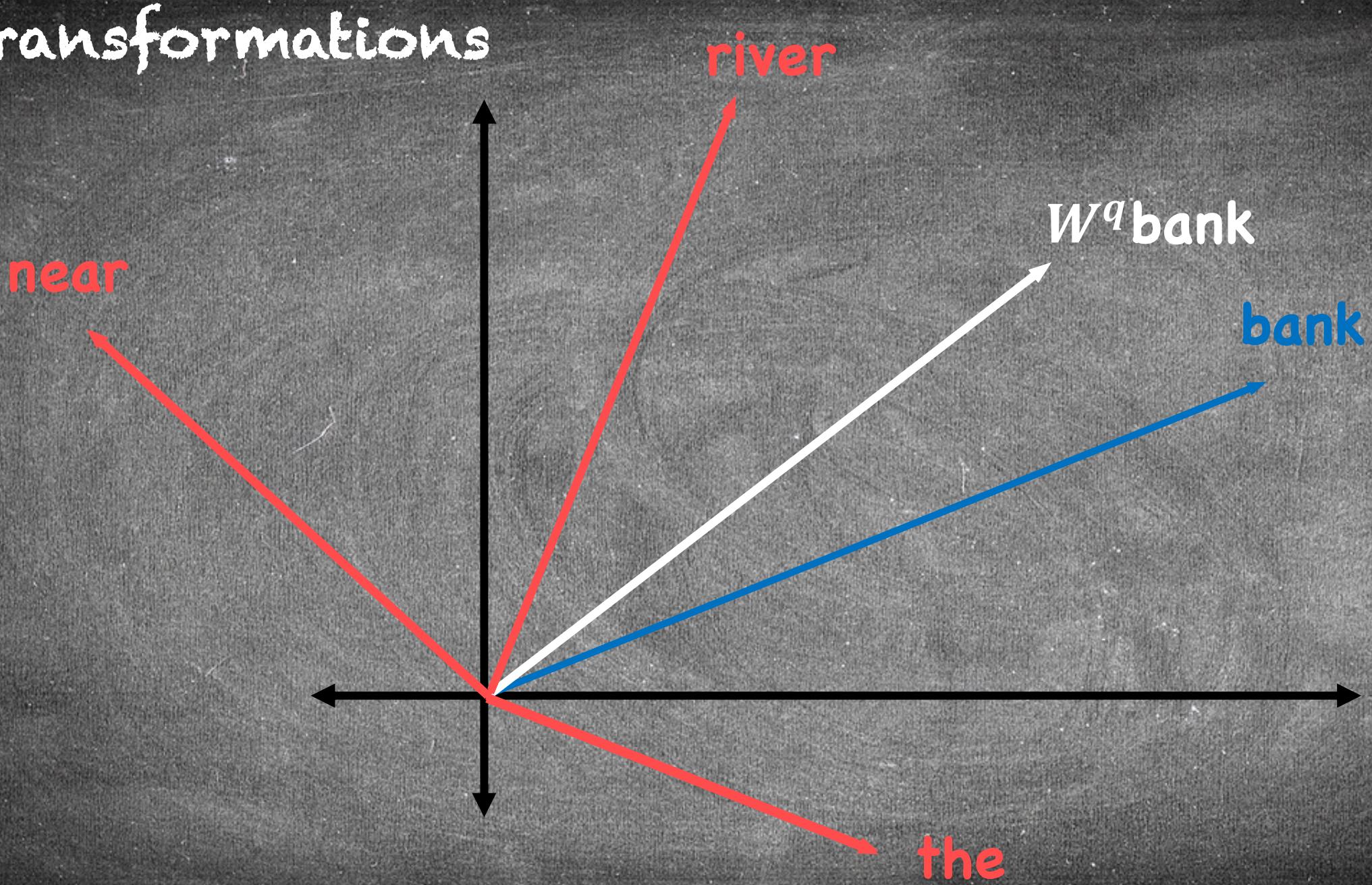
river

bank

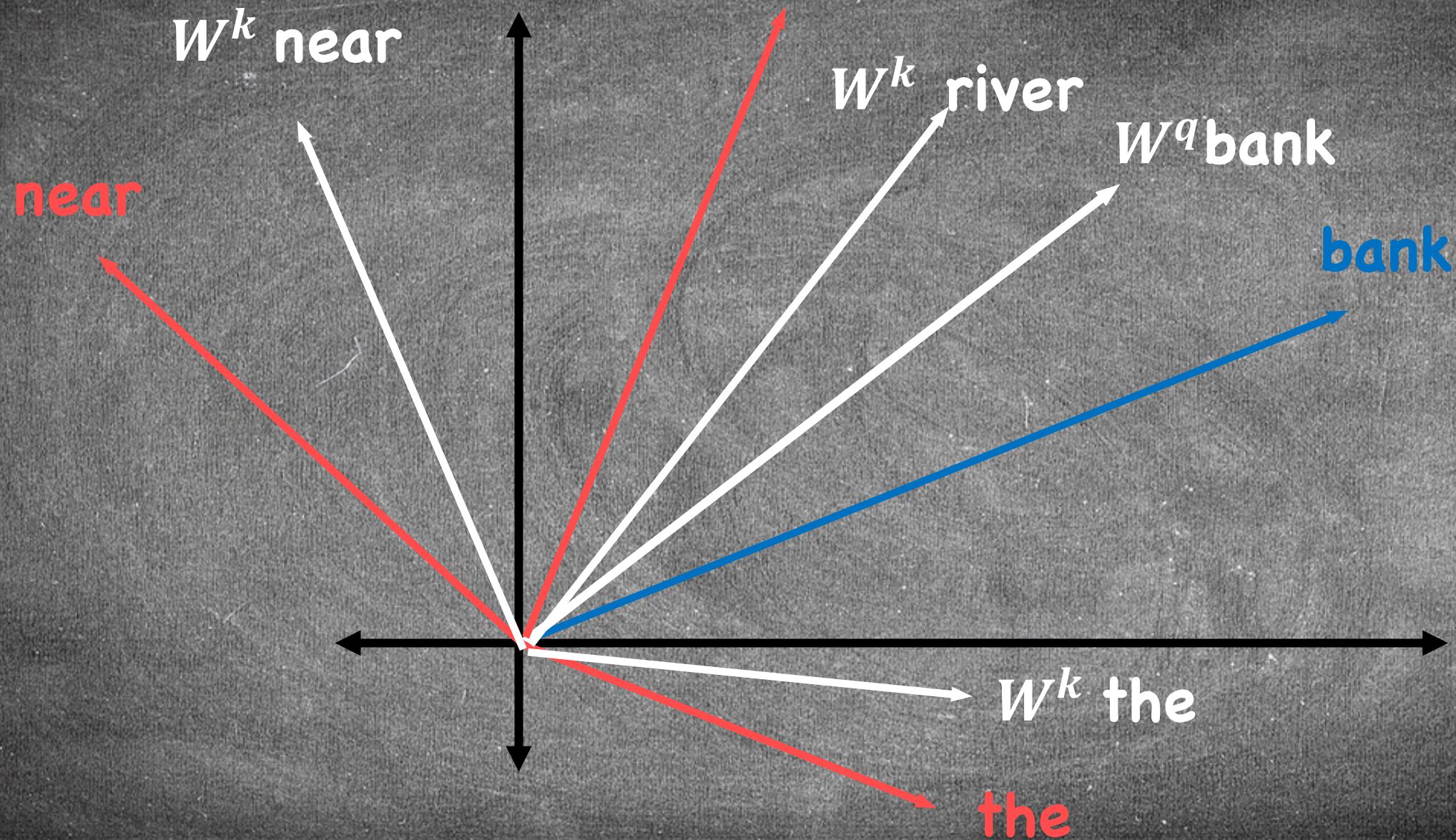
the

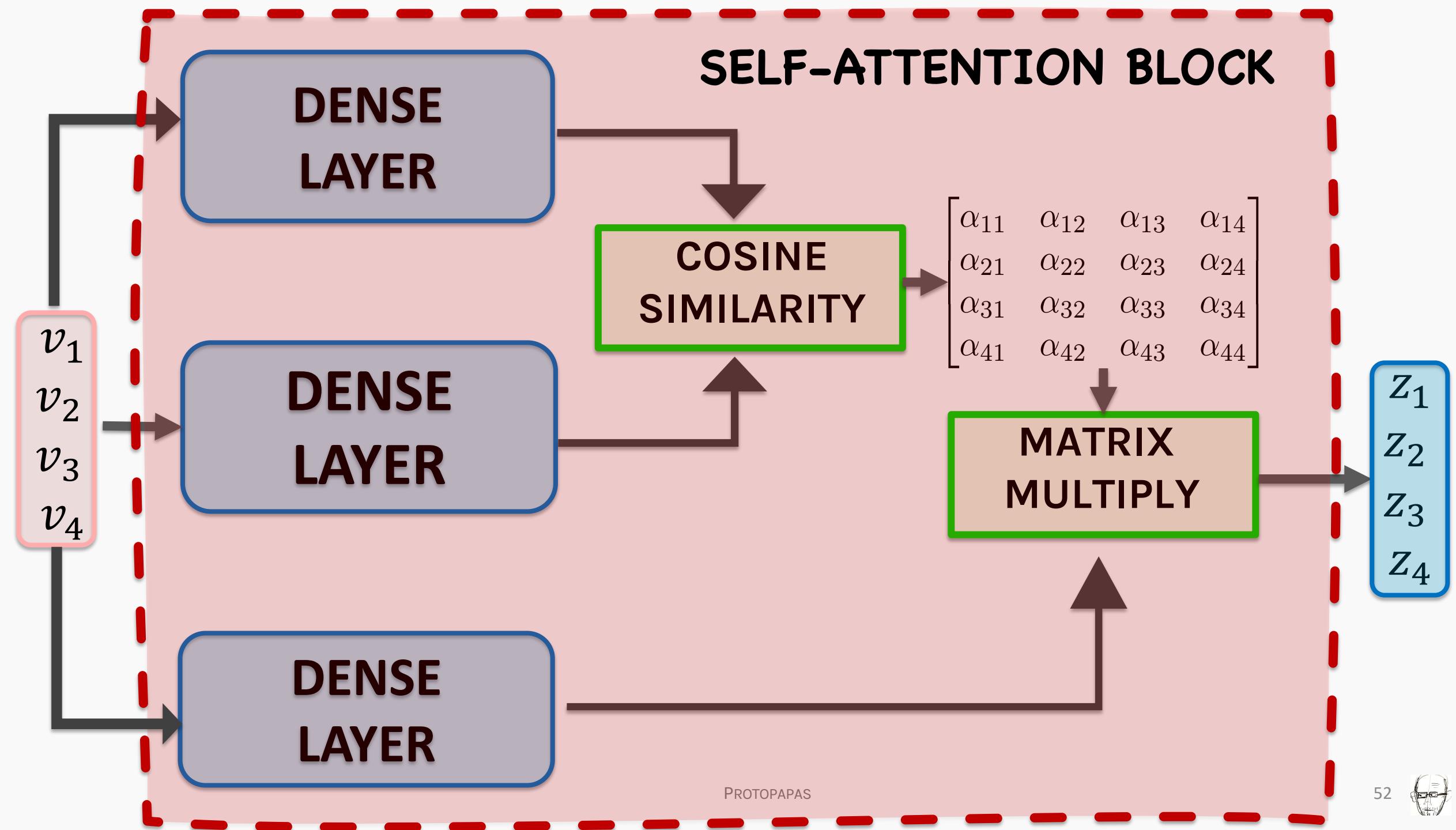


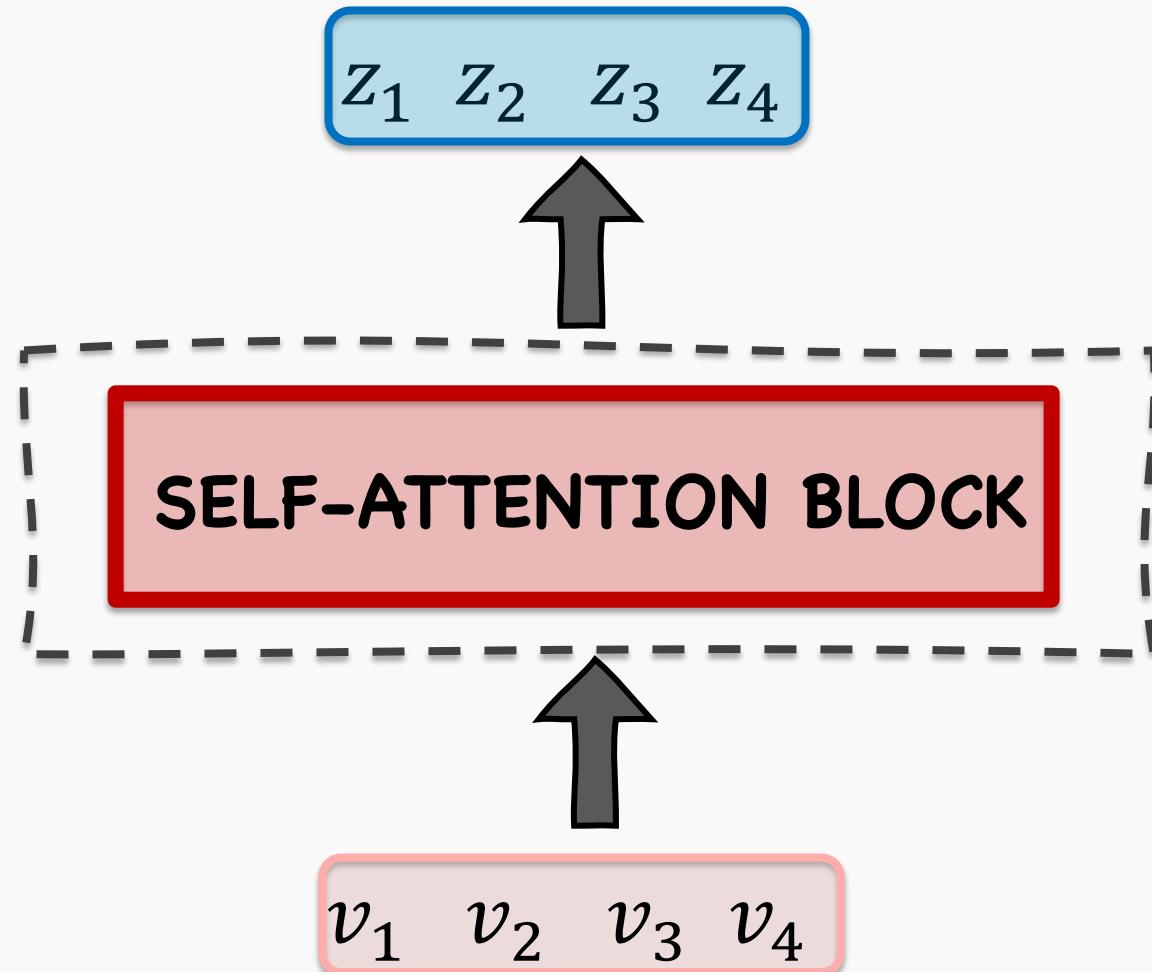
# Transformations

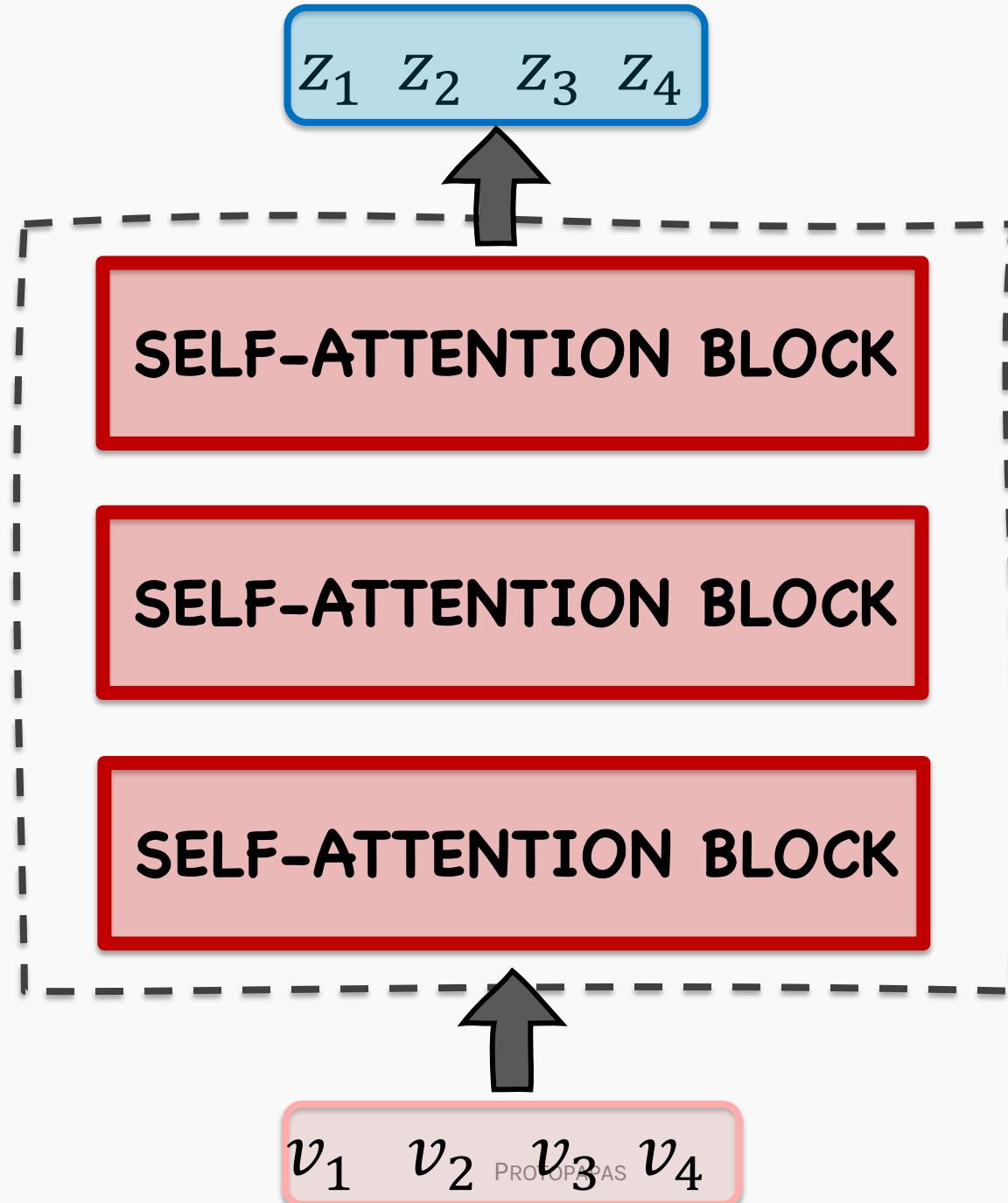


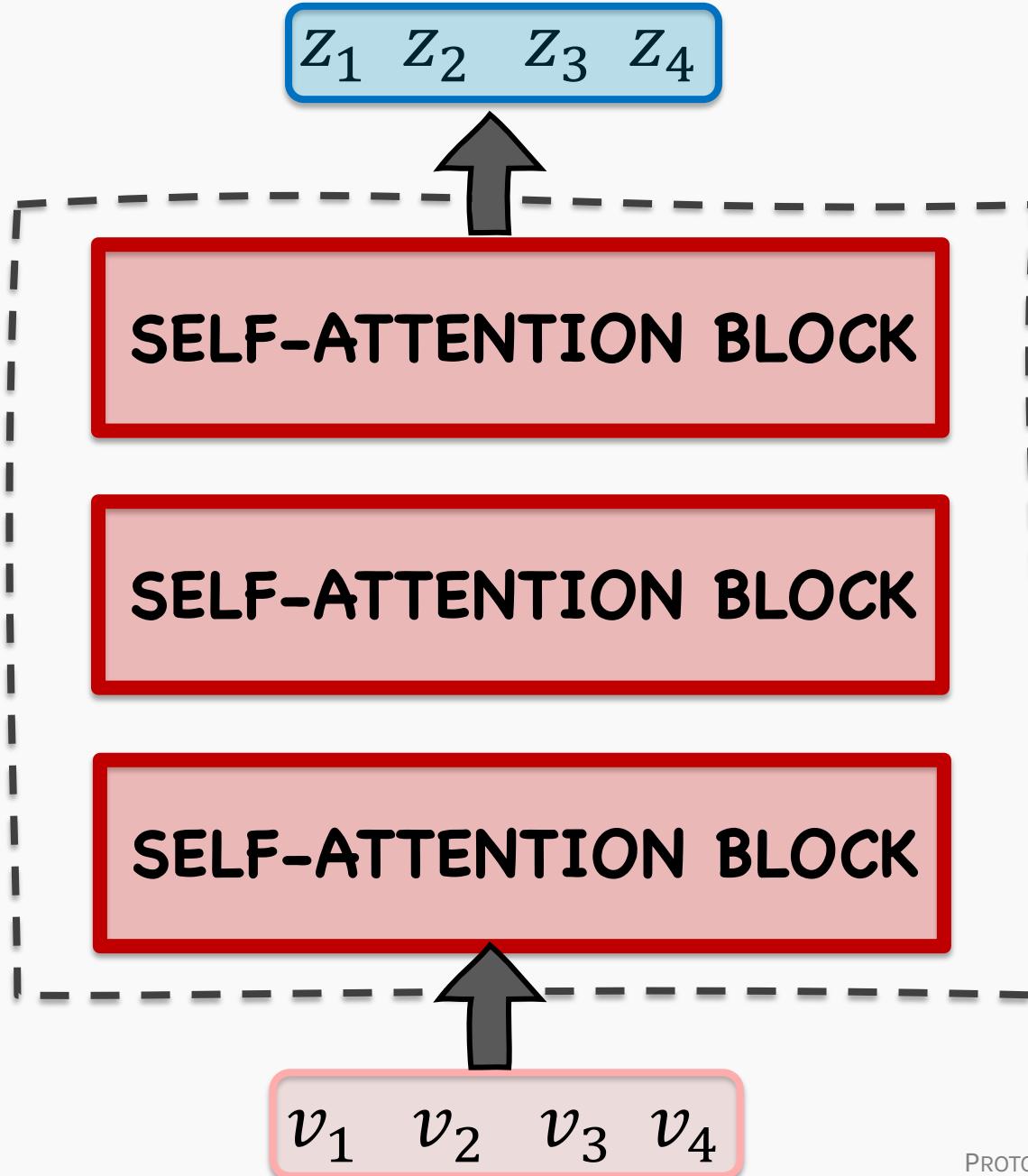
# Transformations











We could stack up these self-attention blocks to get richer and more complex contextual relationships

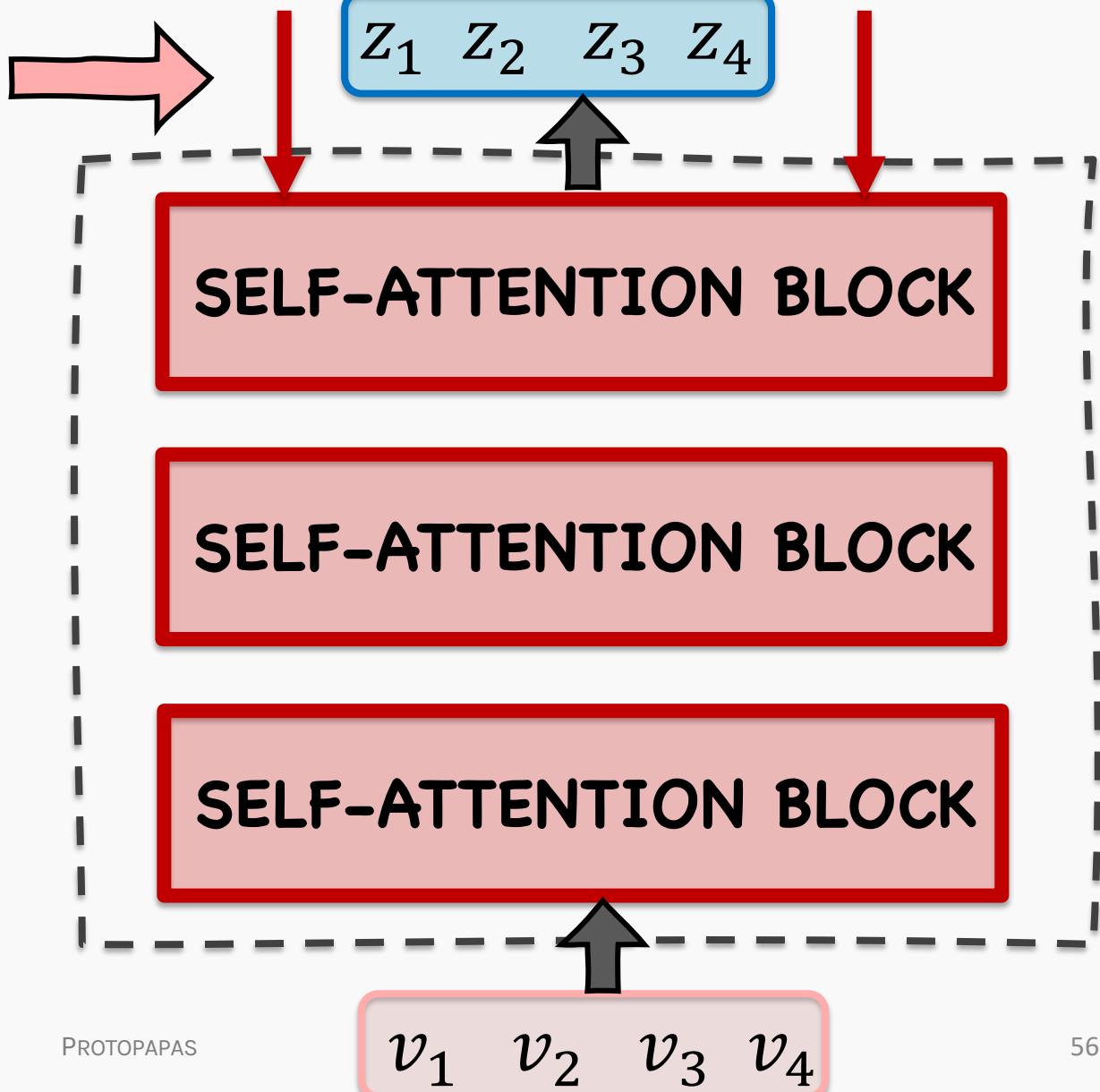


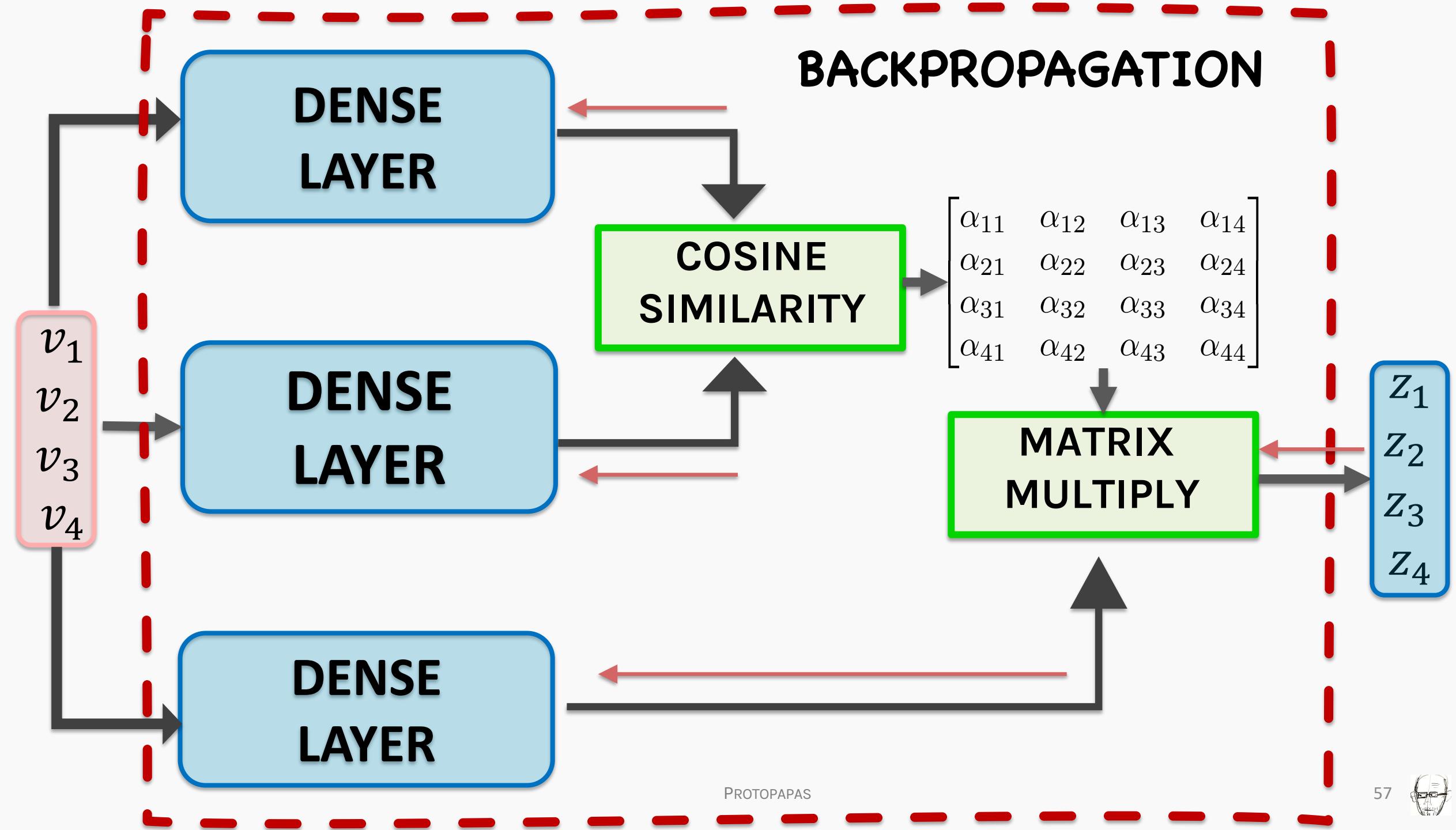
## SENTIMENT ANALYSIS/NAMED ENTITY RECOGNITION

Flow of gradients



And we could train these weights by using backpropagation using masked words or a task like sentiment analysis





# Skip connections



SENTIMENT ANALYSIS/NAMED ENTITY  
RECOGNITION

$z_1 \ z_2 \ z_3 \ z_4$

**SELF-ATTENTION BLOCK**

**SELF-ATTENTION BLOCK**

$v_1 \ v_2 \ v_3 \ v_4$

We could even add skip  
connections between  
blocks to avoid the issue  
of vanishing gradients



# Attention

## ATTENTION STRENGTHS?

- Unlike RNNs, each input is in direct context of every other input  $O(1)$ , hence vanishing gradients are not a significant issue with the attention block
- Unlike RNNs, the operations are not sequentially dependent (Non-Markovian)

| Layer Type     | Complexity per Layer | Sequential Operations | Maximum Path Length |
|----------------|----------------------|-----------------------|---------------------|
| Self-Attention | $O(n^2 \cdot d)$     | $O(1)$                | $O(1)$              |
| Recurrent      | $O(n \cdot d^2)$     | $O(n)$                | $O(n)$              |
| Convolutional  | $O(i \cdot d^2)$     | $O(1)$                | $(\log_k(n))$       |

*d: Dimension of embedding  
n: Length of input sequence*

Non-Markovian      Full context



# Attention

## ATTENTION ISSUES?

- Optimization using attention leads to limited contextual mapping
- There is no positional information encoded



Shivas spoke to Pavlos about attention



PROTOPAPAS



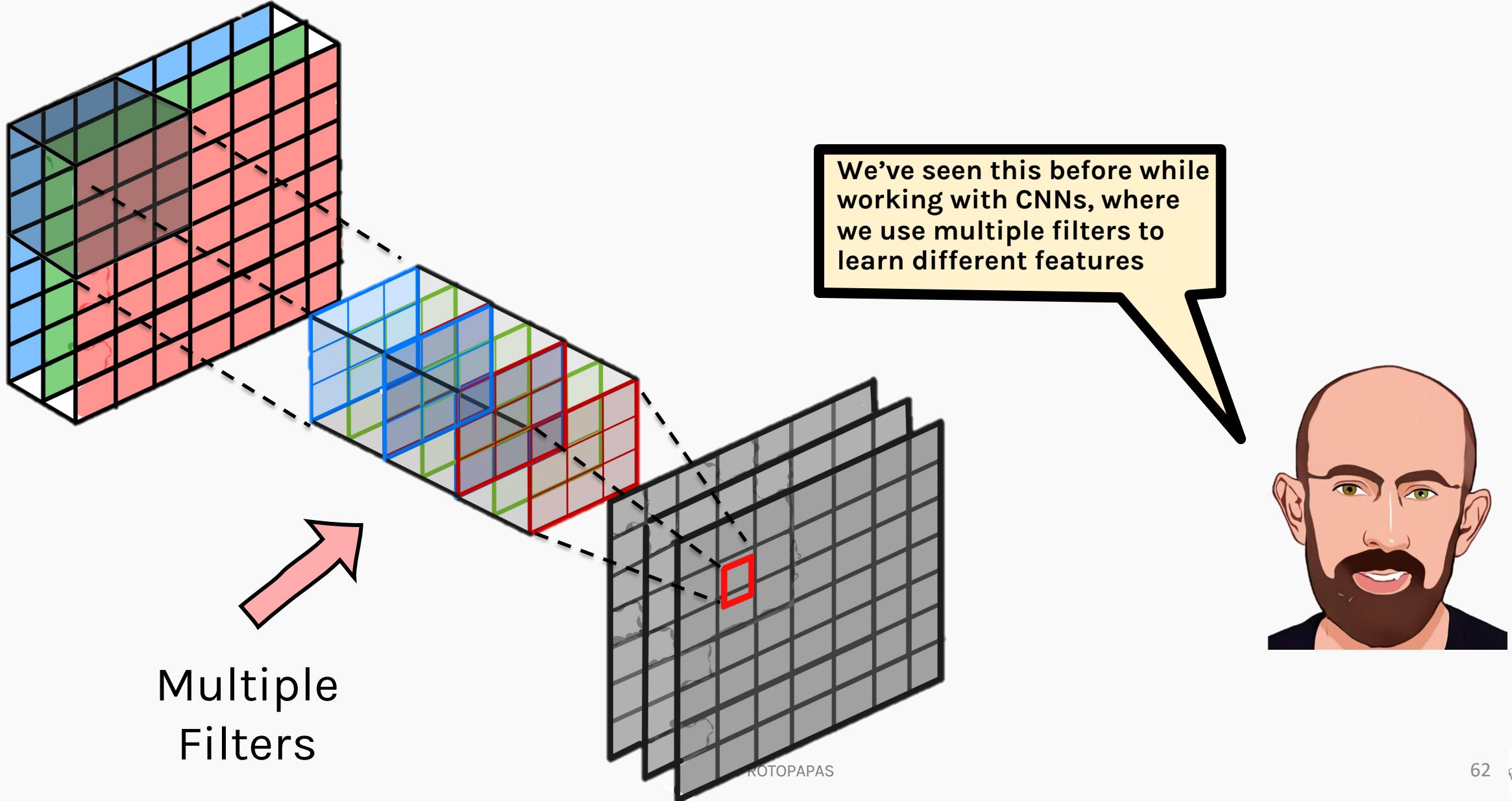
# Attention: Do we have enough attention?



We need to have multiple attention mechanisms to look for different relations



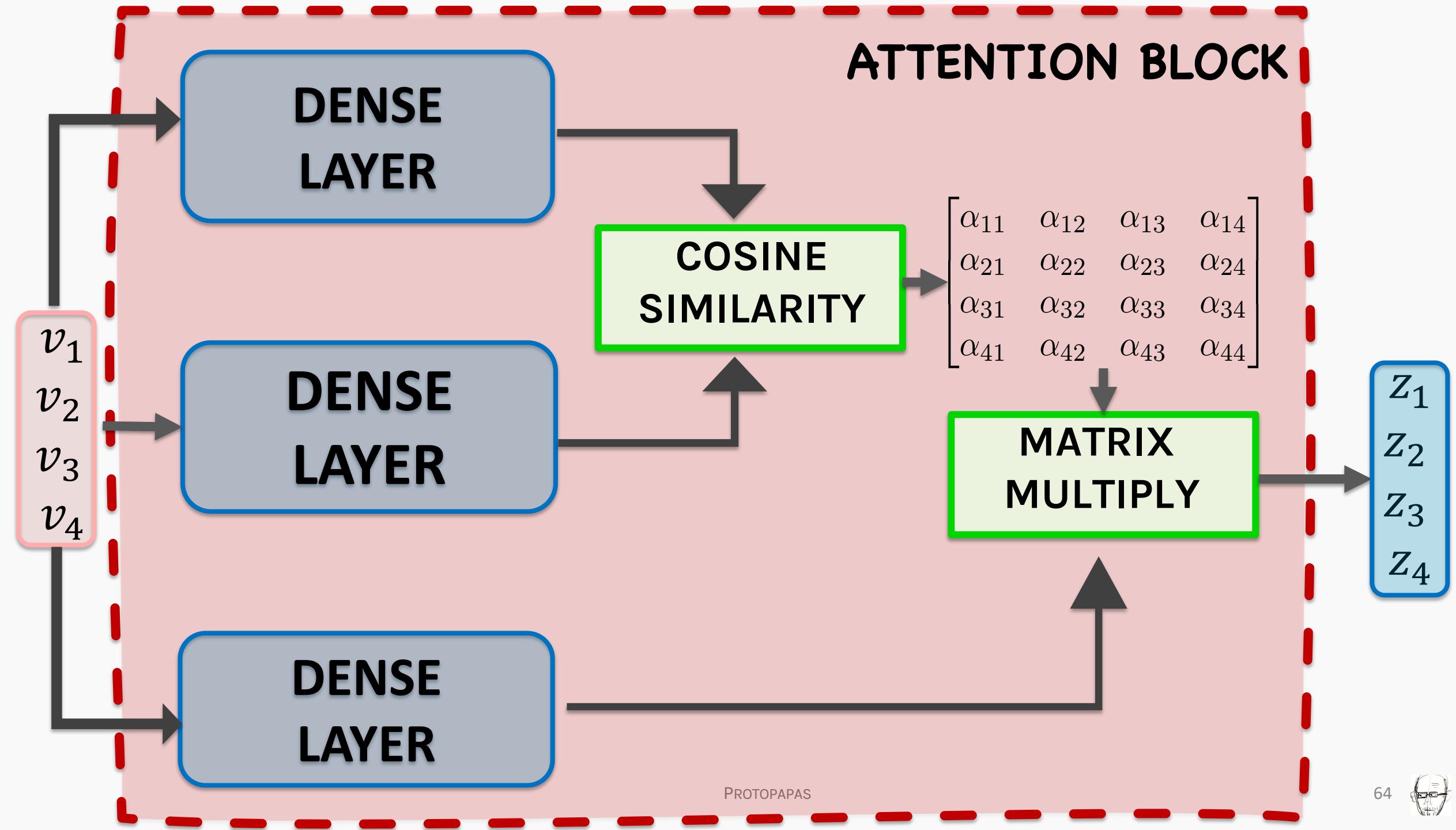
# Analogy - CNN Filters



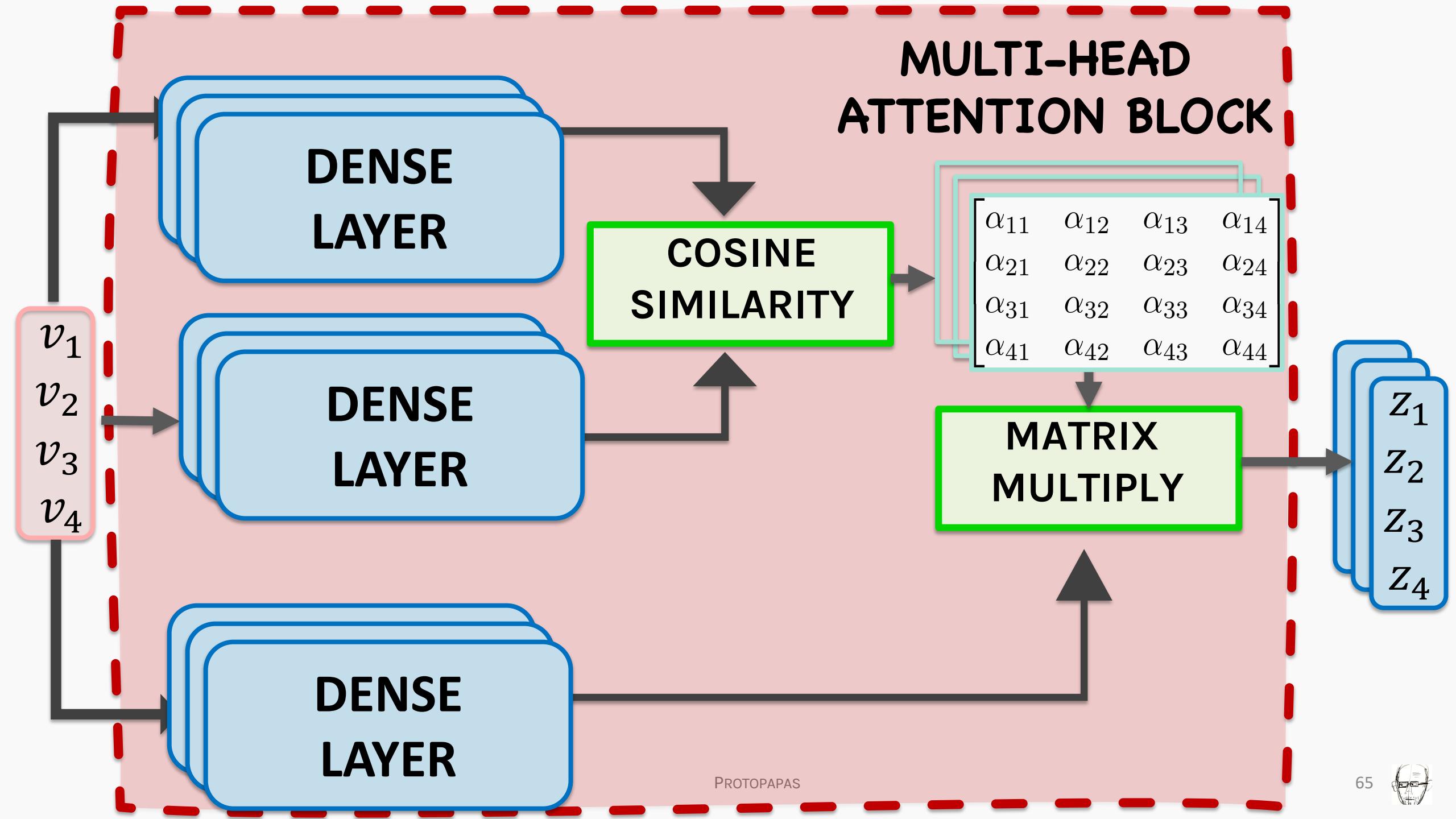
# RECAP: CNNs

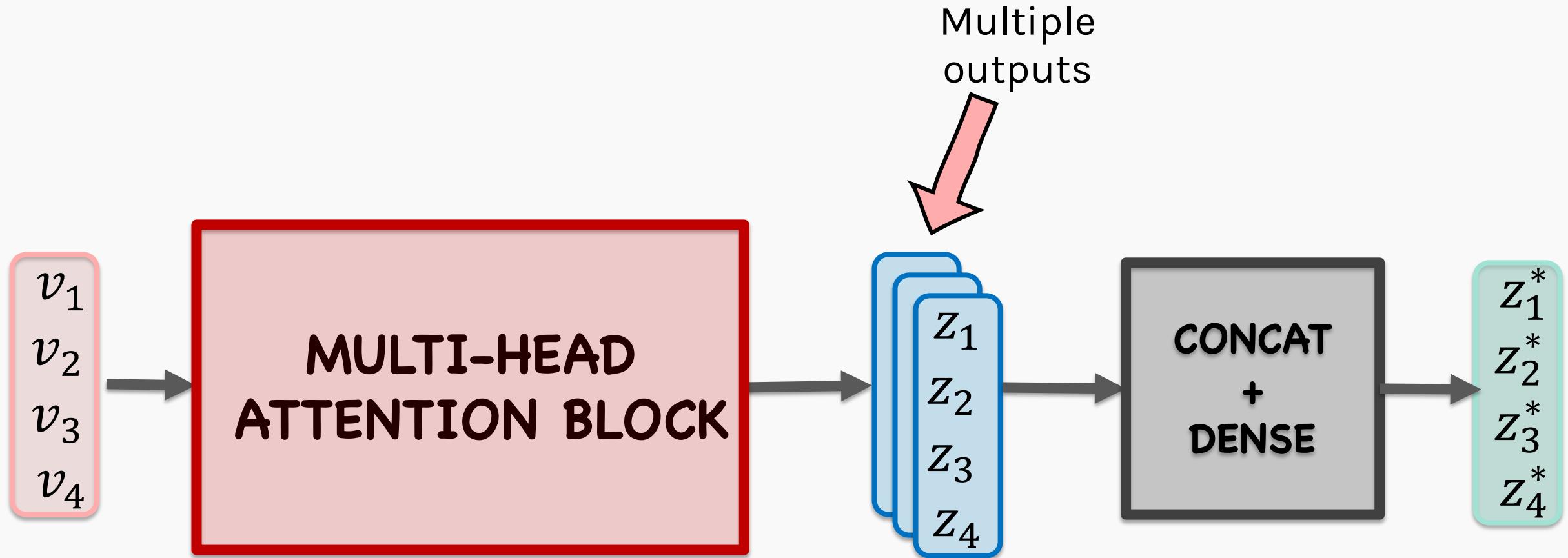
Imagine that we want to recognize swans in an image:

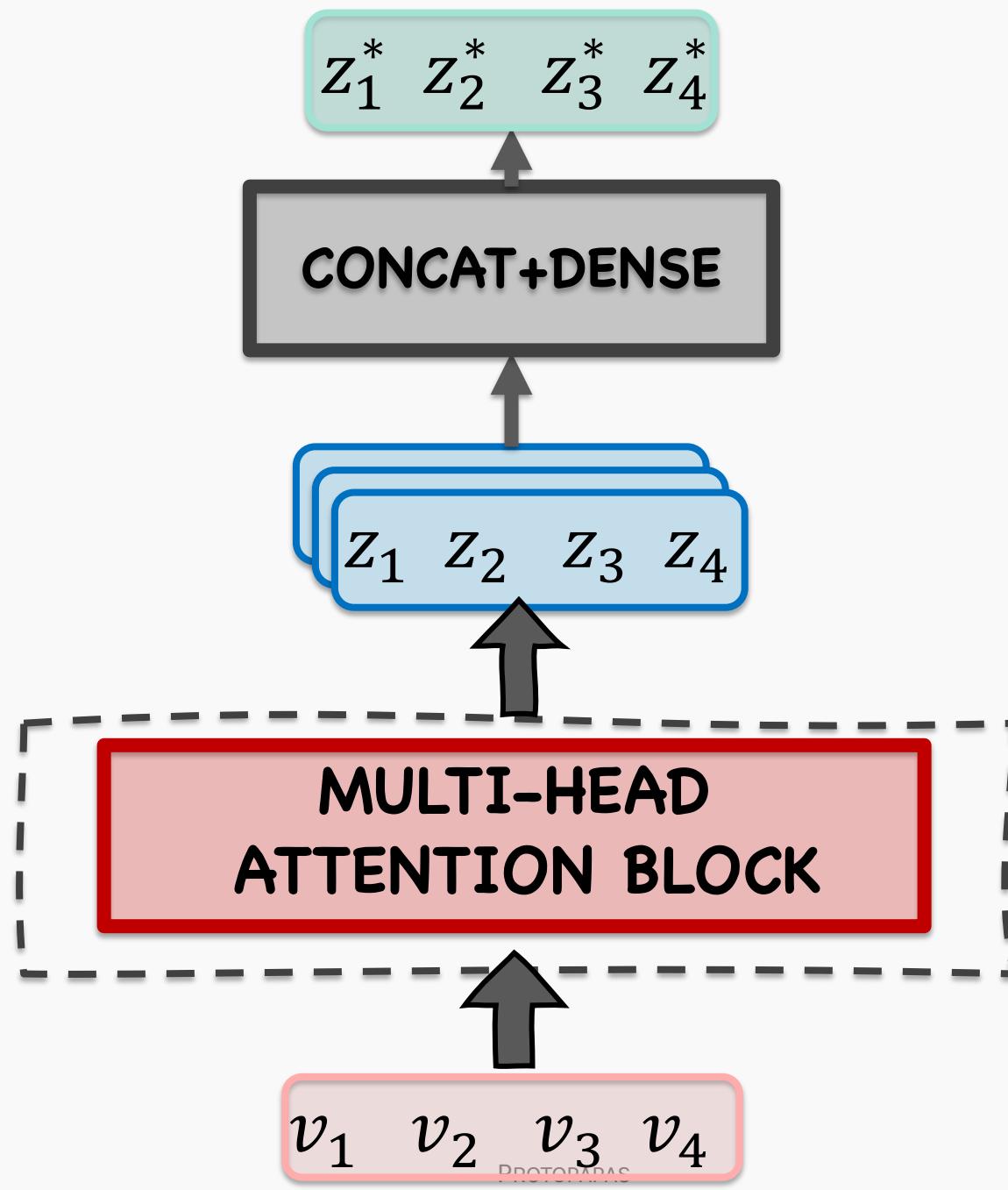


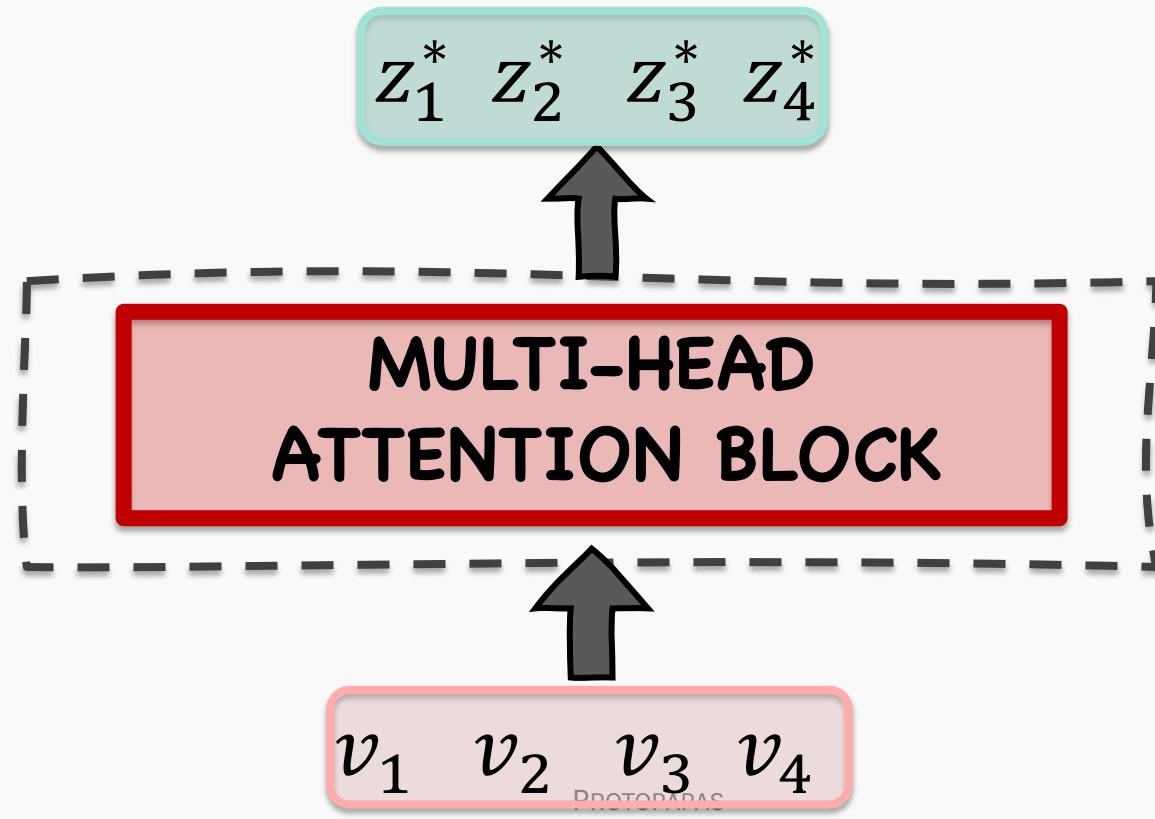


# MULTI-HEAD ATTENTION BLOCK









$$z_1^* \ z_2^* \ z_3^* \ z_4^*$$


MULTI-HEAD  
ATTENTION BLOCK

MULTI-HEAD  
ATTENTION BLOCK

MULTI-HEAD  
ATTENTION BLOCK

$$v_1 \ v_2 \ v_3 \ v_4$$


$$z_1^* \ z_2^* \ z_3^* \ z_4^*$$


MULTI-HEAD  
ATTENTION BLOCK

MULTI-HEAD  
ATTENTION BLOCK

MULTI-HEAD  
ATTENTION BLOCK

$$v_1 \ v_2 \ v_3 \ v_4$$

Now we can potentially look for richer contextual mappings in a sentence without worrying about vanishing gradients



# Attention

## MULTI-HEAD ATTENTION ISSUES?

- No weights trained in the process
- Optimization using attention leads to limited contextual mapping
- There is no positional information encoded



Shivas spoke to Pavlos about attention



# Attention

## MULTI-HEAD ATTENTION ISSUES?

- No weights trained in the process
- Optimization using attention leads to limited contextual mapping
- There is no positional information encoded



Pavlos spoke to Shivas about attention



# What we want

## LANGUAGE MODEL WISHLIST

- Position and order of words are the essential parts of any language
- Recurrent Neural Networks (RNNs) inherently take the order of word into account
- Multi-head attention blocks do not take such an order by design, so there's the need to incorporate the order of the words separately

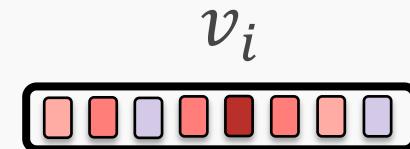


### IDEA #255: Positional Encoding

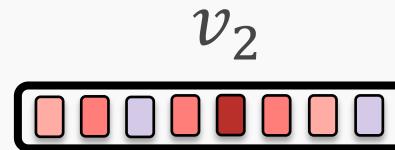
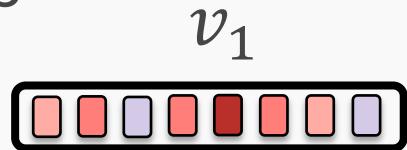


# Positional Encoding

Assume an input embedding  $v_i$  of some dimension for the word ‘Shivas’ at the position  $i$  in the sentence



This input embedding will be the **same** for any position in the sentence

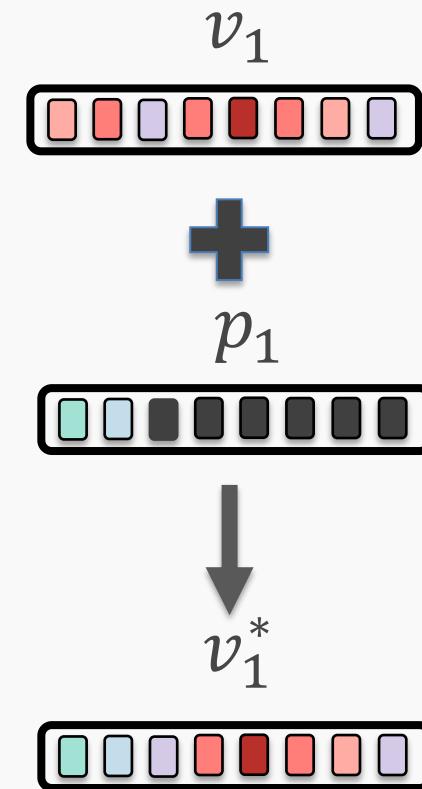


We hope to modify the embedding with some **positional information**

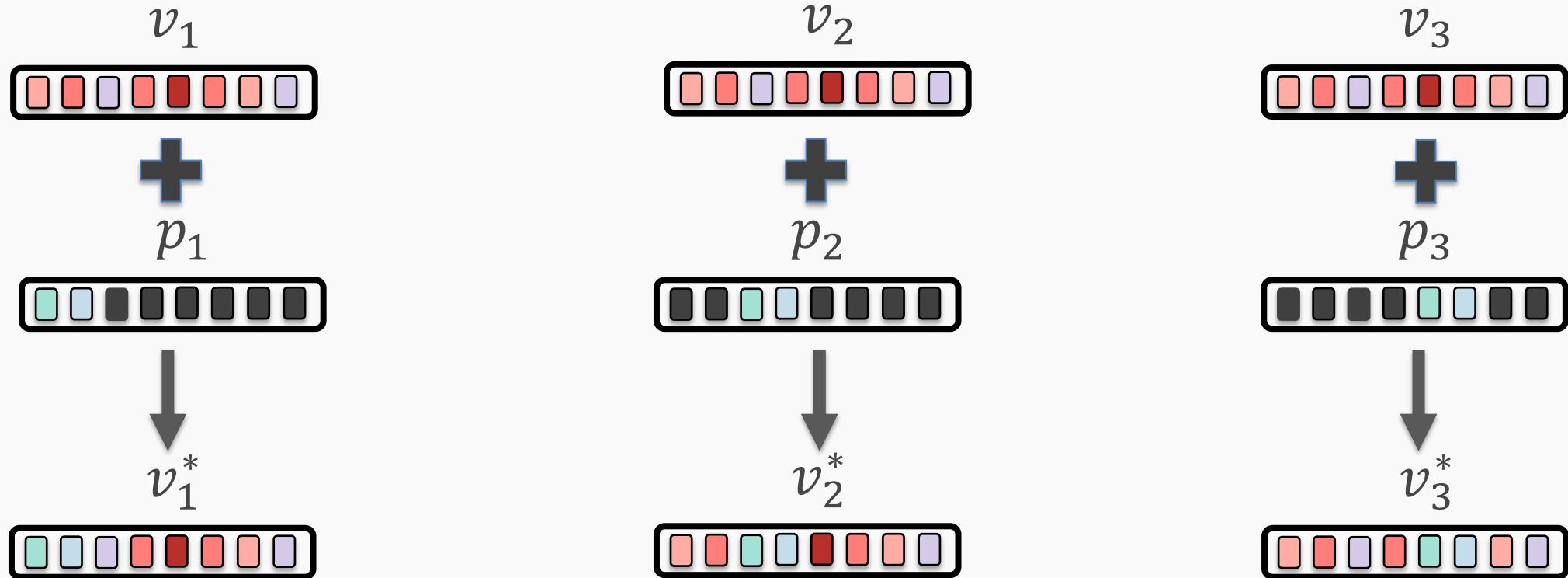


# Positional Encoding

- A very simple way to do this would be to **modify** the input embedding  $v_i$  with a positional vector  $p_i$  which encodes some information of the position of the input embedding
- Thus, the same input embedding  $v_i$  will be a different value  $v_i^*$  depending on the position of the embedding in the sentence



# Positional Encoding



In the above case, although  $v_1 = v_2 = v_3$ ,  $v_1^* \neq v_2^* \neq v_3^*$



# Positional Encoding

$p_1$



$p_2$



$p_3$



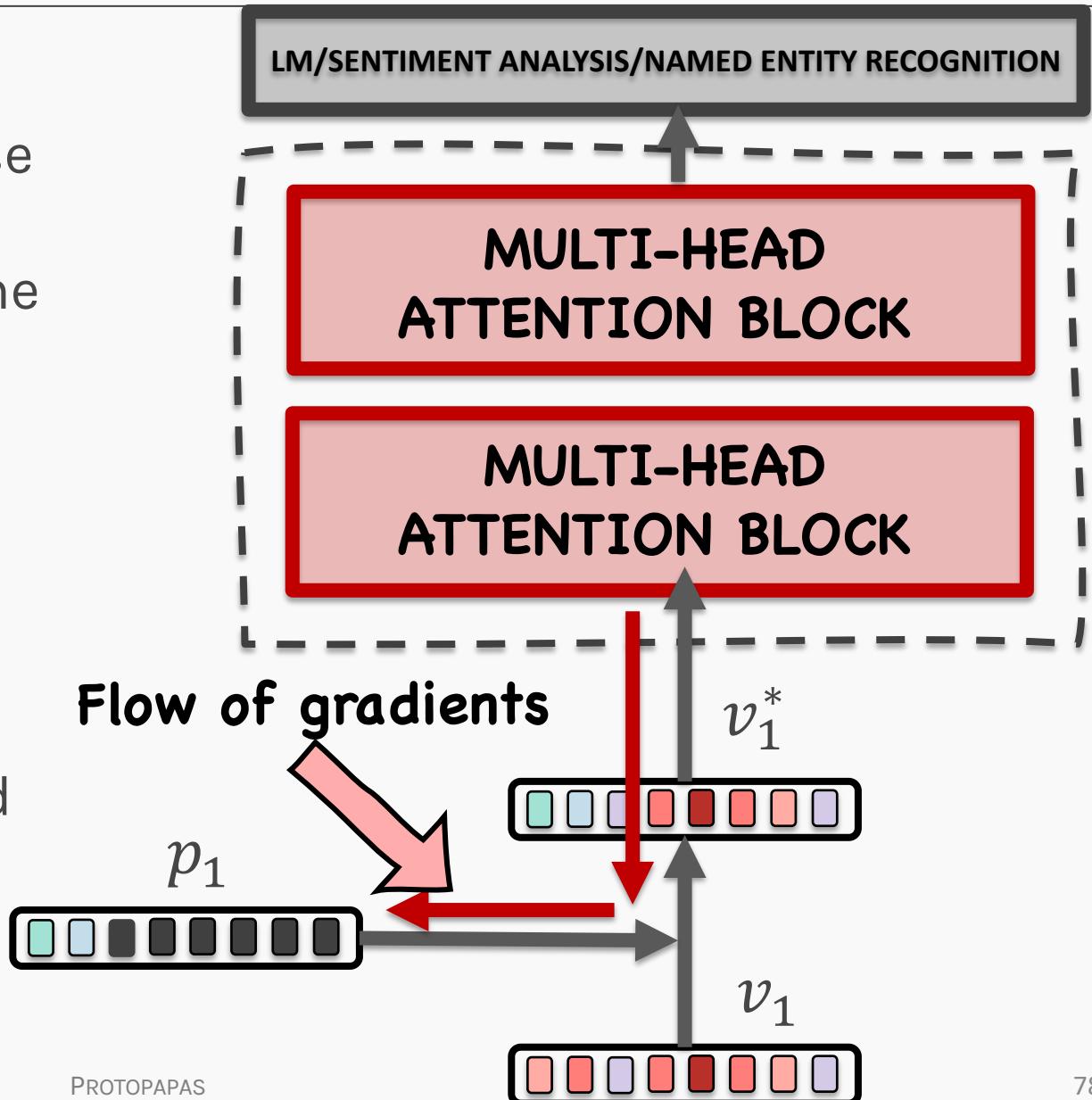
But how do we find  
these positional  
embedding vectors?

Don't worry Shivas, we  
have several options to  
choose from...



# Positional Encoding

- The no-nonsense way to find these positional encodings would be to learn them during training (like the Query, Key & Value transformations)
- But the number of learnable parameters in a stacked multi-head attention block can massively grow, and this can lead to poor training



# Positional Encoding

## POSITIONAL EMBEDDING WISHLIST

- It should be a unique embedding for each timestep
- Relative encodings must remain consistent across sentences of different lengths
- It should generalize to longer sentences
- It should be bounded & deterministic

Okay Google, get in line,  
this problem was  
solved in 14<sup>th</sup> century by  
the great Galileo Galilei



# Positional Embedding – Motivation



# Positional Embedding – Motivation

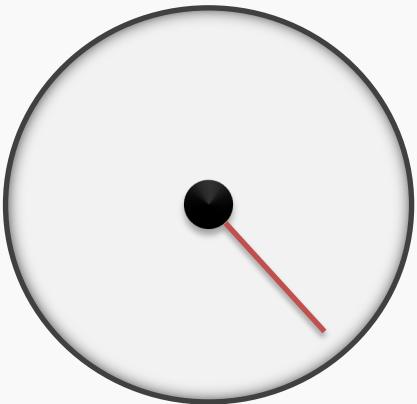
- The clock was an ingenious, compact solution to keep time
- Using the H:M:S system for hour, minute and second, we actually read a tuple of three numbers (H,M,S), with each dimension representing a **unique** time of the day
- We achieve this by setting separate frequencies for the hour, minute & second



The mechanical clock



# Positional Embedding – Motivation



Even though the seconds hand repeats every minute, the overall tuple is unique

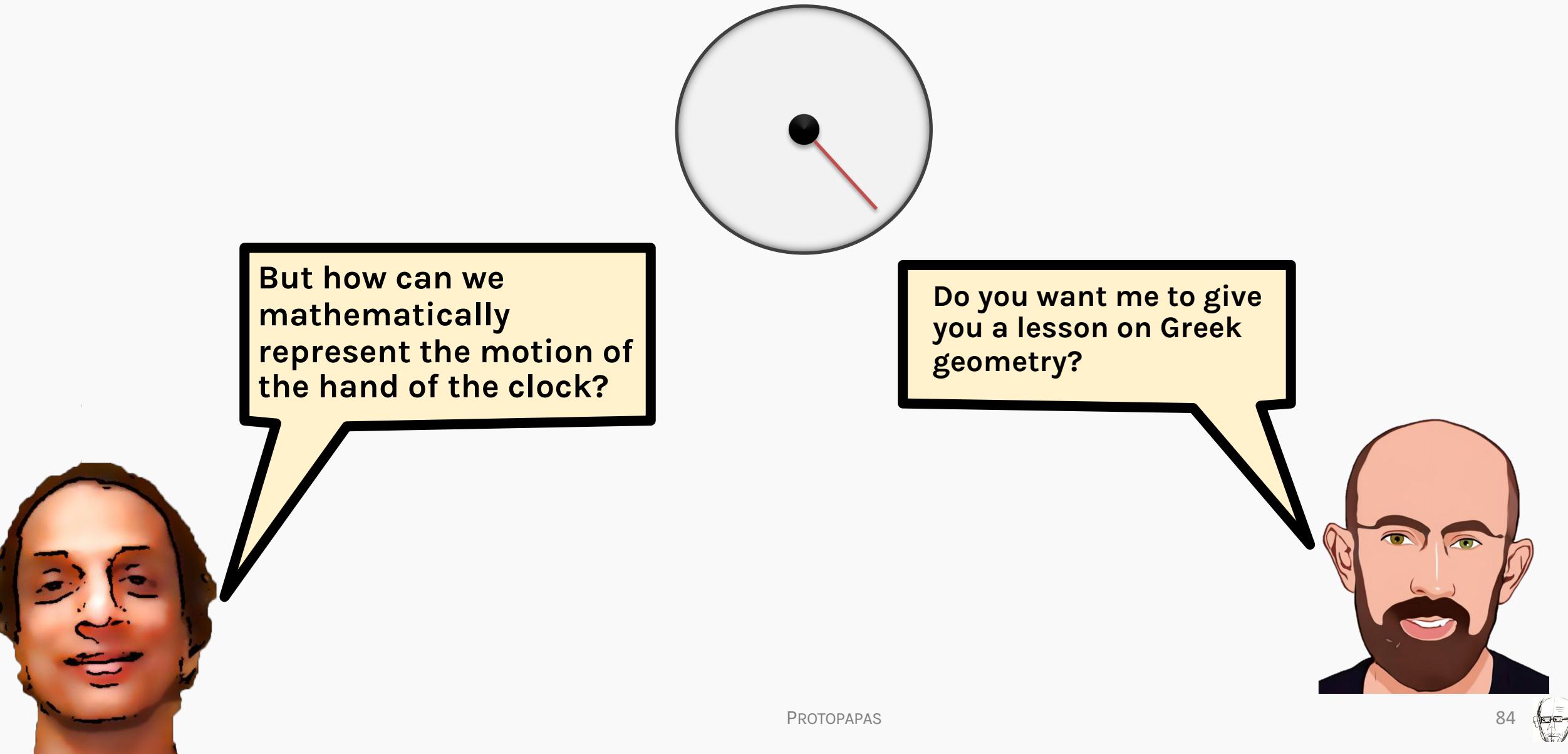


# Positional Embedding – Motivation

- In principle, we could add more hands to the clock, for days of the week, week of the month, month of the year etc.
- With enough hands, we could uniquely represent any time series from the start of the universe to the end
- This powerful idea can be used to generate scale independent positional encodings

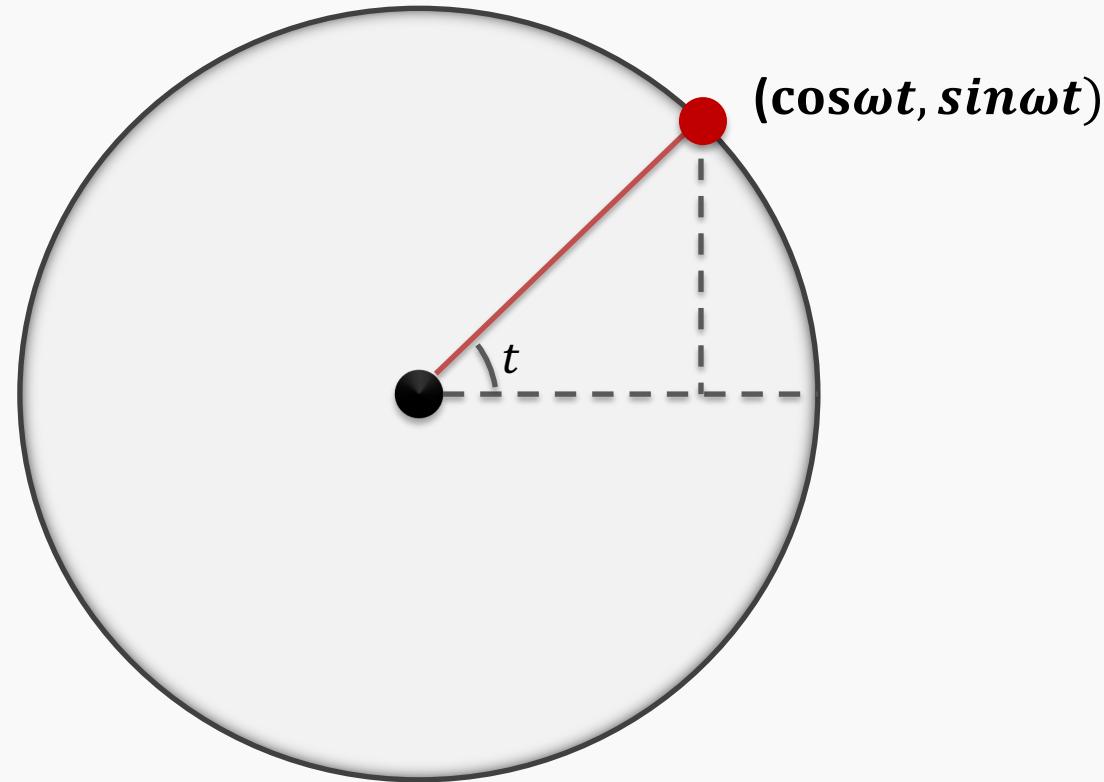


# Positional Embedding - Motivation

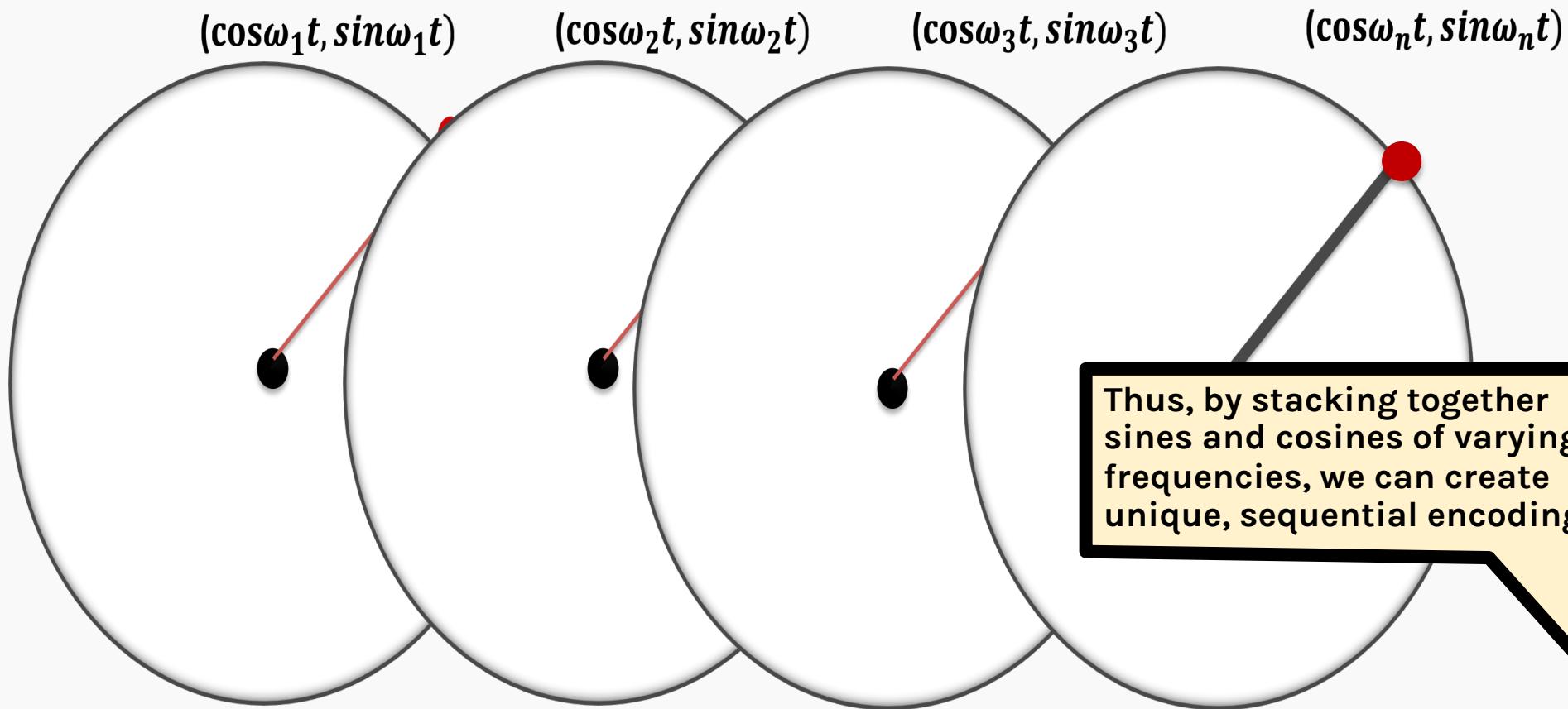


# Positional Embedding - Motivation

- We can sufficiently define the path of a unit length around a circle by two hyperparameters
  - Angle of rotation  $t$
  - Frequency of rotation  $\omega$
- The combination the sine and the cosine together can completely define the unit circle

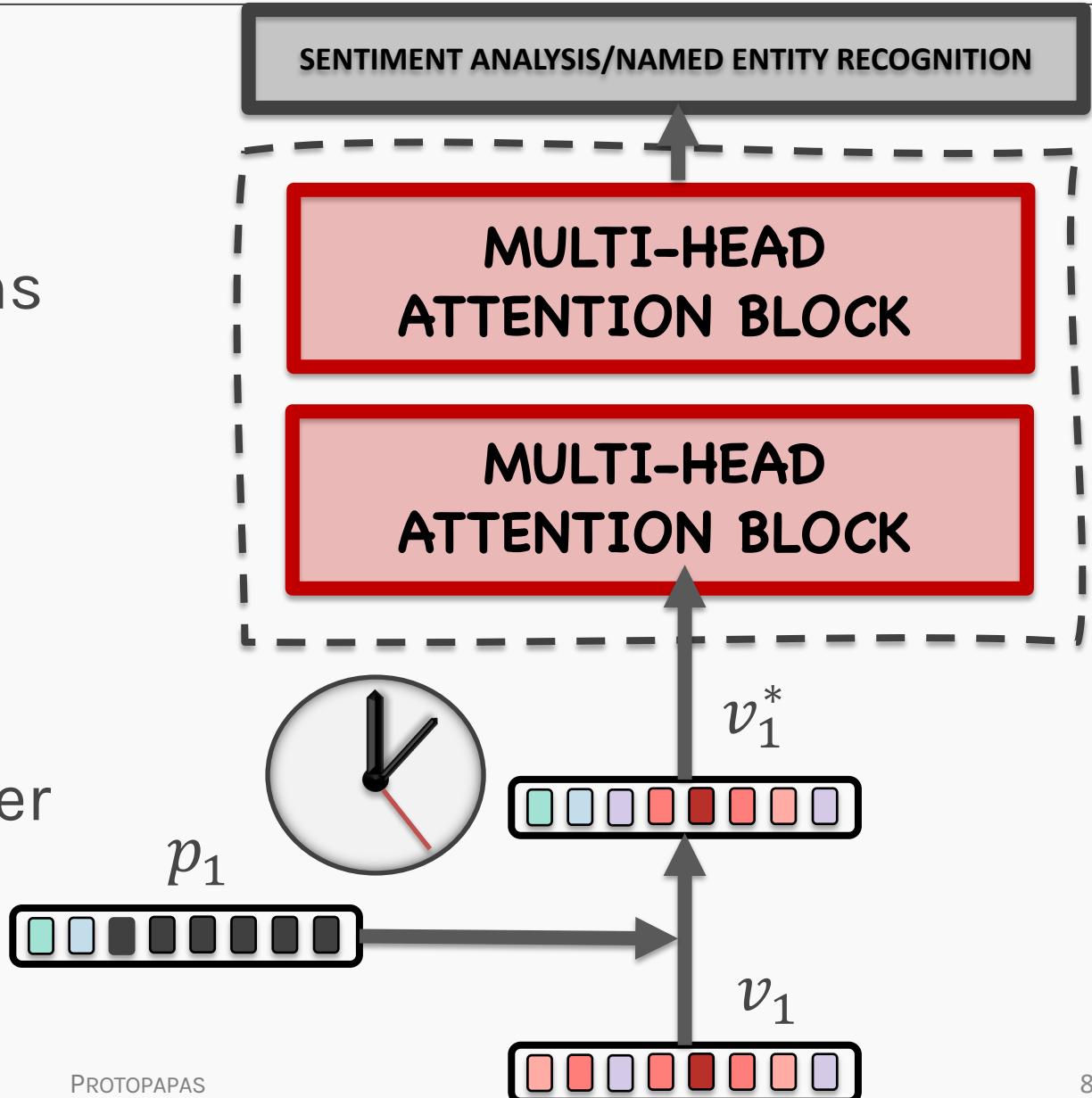


# Positional Embedding - Motivation



# Positional Encoding

- In the experimental results, the positional encodings using deterministic functions were found to be as effective as those learned using backpropagation
- However, since this method more general and much faster to implement, it is usually preferred



# Positional Embedding

## TECHNICAL DETAILS

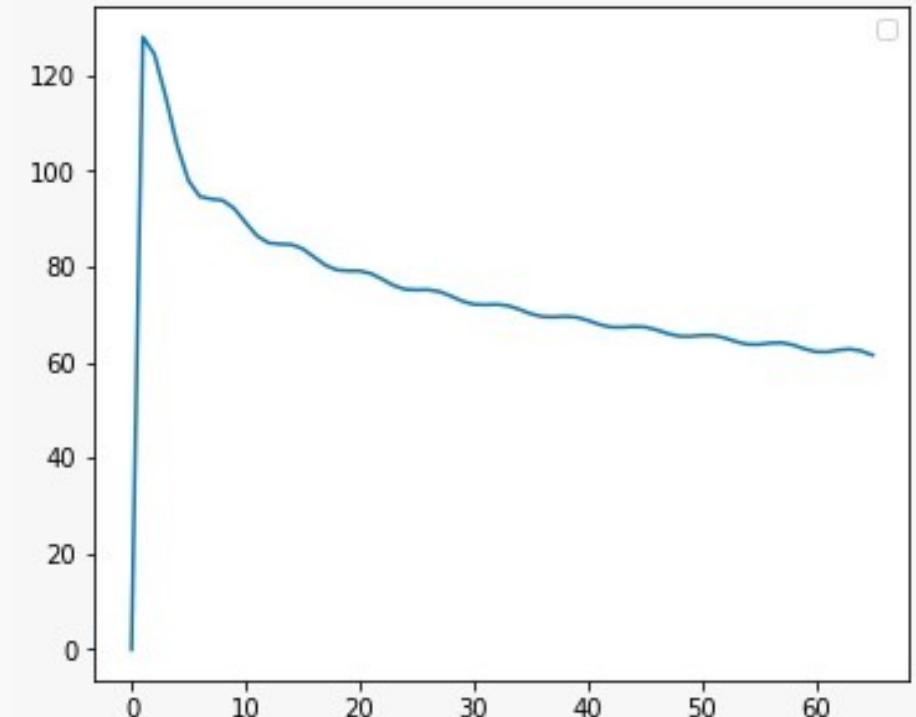
Let  $t$  be the desired position in an input sentence,  $\vec{p}_t \in \mathbb{R}^d$  be its corresponding encoding and  $d$  be the encoding dimension.

Then  $f: \mathbb{N} \rightarrow \mathbb{R}^d$  is the function that produces  $\vec{p}_t$  and is defined as:

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

Where,

$$\omega_k = \frac{1}{10000^{\frac{2k}{d}}}$$



X-axis is time (position), y-axis is  $w_k$

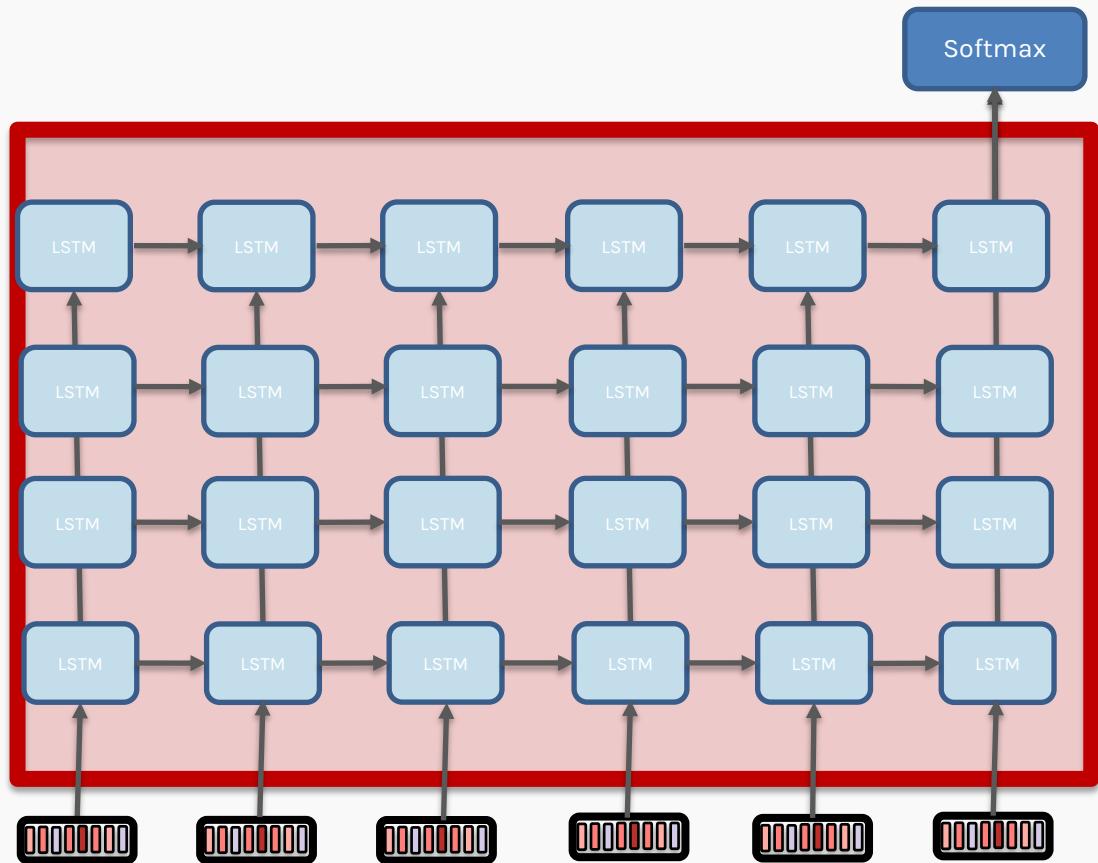


# Bringing it all together



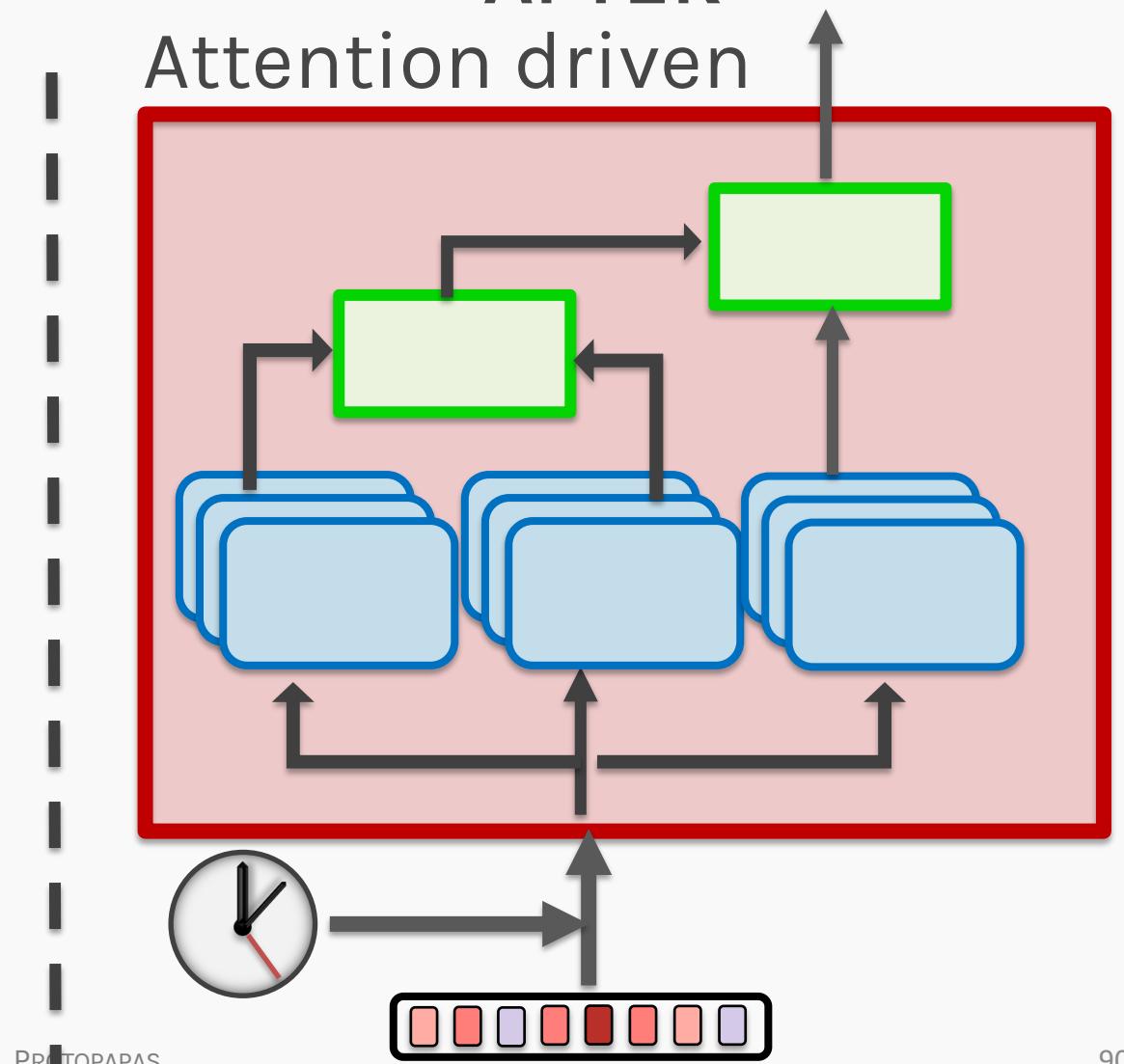
# Comparison – RNN v/s Transformer

**BEFORE**



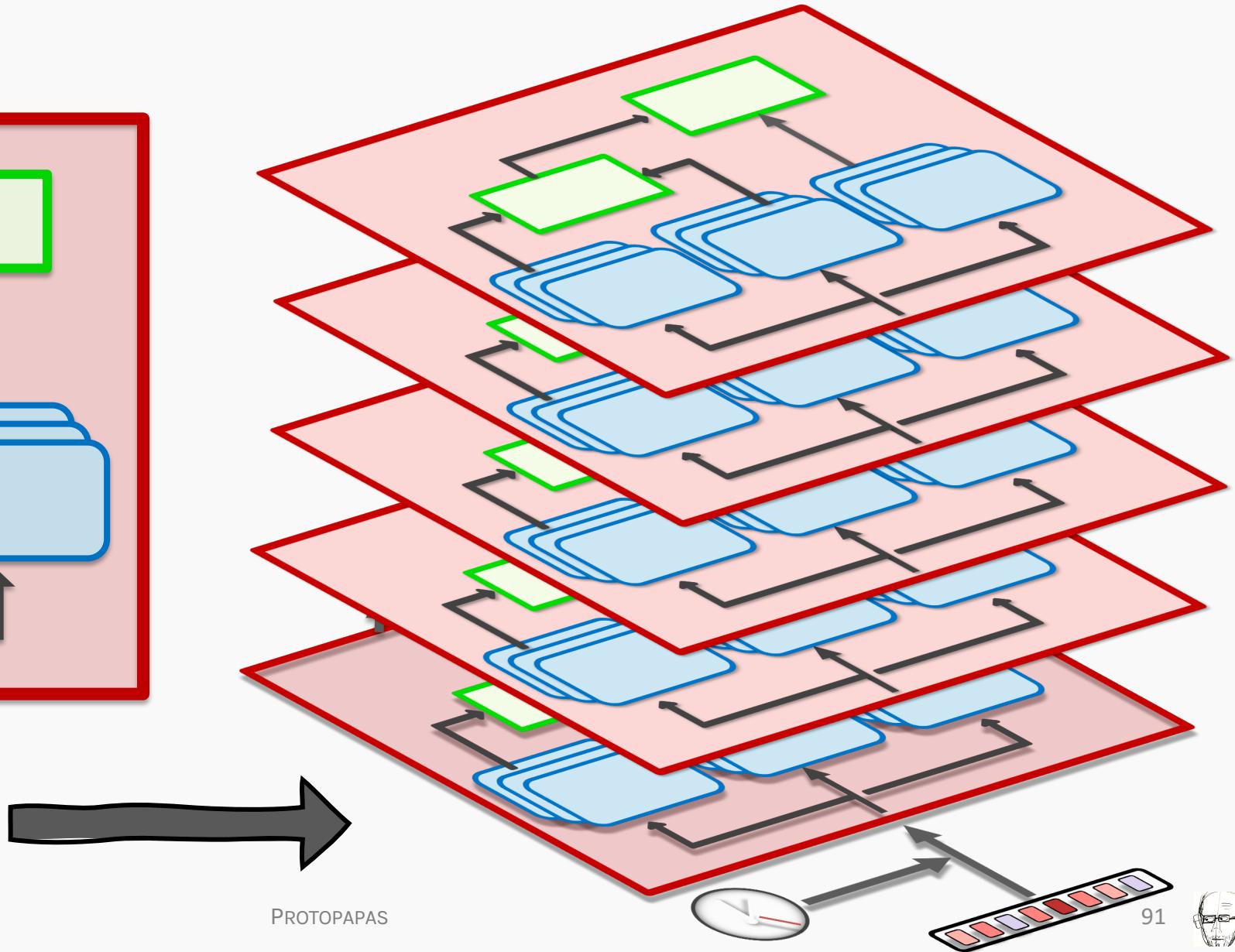
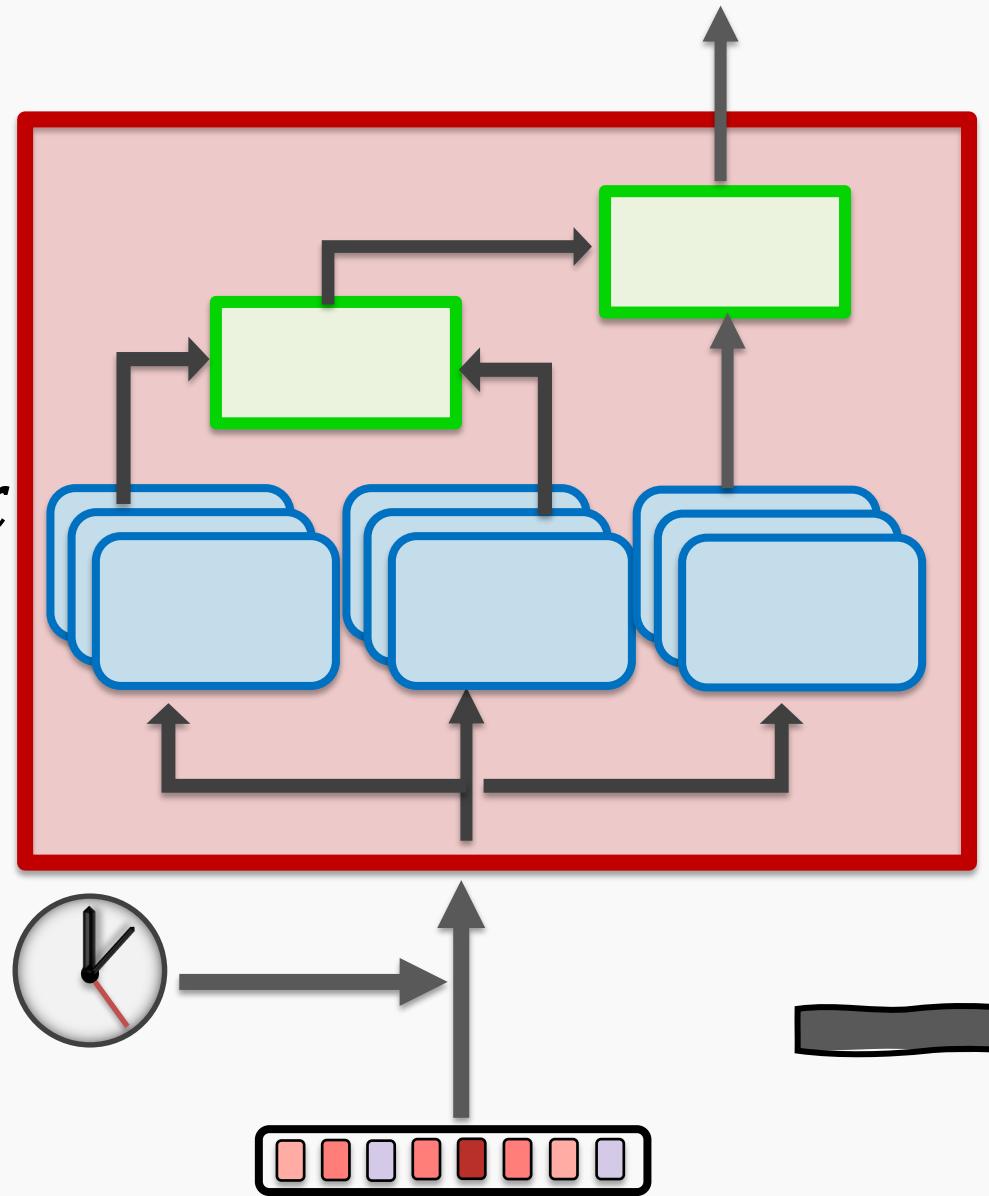
Recurrent units

**AFTER**  
Attention driven



# Transformer as a 3-D model

$N_x$



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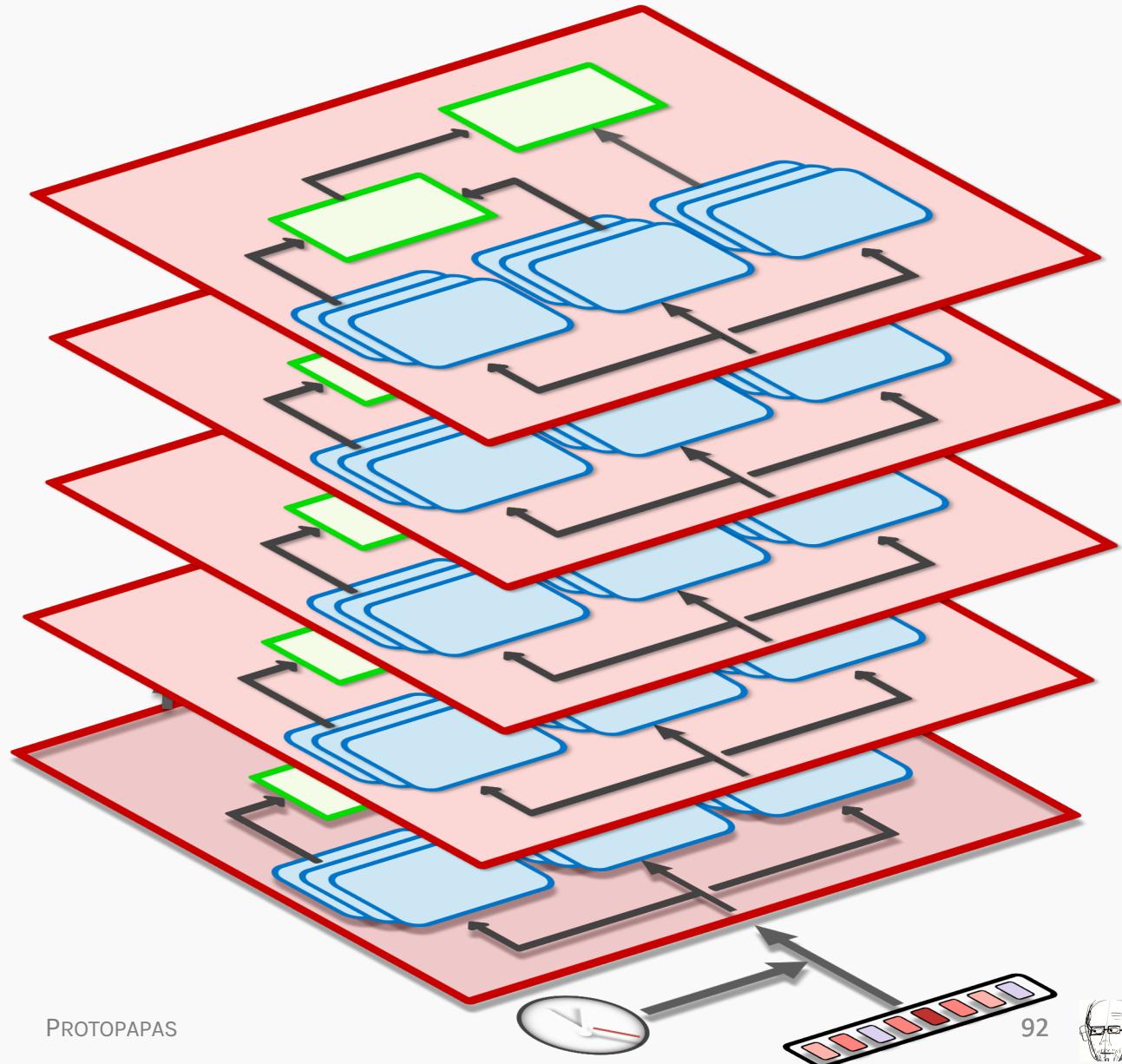
91



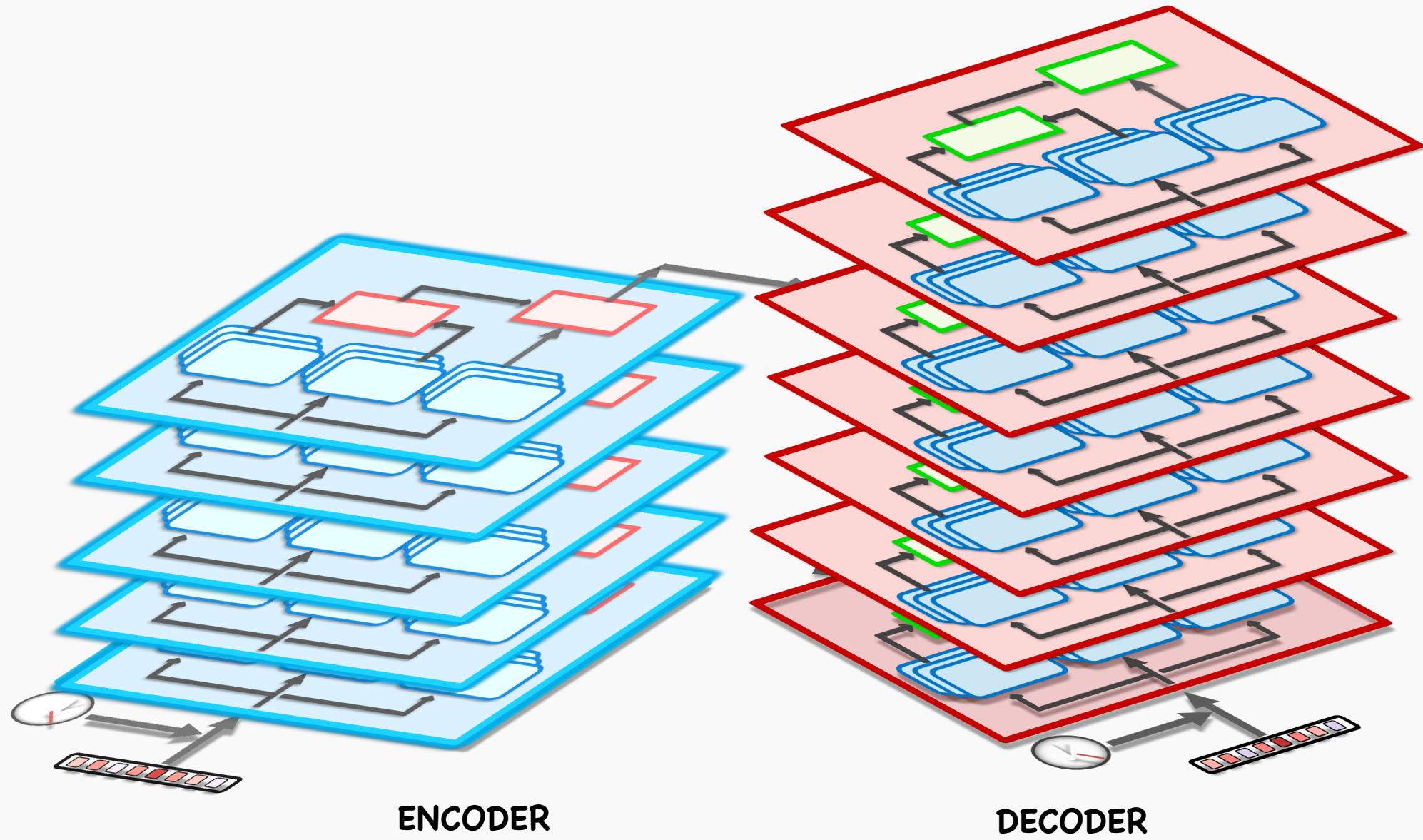
# Transformers - Summary

## Language Model Wishlist?

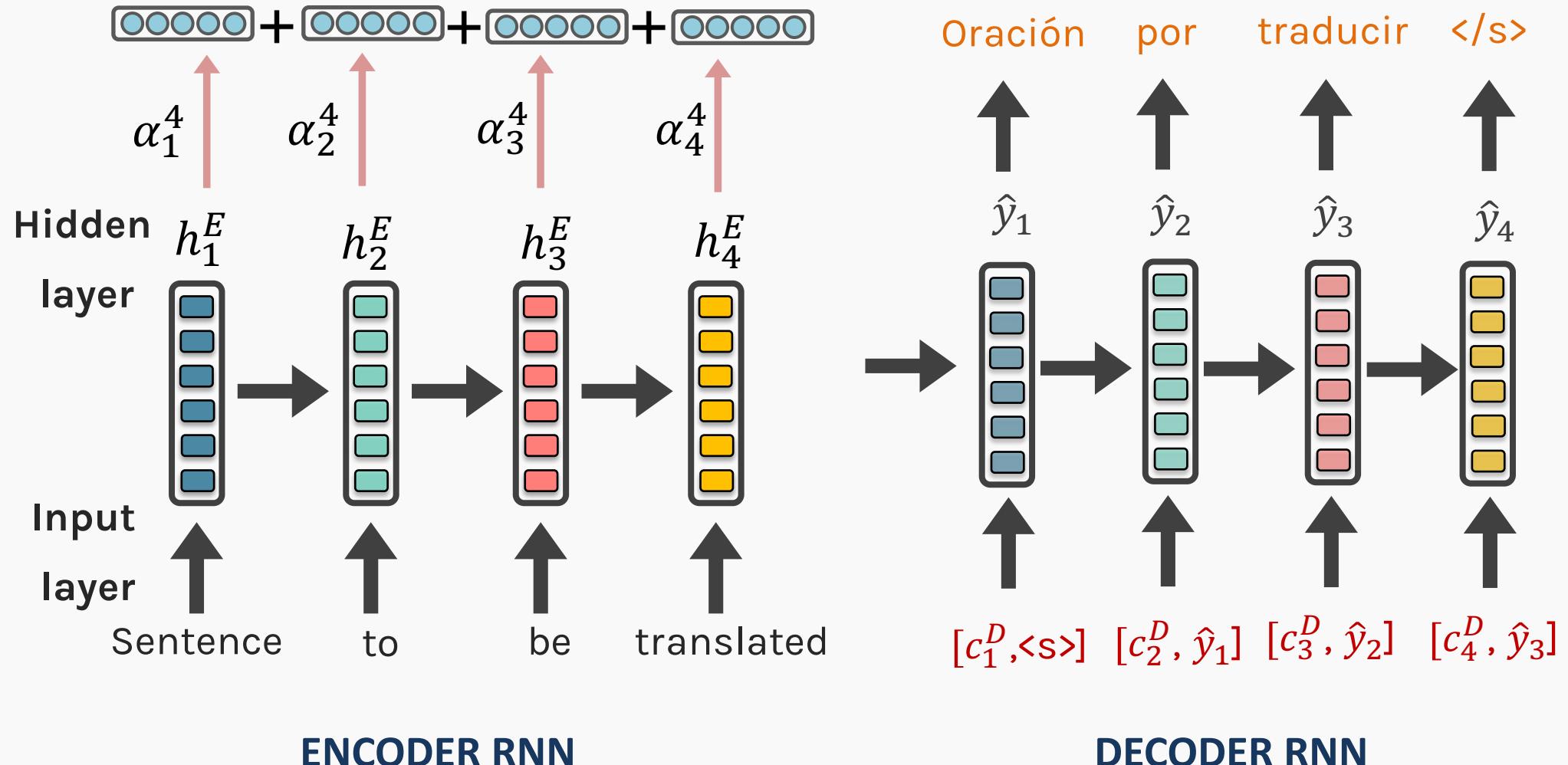
- We want to have strong contextual relations between words - **DONE**
- We want words to have sequential information - **DONE**
- We need an architecture that can be trained in parallel (non-Markovian property) - **DONE**



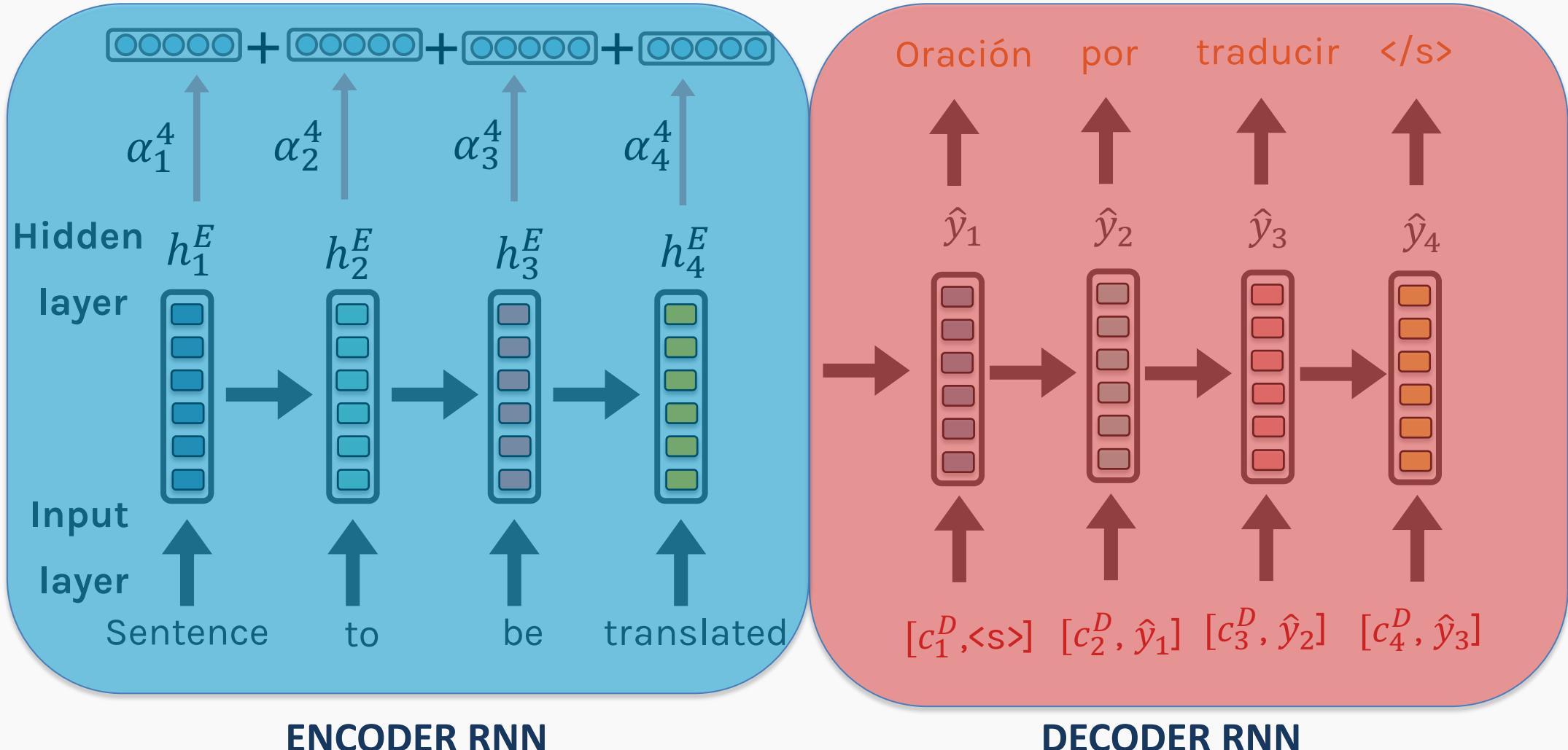
# Transformers - Summary



# RECAP: Seq2Seq + Attention

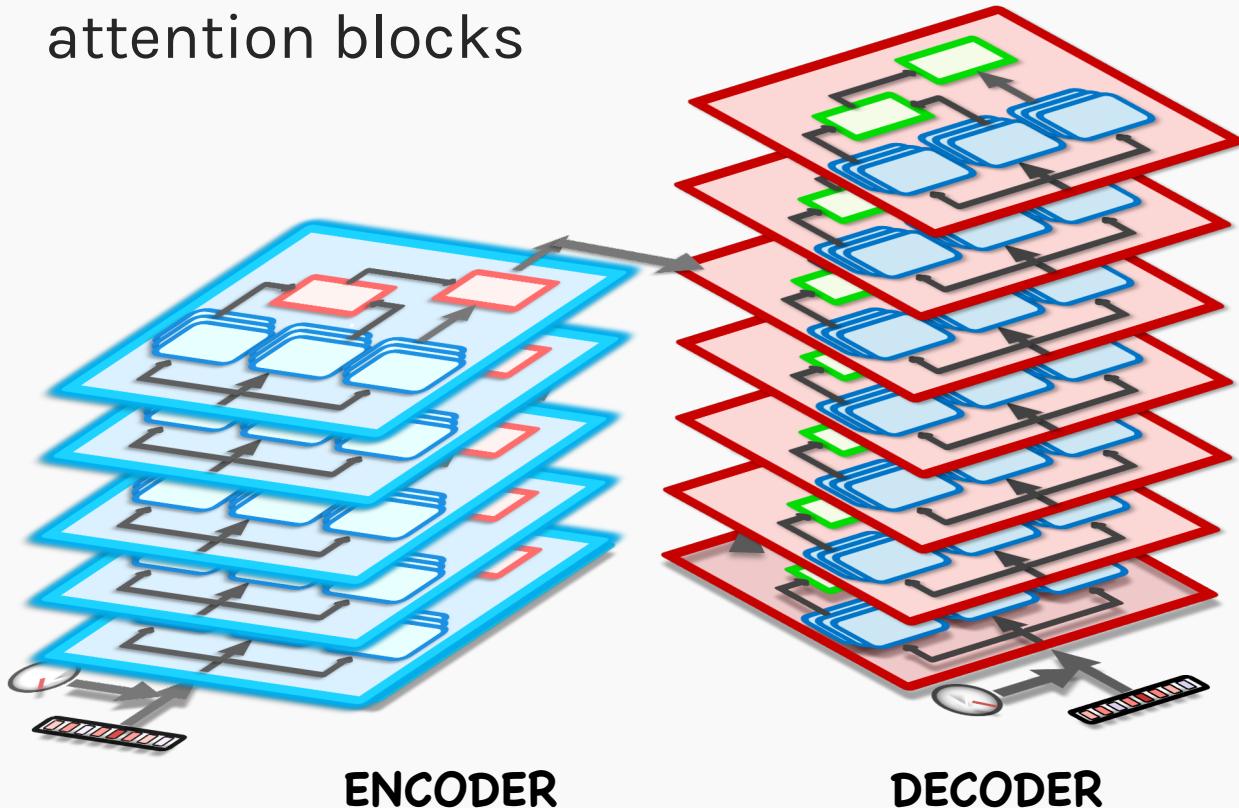


# RECAP: Seq2Seq + Attention

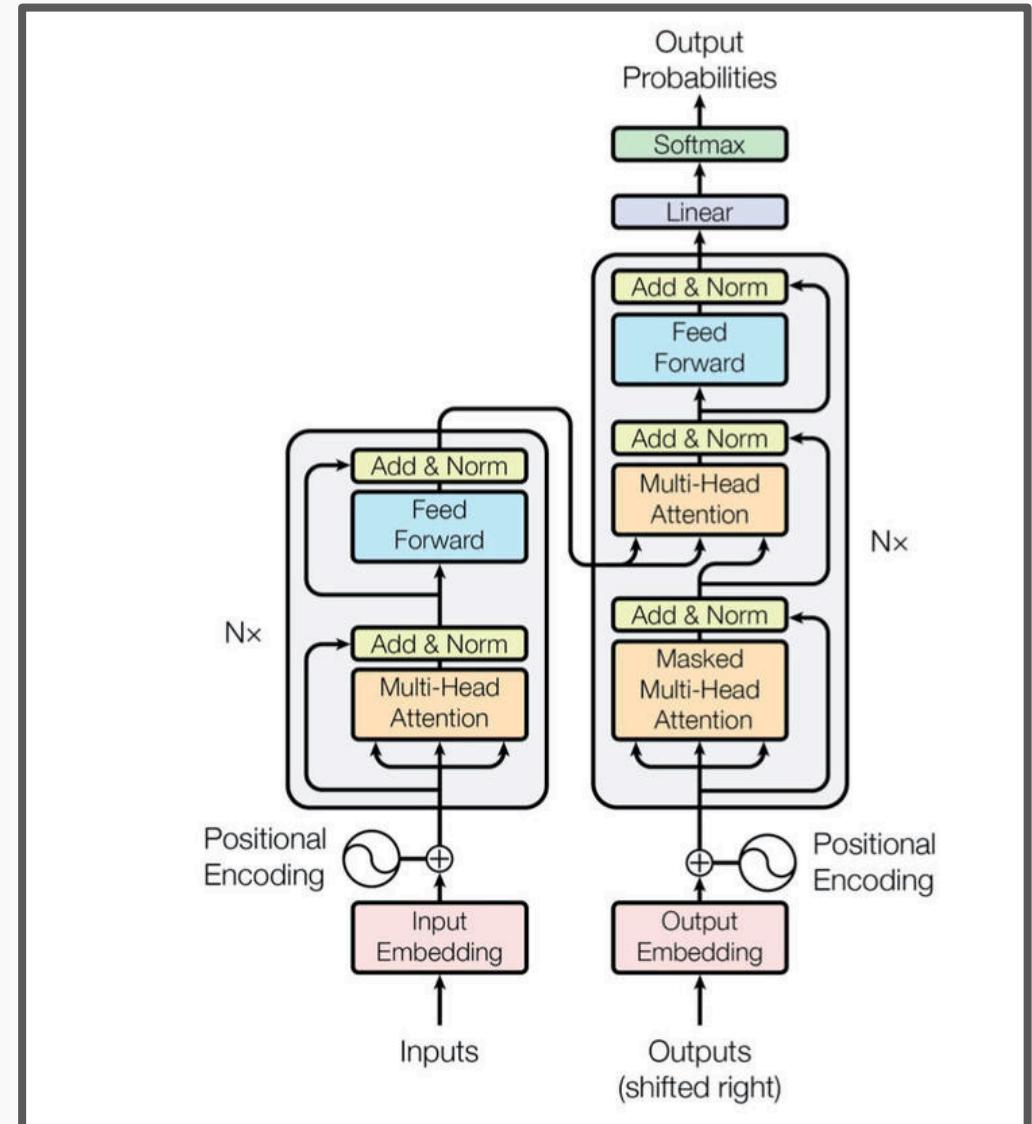


# Transformers - Summary

Transformers consist of an Encoder-Decoder architecture, but instead of using RNNs, we use stacked multi-head attention blocks

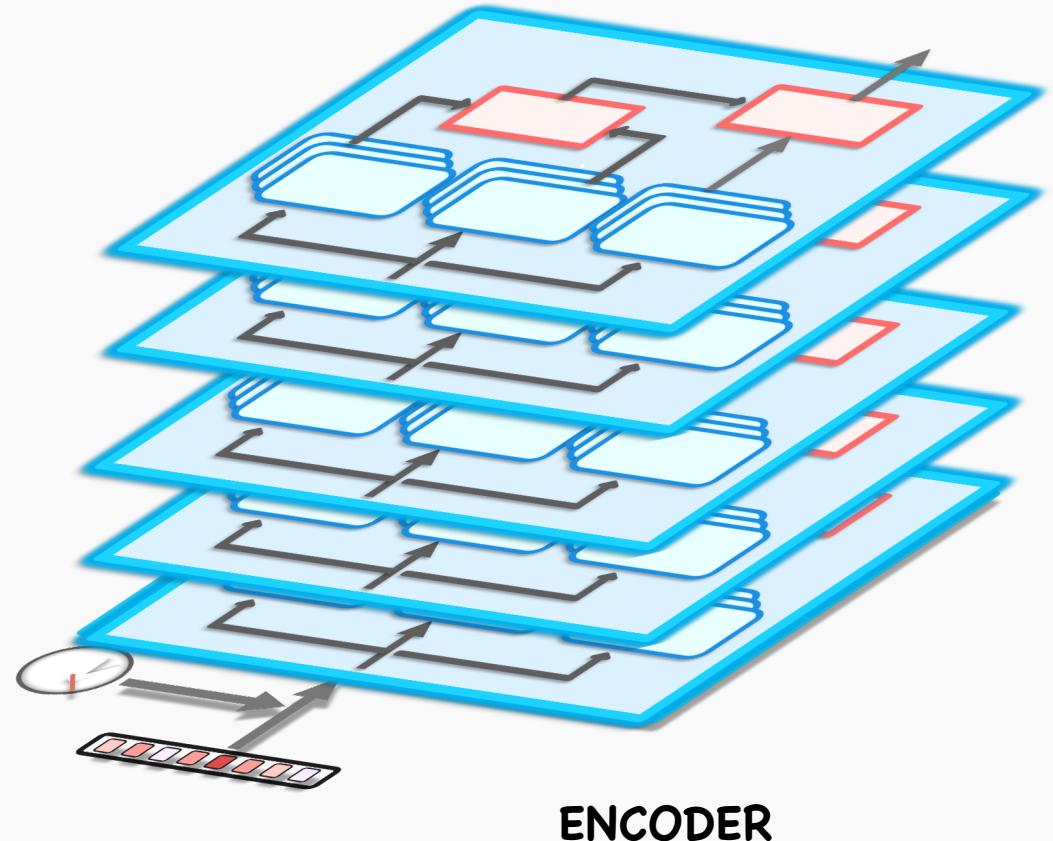


PROTOPAPAS



# From Transformers to BERT

- Instead of an **Encoder-Decoder** architecture for machine translation, what if we just use the encoder for Language Model and other NLP tasks
- This led to the new architecture called **Bidirectional Encoder Representations from Transformers**, or more commonly known as BERT



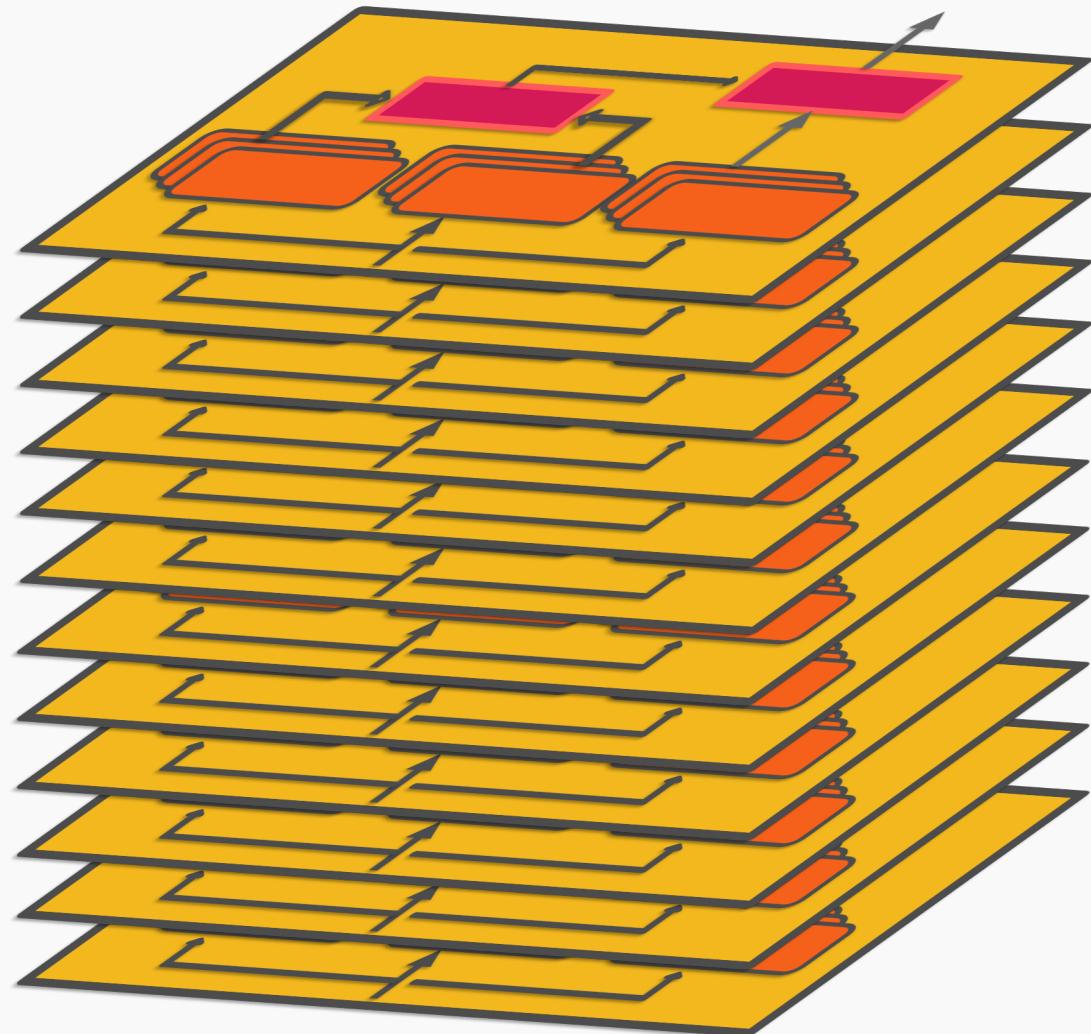
# Bidirectional Encoder Representations from Transformers (BERT)



# BERT

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- The BERT model broke several records across various language model tasks
- The source-code and pre-trained BERT models are all open-source and can be easily adapted to individual tasks
- This makes BERT a prime candidate for transfer learning applications



# Flavors of BERT

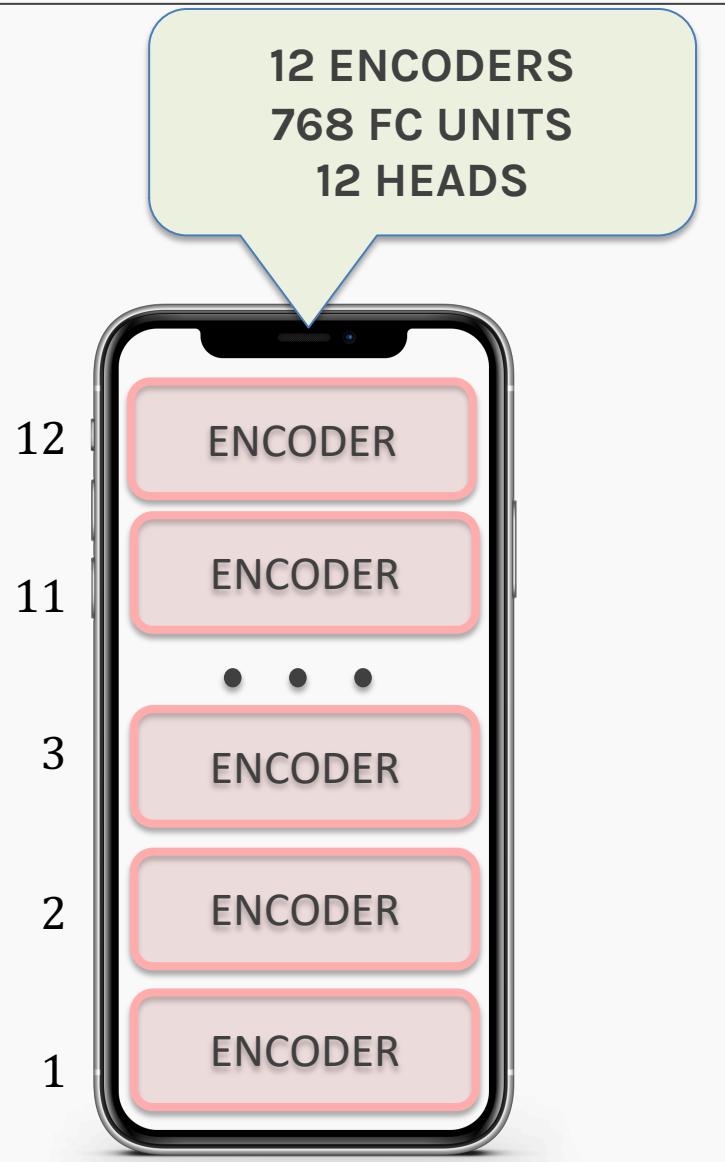
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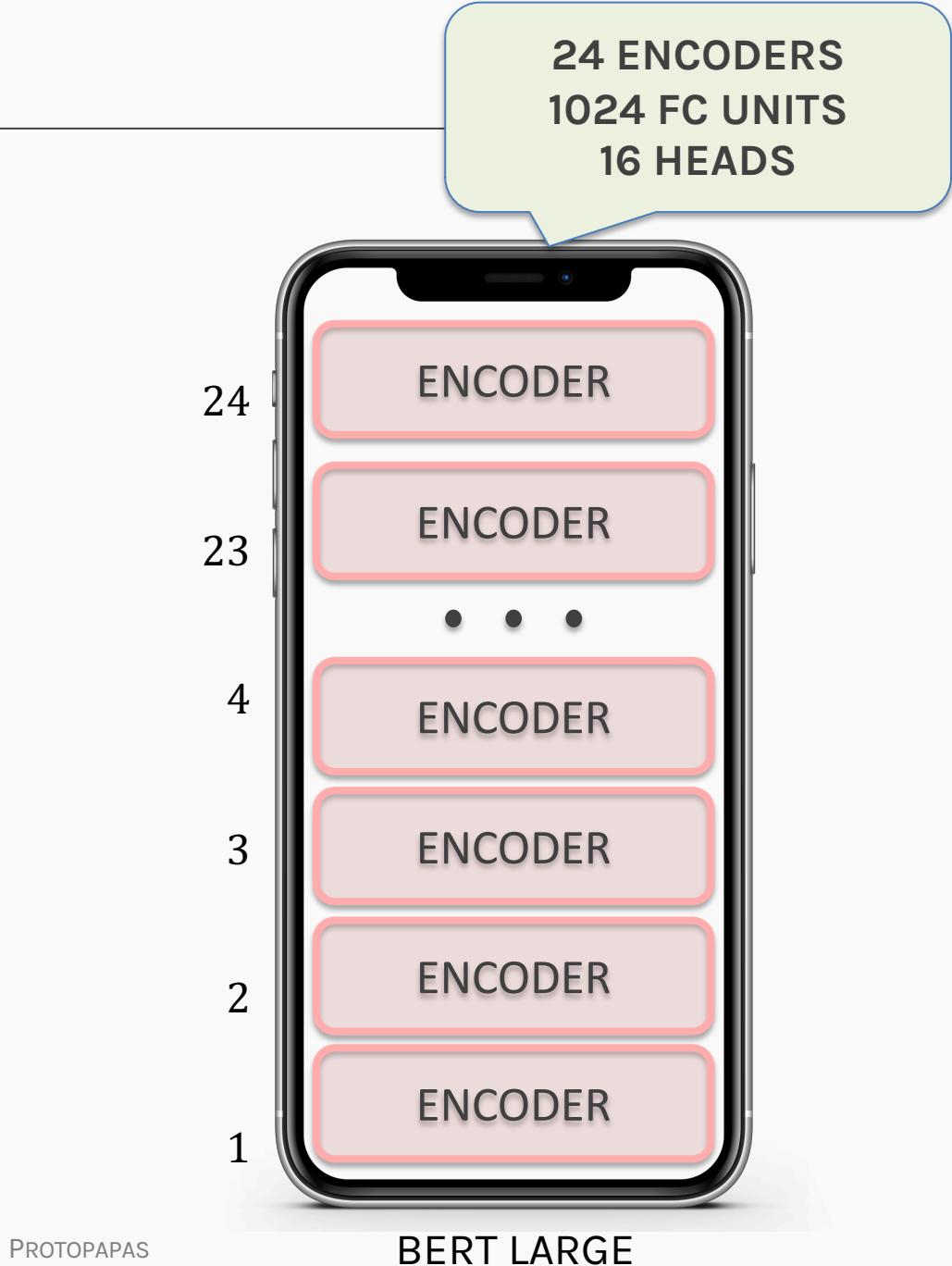
PROTOPAPAS



# Flavors of BERT



BERT BASE



BERT LARGE

PROTOPAPAS

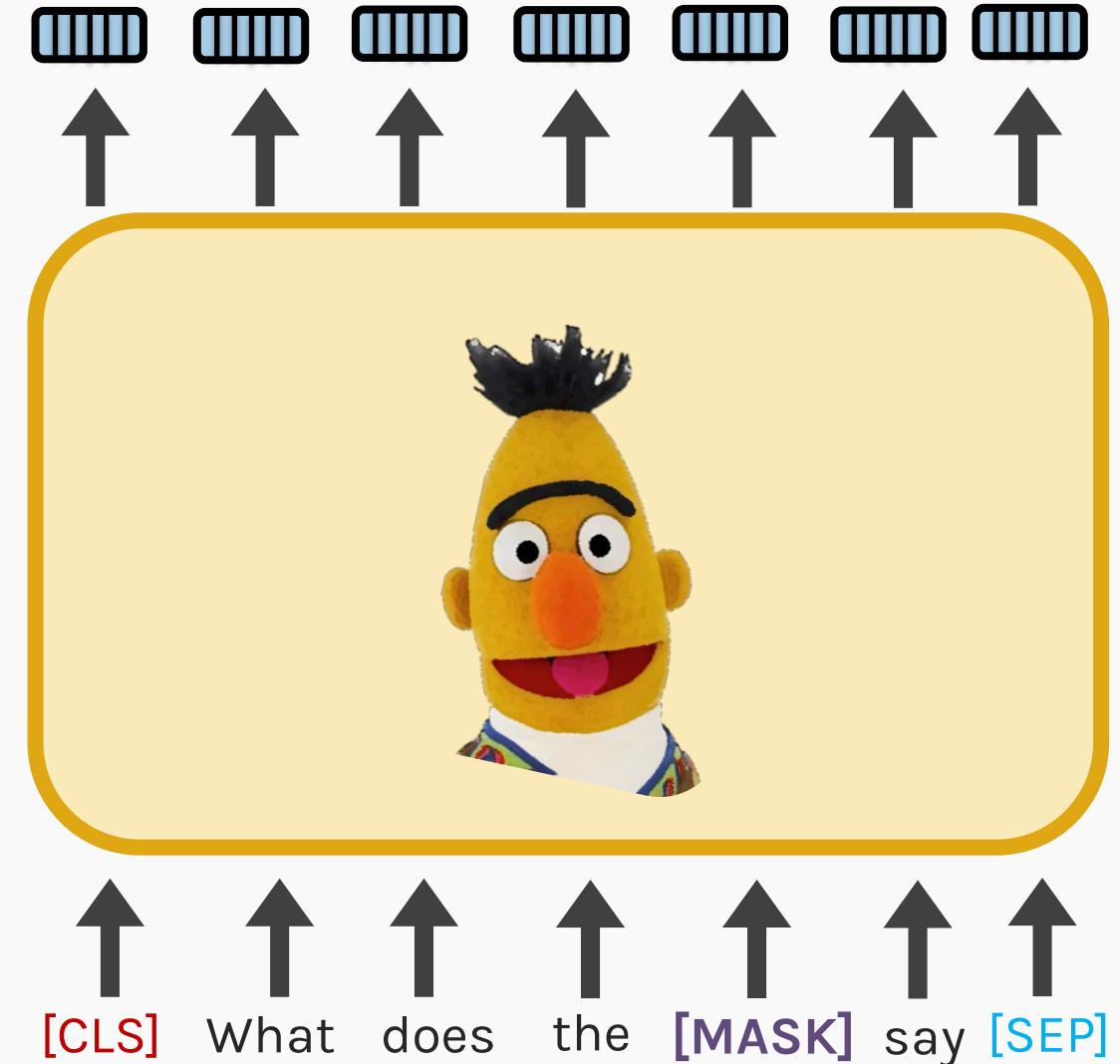


# BERT

## TECHNICAL DETAILS

- Input sequences to BERT must have the following special tokens:
  - [MASK] – Masking token
  - [SEP] – Separator token
  - [CLS] – Classifier Token

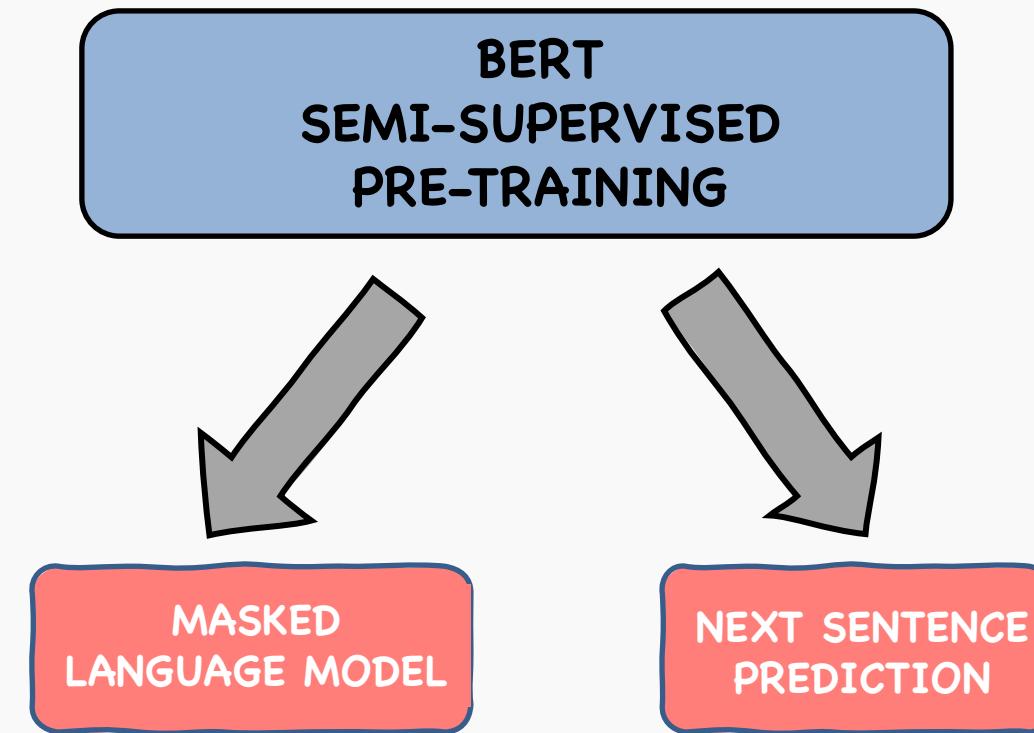
What are these new tokens you ask? Hold on!



# How to train a BERT?



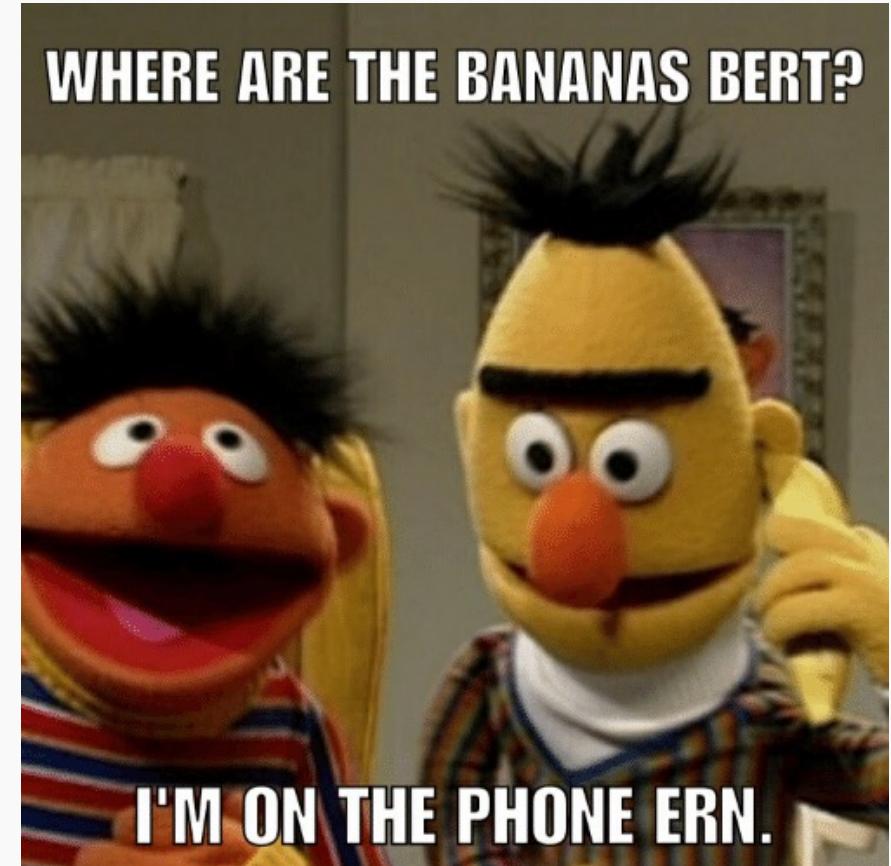
# How to train a BERT



# How to train a BERT?

## TRAINING ISSUES?

- If BERT takes the entire sequence as an input, how can we train it as a language model?
- How could we classify if two chosen sentences follow each other or are out of place if the output is also a sequence of tokens?



# MASKED LANGUAGE MODELING

PROTOPAPAS



# RECAP: Language Model

Shivas was hit by a bus as he was crossing the street

Shivas was hit by a \_\_



So, what do we do?



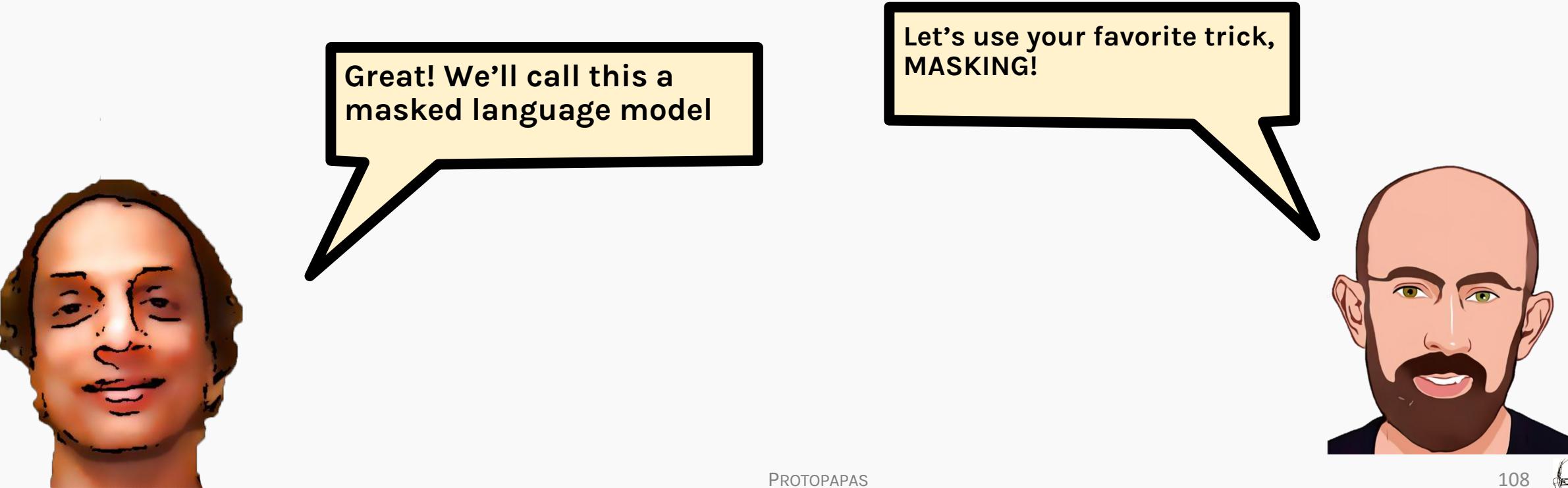
This sort of language modeling is not possible with BERT, because it inputs the entire sequence at once



# Masked Language Model

Shivas was hit by a bus as he was crossing the street

Shivas was hit by a [MASK] as he was ...

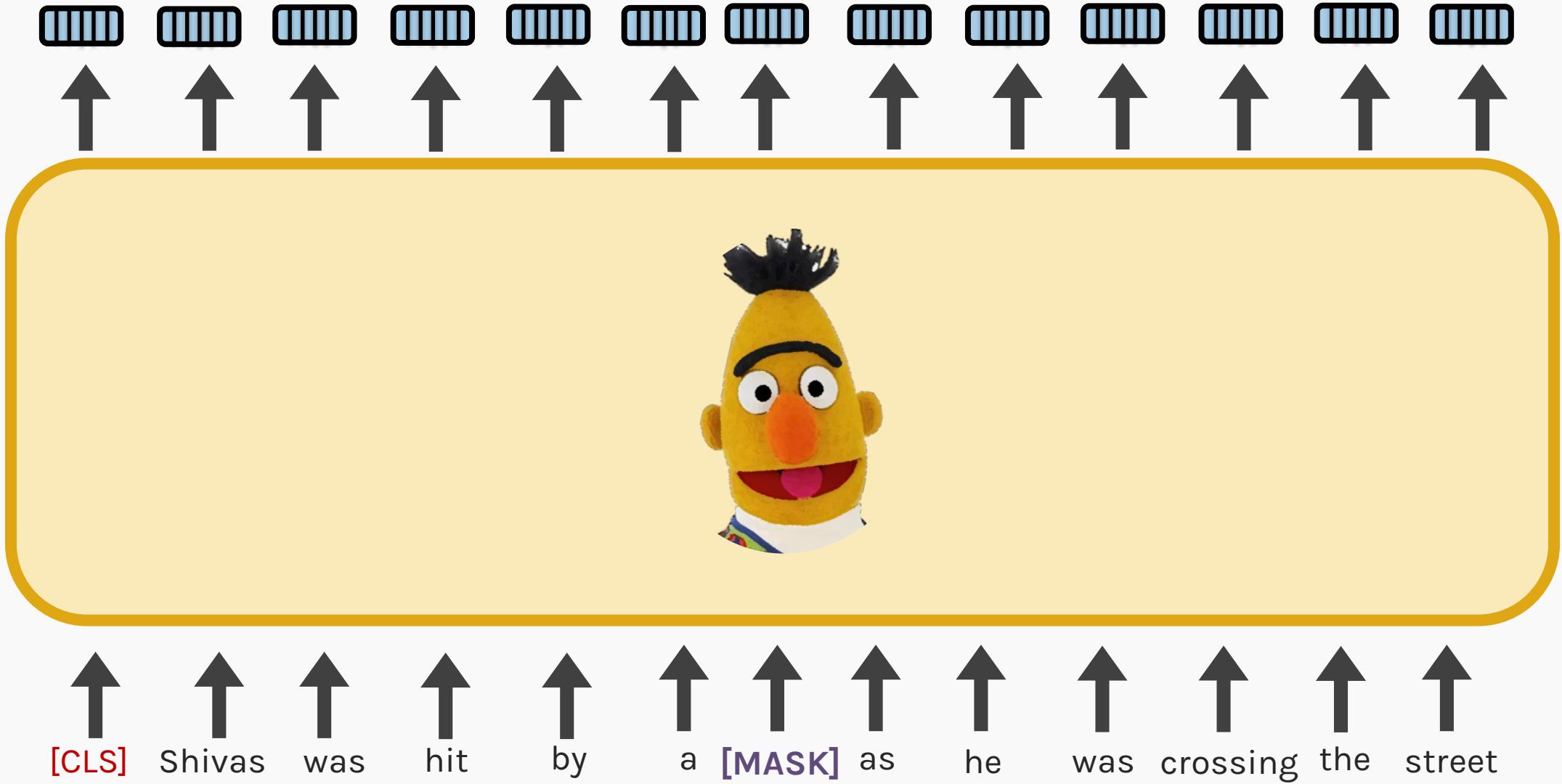


Great! We'll call this a  
masked language model

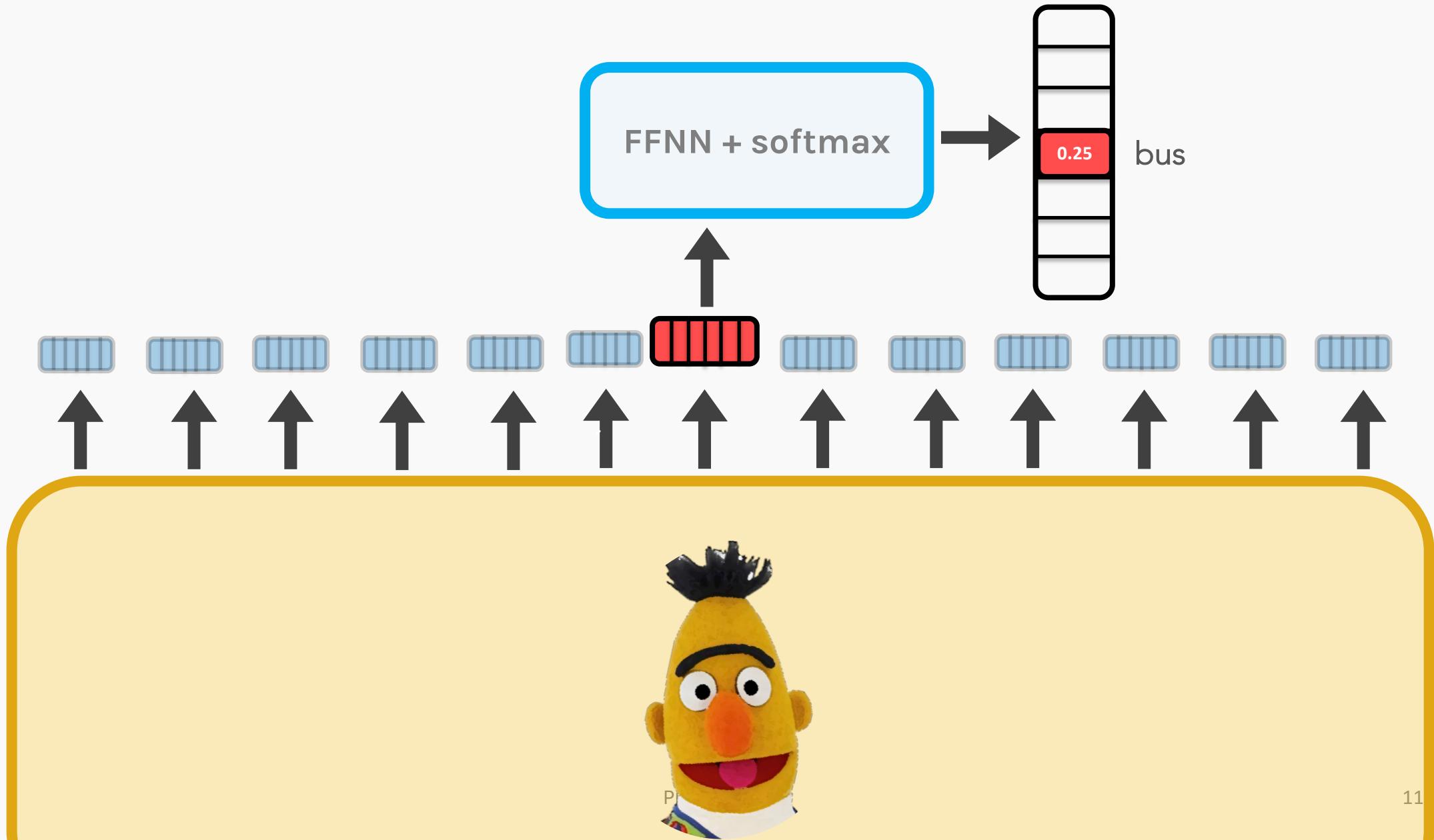
Let's use your favorite trick,  
MASKING!



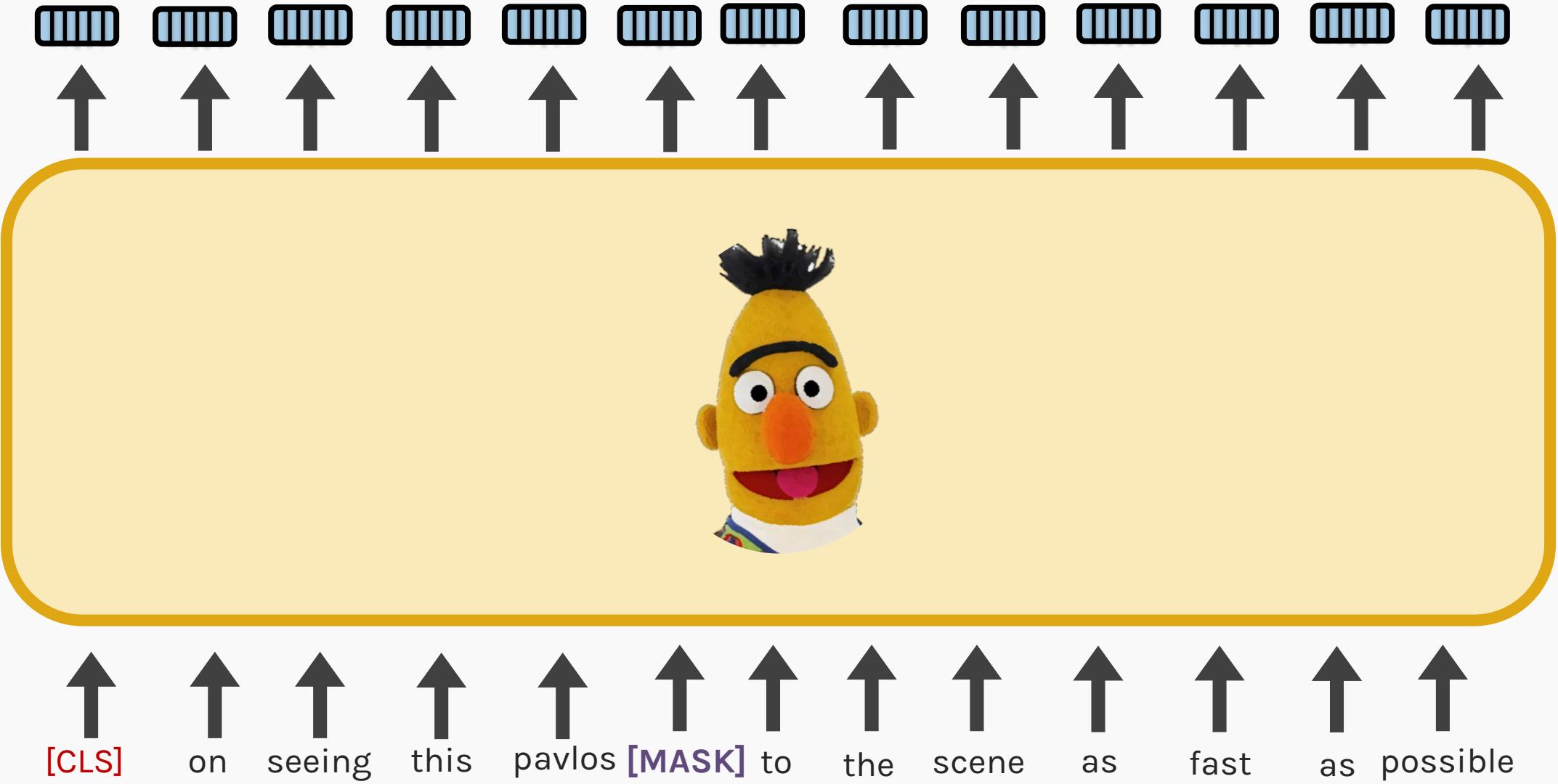
Shivas was hit by a **bus** as he was crossing the street



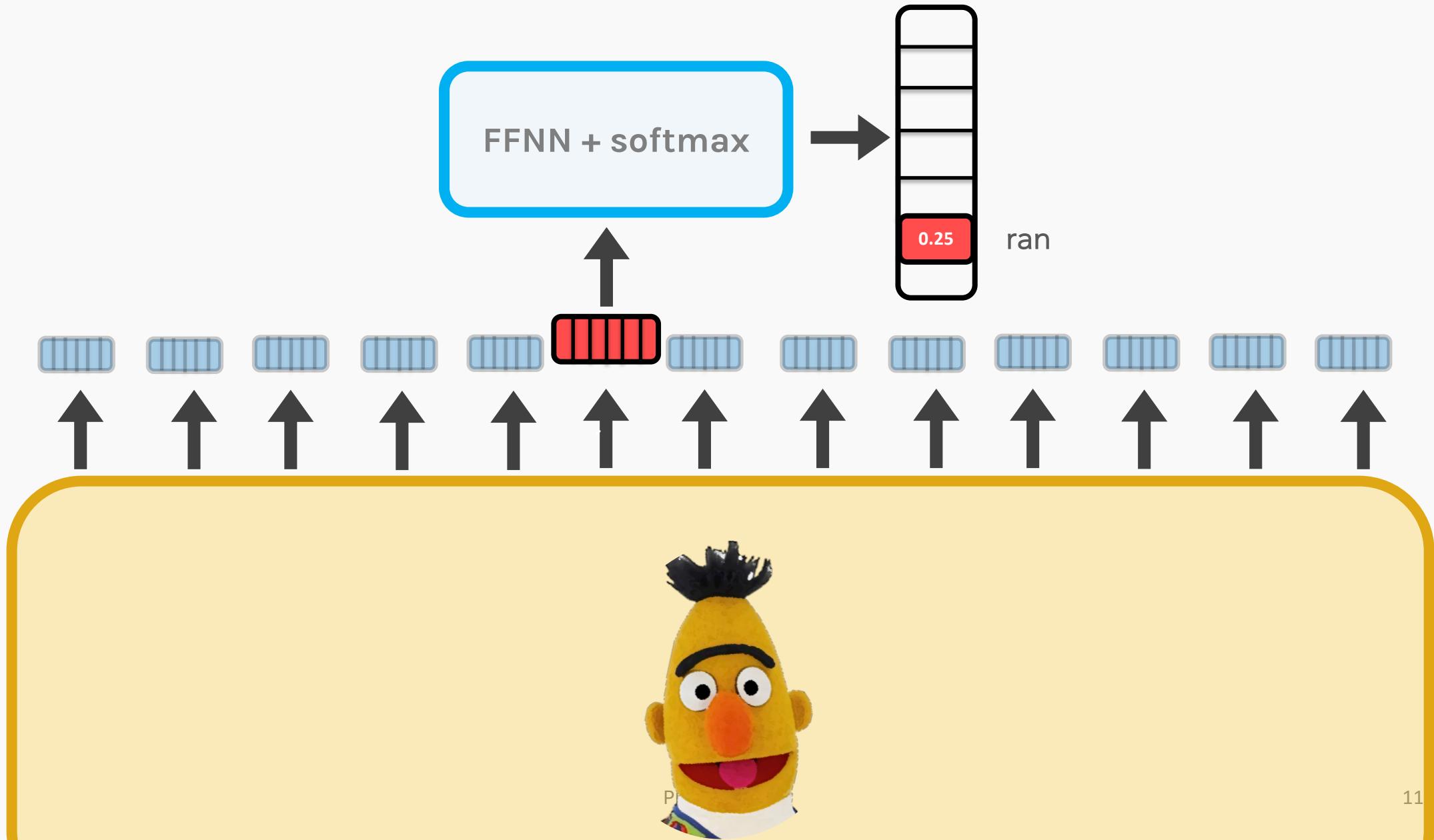
Shivas was hit by a bus as he was crossing the street



On seeing this, Pavlos ran to the scene as fast as possible

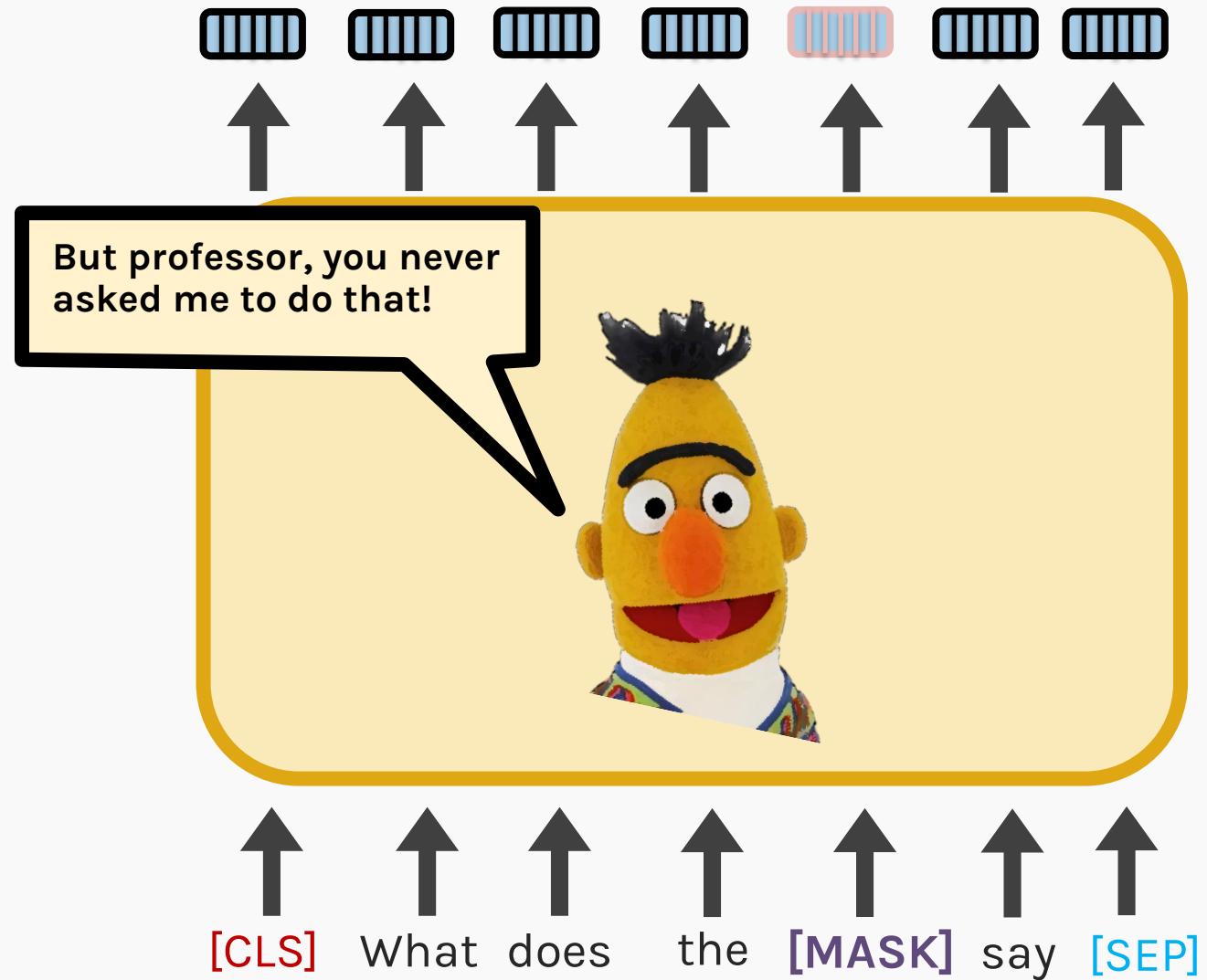


On seeing this, Pavlos ran to the scene as fast as possible

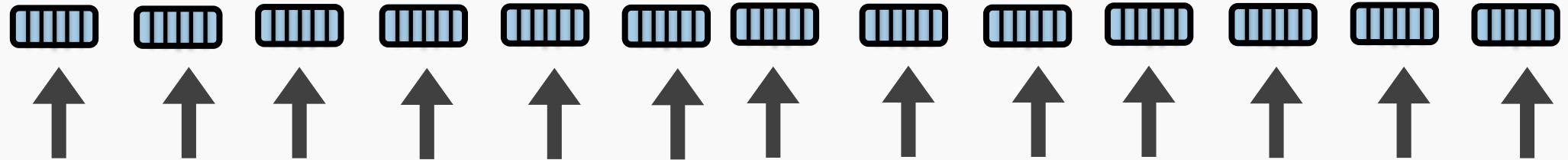


## MASKING ISSUES?

- The model learns how to correctly predict the masked words but completely ignores other words.



Shivas was **hit** by a bus as he was crossing the street



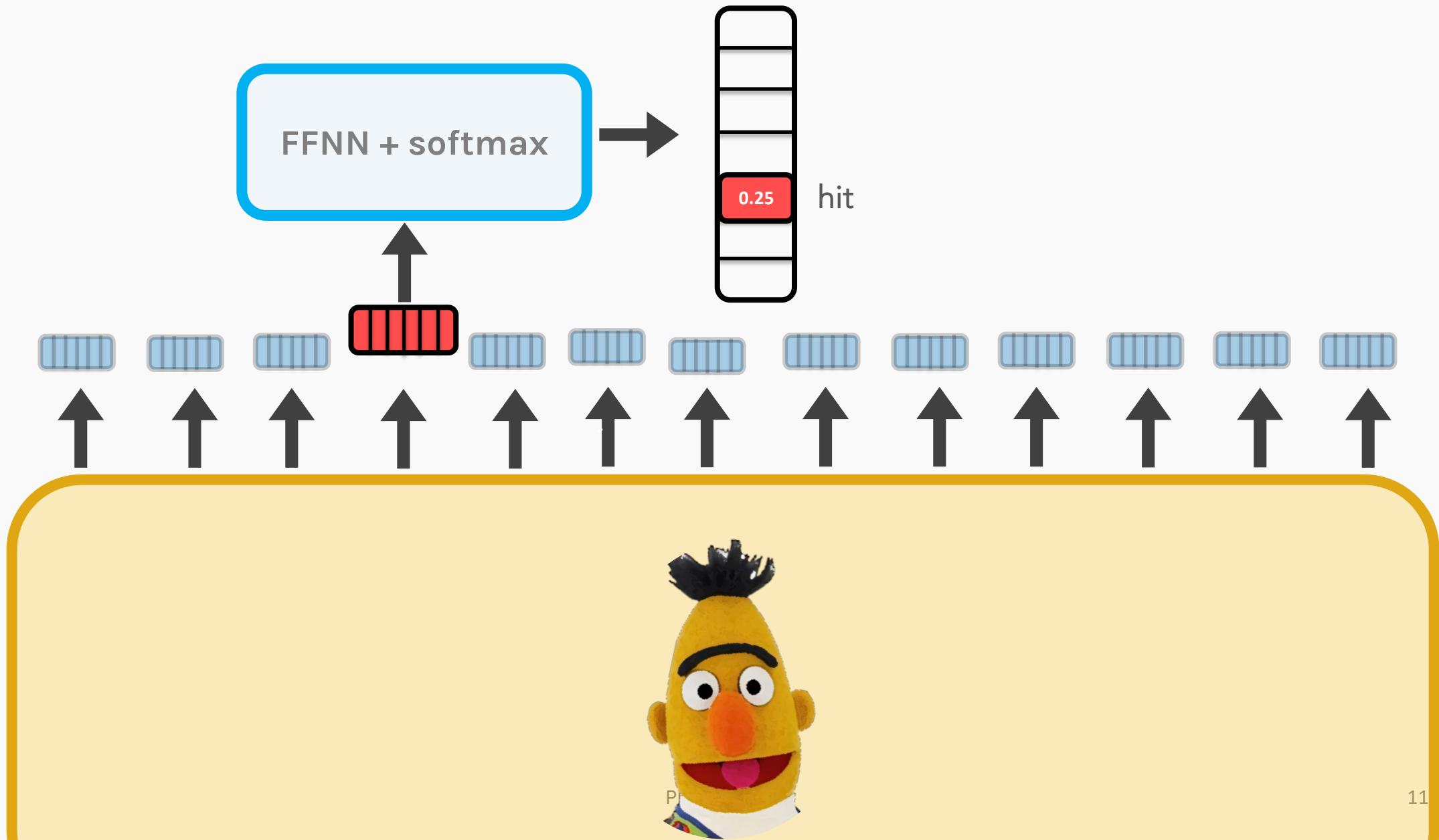
Occasionally, we randomly pick a *unmasked word* and ask the network to predict it



[CLS] Shivas was **hit** by a [MASK] as he was crossing the street



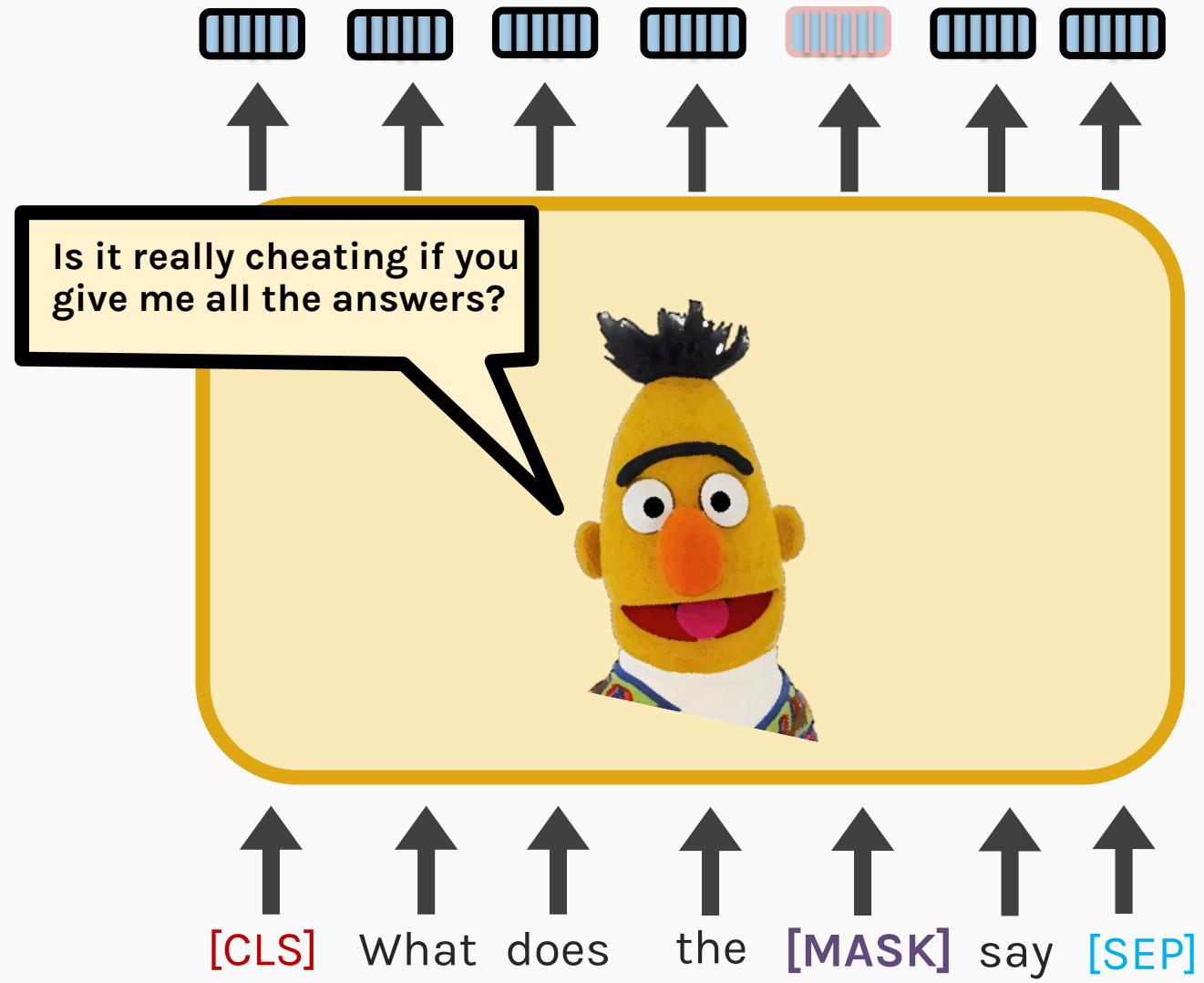
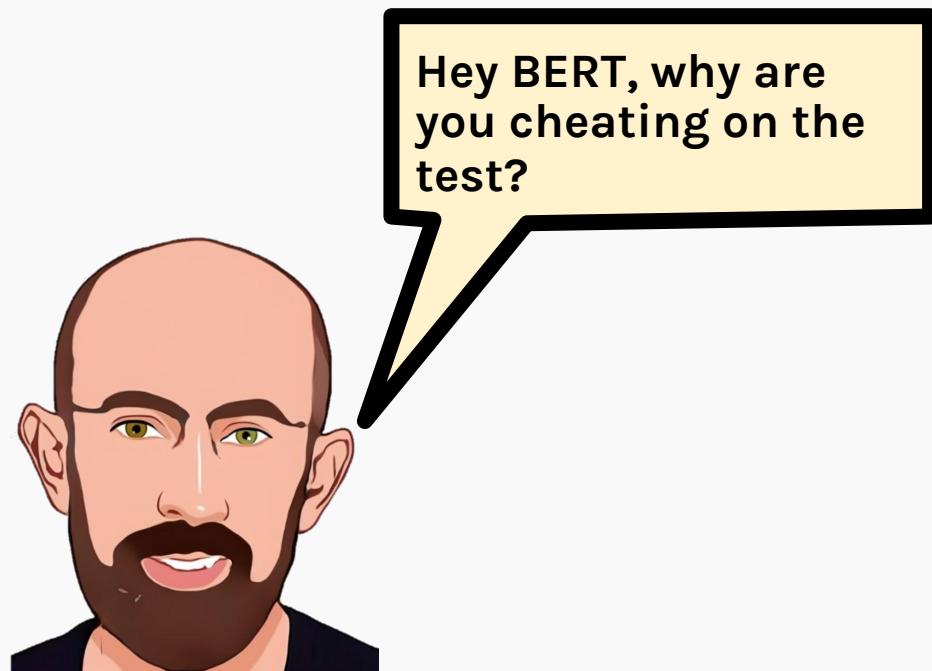
Shivas was hit by a bus as he was crossing the street



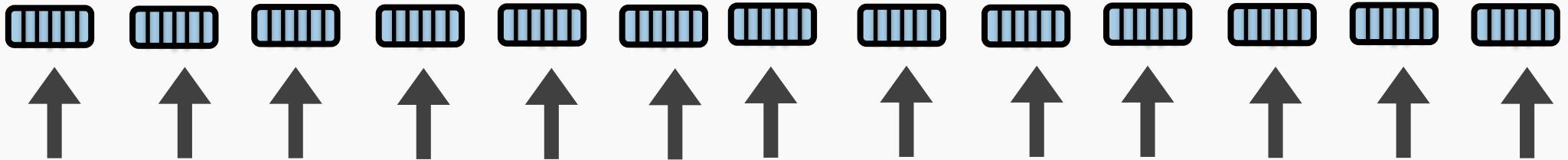
# BERT

## ISSUES?

- The model uses an identity mapping to return unmasked words



Shivas was **hit** by a bus as he was crossing the street



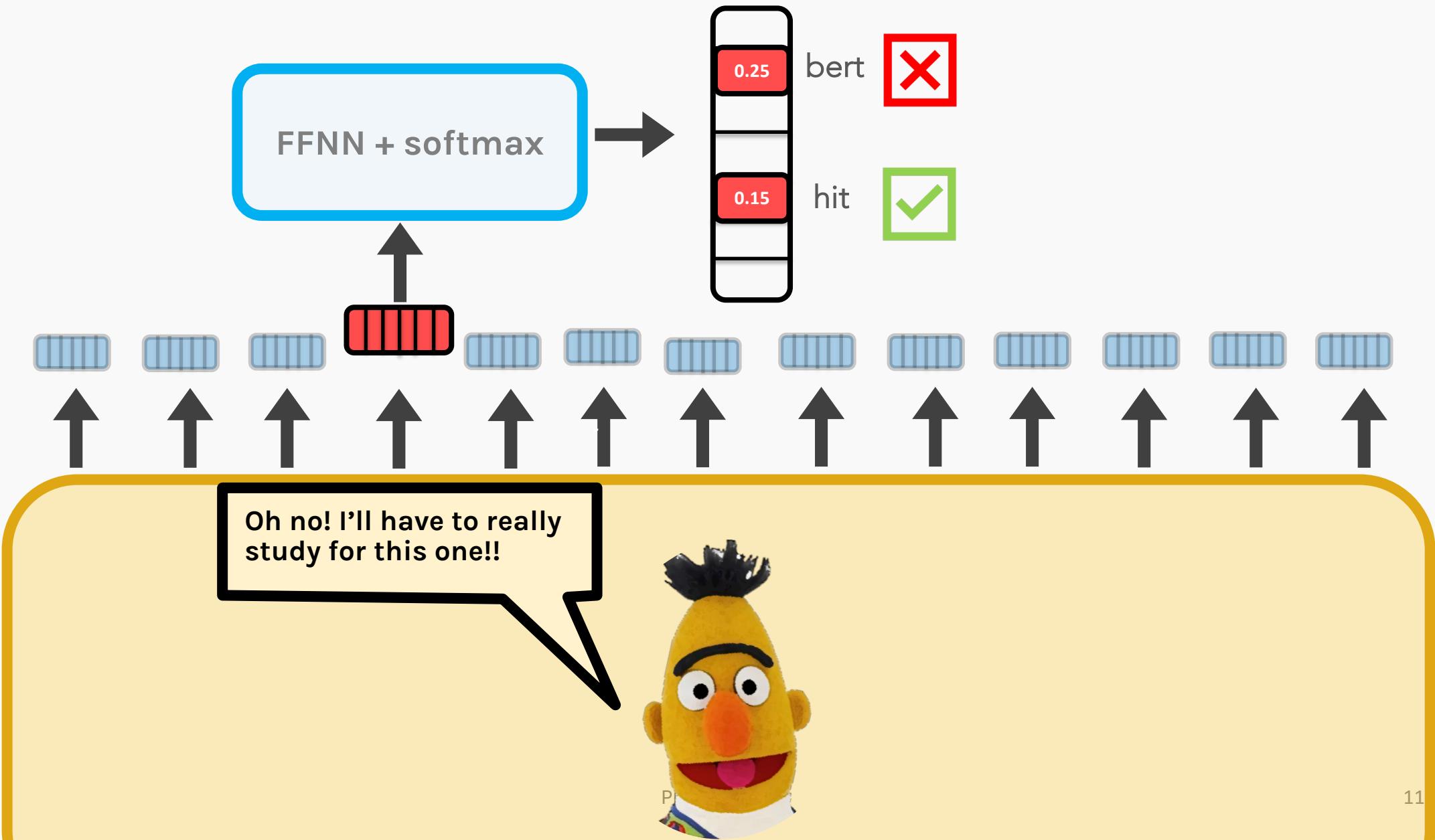
For every unmasked word selected, we can either give the correct input, or a random



[CLS] Shivas was **bert** by a [MASK] as he was crossing the street



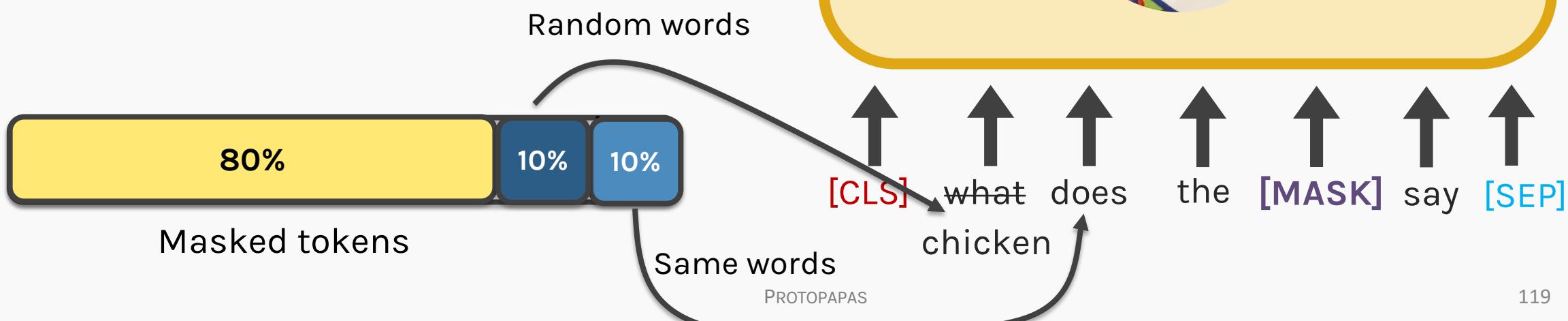
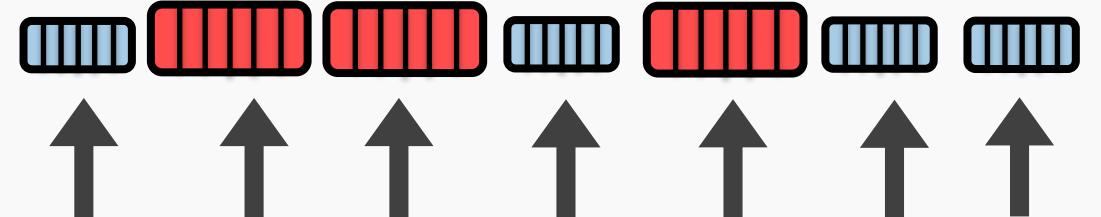
Shivas was hit by a bus as he was crossing the street



# BERT

## MASKING DETAILS

- BERT's language modeling task masks 15% of the input and asks the model to predict the missing word
- 80% of the selected tokens are masked, 10% are the same words and 10% are randomly replaced words



# NEXT SENTENCE PREDICTION



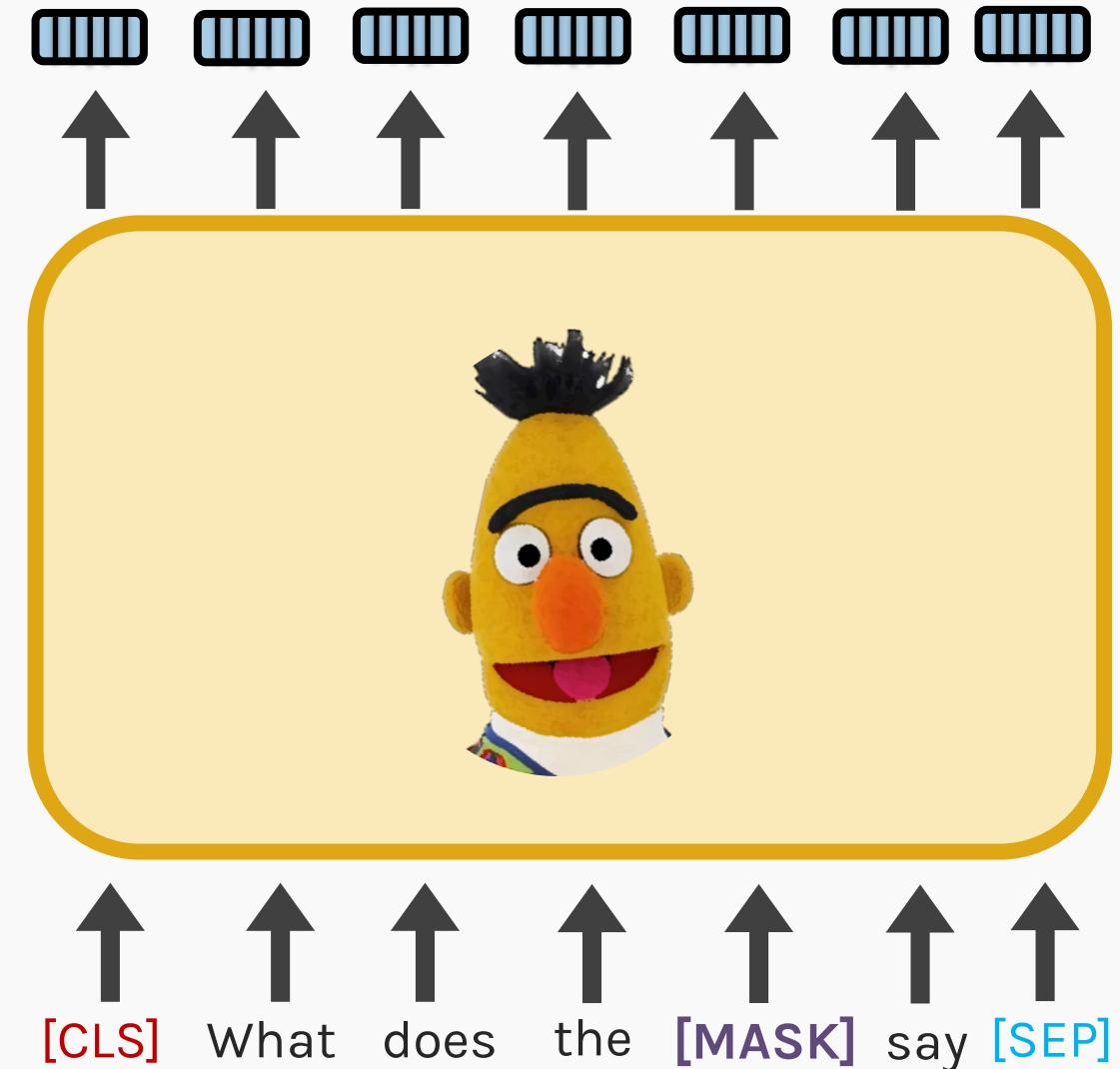
# Two sentence task

## TECHNICAL DETAILS

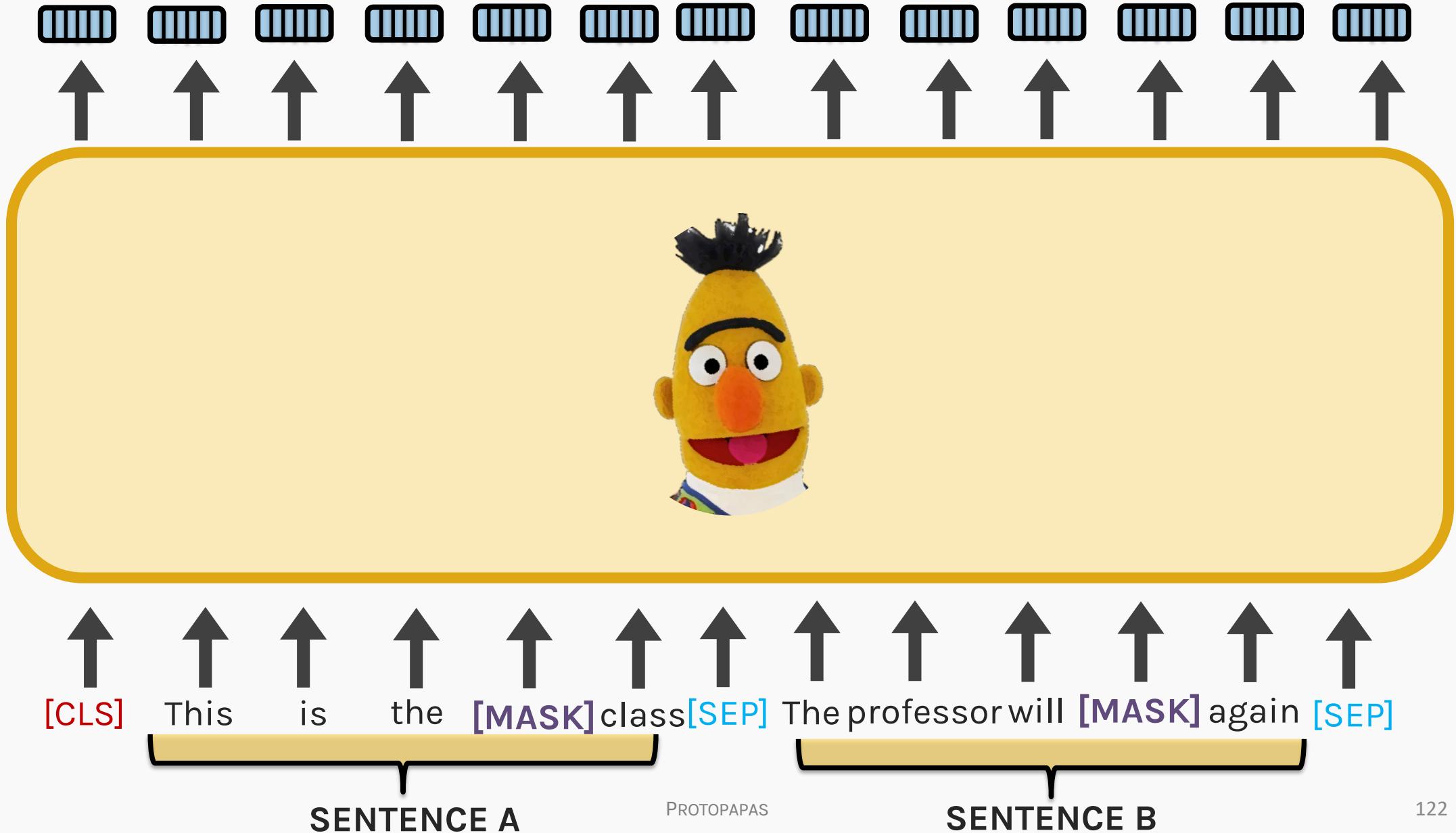
- To make BERT better at handling relationships between multiple sentences, the pre-training process includes an additional task:

Given two sentences (A and B), is B likely to be the sentence that follows A, or not?

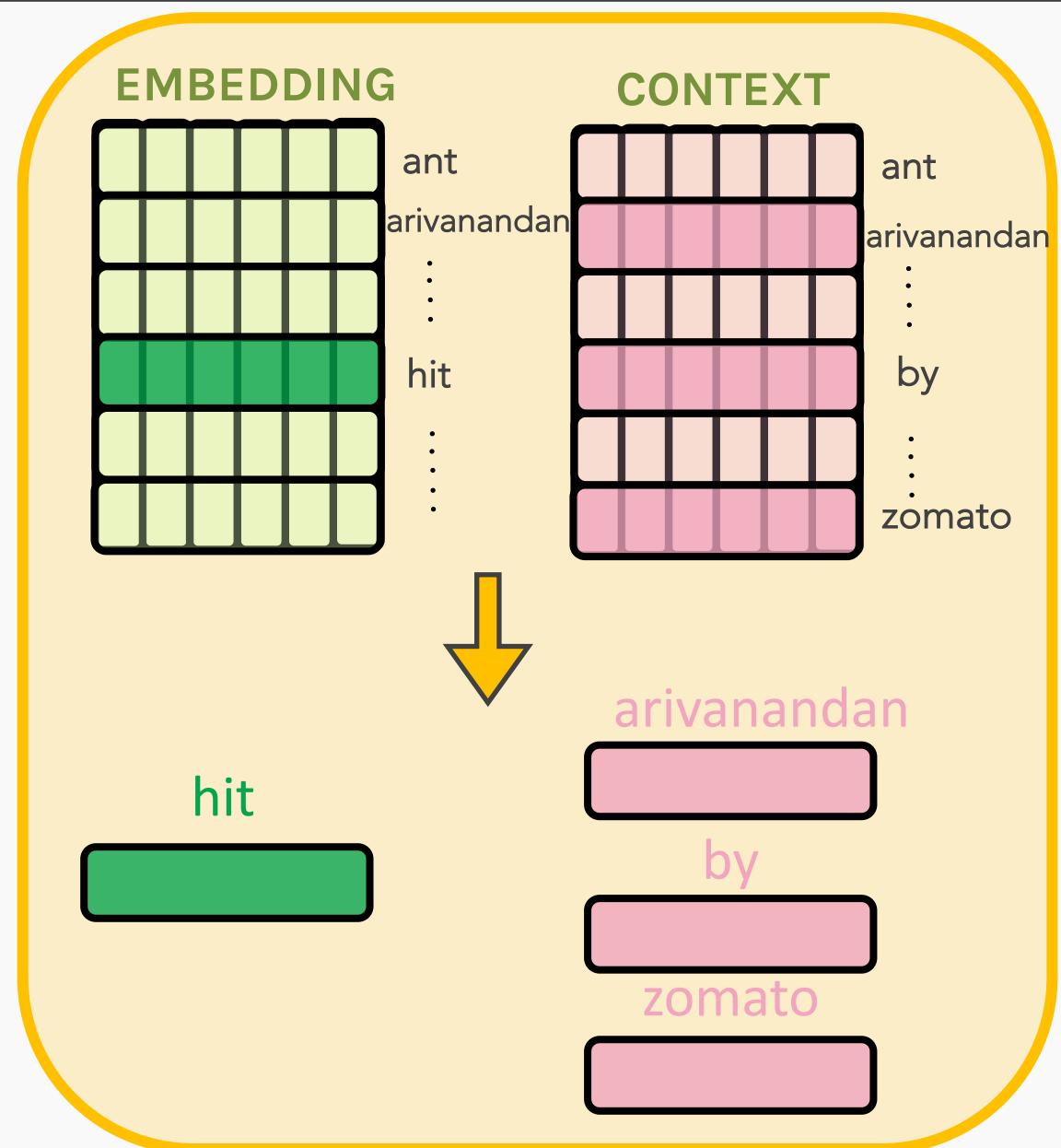
The individual sentences are separated by the **[SEP]** tag mentioned before



## Two sentence task



# RECAP: Negative Sampling

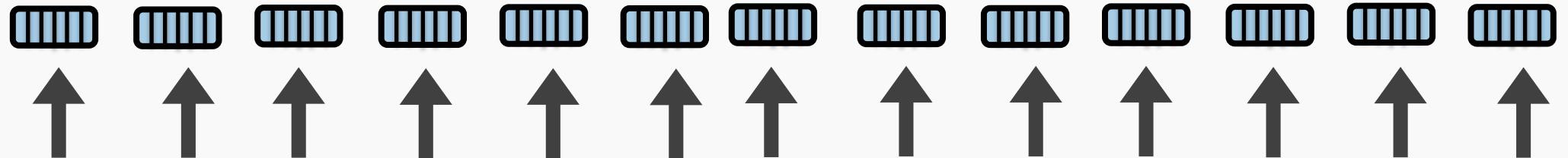


| input<br>(centre)<br>word, $w_c$ | output word, $w_o$ | Input ·<br>Output | Sigmoid() | Target |
|----------------------------------|--------------------|-------------------|-----------|--------|
| hit                              | was                | -0.91             | 0.25      | 1      |
| hit                              | arivanandan        | -1.11             | 0.25      | 0      |
| hit                              | by                 | 0.2               | 0.55      | 1      |
| hit                              | zomato             | 0.74              | 0.68      | 0      |

- Just as in word2vec training, we generate ***negative samples*** of sentences
- These sentences could follow each other ( $TARGET = 1$ ) or can be selected at random ( $TARGET = 0$ )
- The training will be using a simple classifier



This is the last class. The professor will explain again



To assess if the two sentences follow each other, we use the embedding of the [CLS] tag from the start of the sentence



[CLS] This is the [MASK] class [SEP] The professor will [MASK] again [SEP]

SENTENCE A

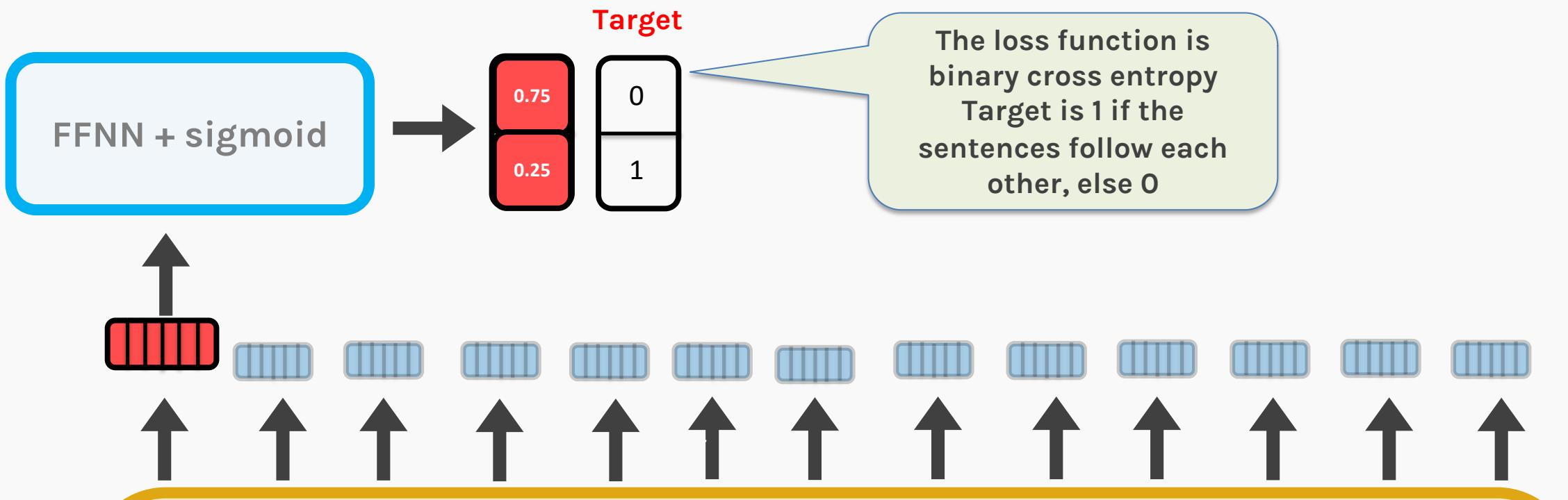
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SENTENCE B

124



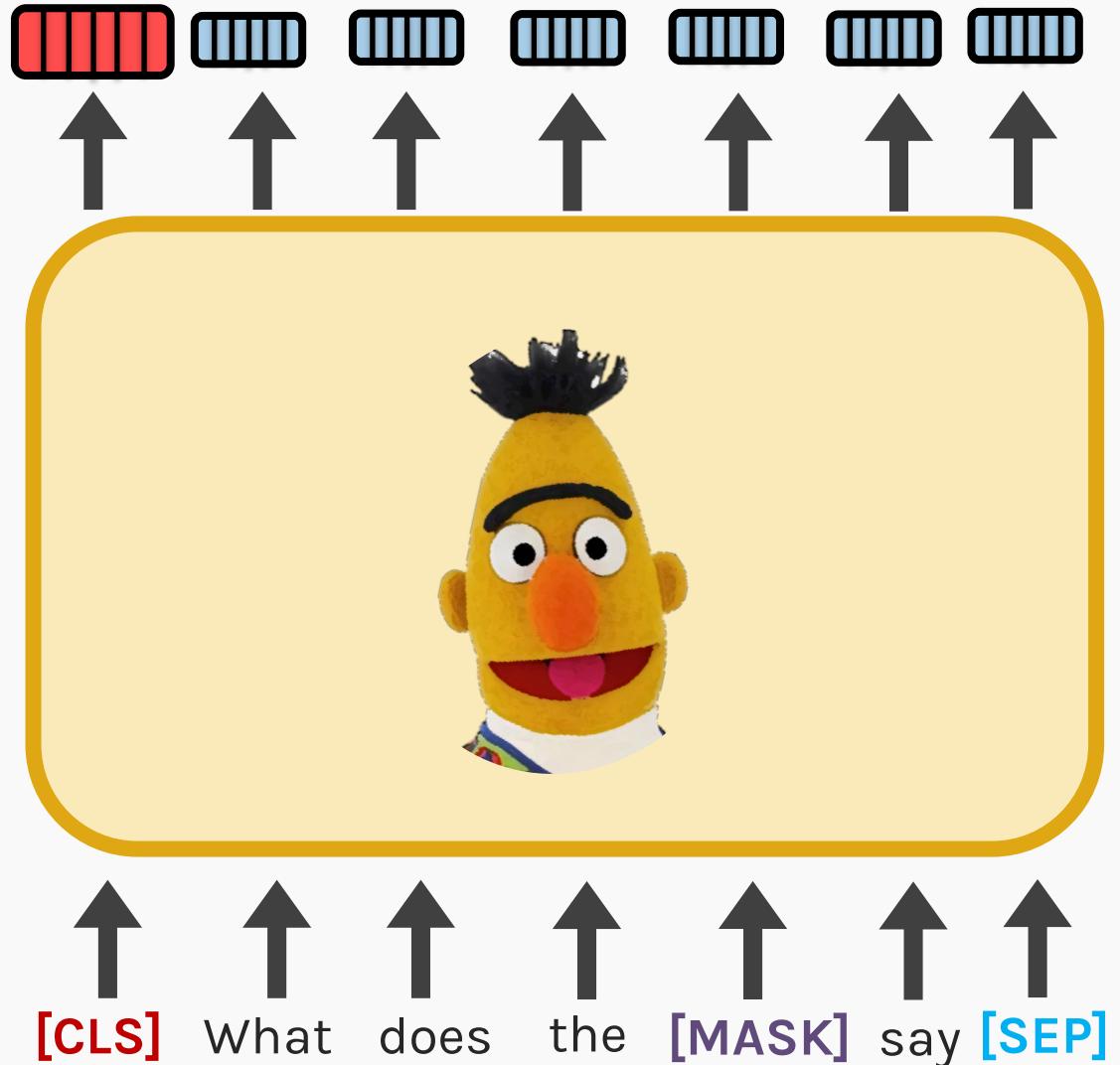
This is the last class. The professor will explain again



# How to train BERT?

## CLIFF NOTES

- Using a large corpus (e.g. wikipedia texts), we pre-train a BERT model for two tasks:
  - Masked word prediction
  - Next sentence prediction
- We train BERT with the two tasks simultaneously with a goal of minimizing the combined loss function
- The [MASK] tag is used for the language model task, and the [CLS] and [SEP] tag helps to train the sentence



# How to use a BERT?



# How to use a BERT?

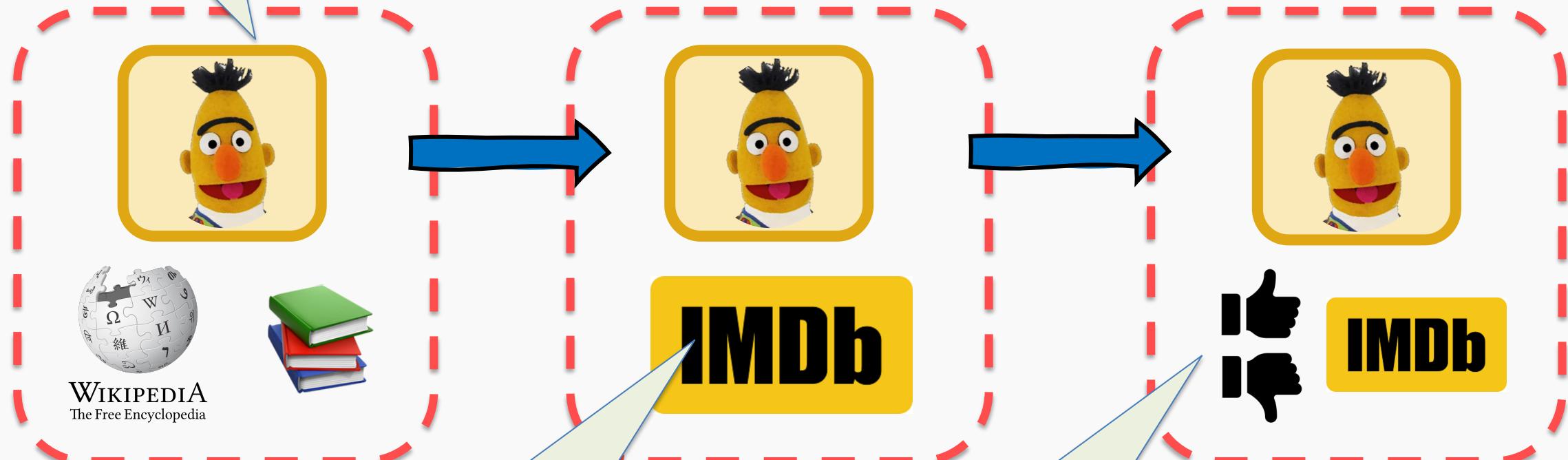
You will (almost)  
never train a BERT  
from scratch

There are three main steps in using BERT for a given NLP task

## Pre-training

## Fine-tuning

## Language tasks



We don't use the  
labels in the fine-  
tuning step

The final step is the  
supervised learning  
using labels



# How to use BERT?

BERT can be used for a wide variety of language tasks

## Classification tasks (e.g. Sentiment analysis):

Done by adding a classification layer on top of the Transformer output for the [CLS] token.

## Named Entity Recognition (NER)

Using BERT, a NER model can be trained by feeding the tokens into a classification layer that predicts the NER label.

More on this in my demo!  
Don't miss it!

## Question Answering tasks

Using BERT, a Q&A model can be trained by learning two extra vectors that mark the start and the end of the answer.



# Concluding remarks

## BERT ISSUES?

- The vanilla BERT (base) has **109,482,240** trainable parameters; with such a massive size, it can only be trained by large corporations with massive resources.
- The sheer size also makes it extremely slow to train.
- The fine-tuning is not straight-forward and requires lots of tweaks and experimentation (for e.g. you must use the same tokenizer used during pre-training).

Hey! I never said that I was perfect!

Vanilla BERT cannot be used for natural language generation (GPT can be used instead)



**THANK YOU**

PROTOPAPAS

