COMP6211I: Trustworthy Machine Learning

Lecture 4

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Course information

- Exam on next Monday (Feb 20) during the class time
- Remember to sign-up paper presentation sign-up
- Remember to submit project proposal (due on Feb 24) (1/2 page)
  - Don’t worry if you couldn’t find teammates

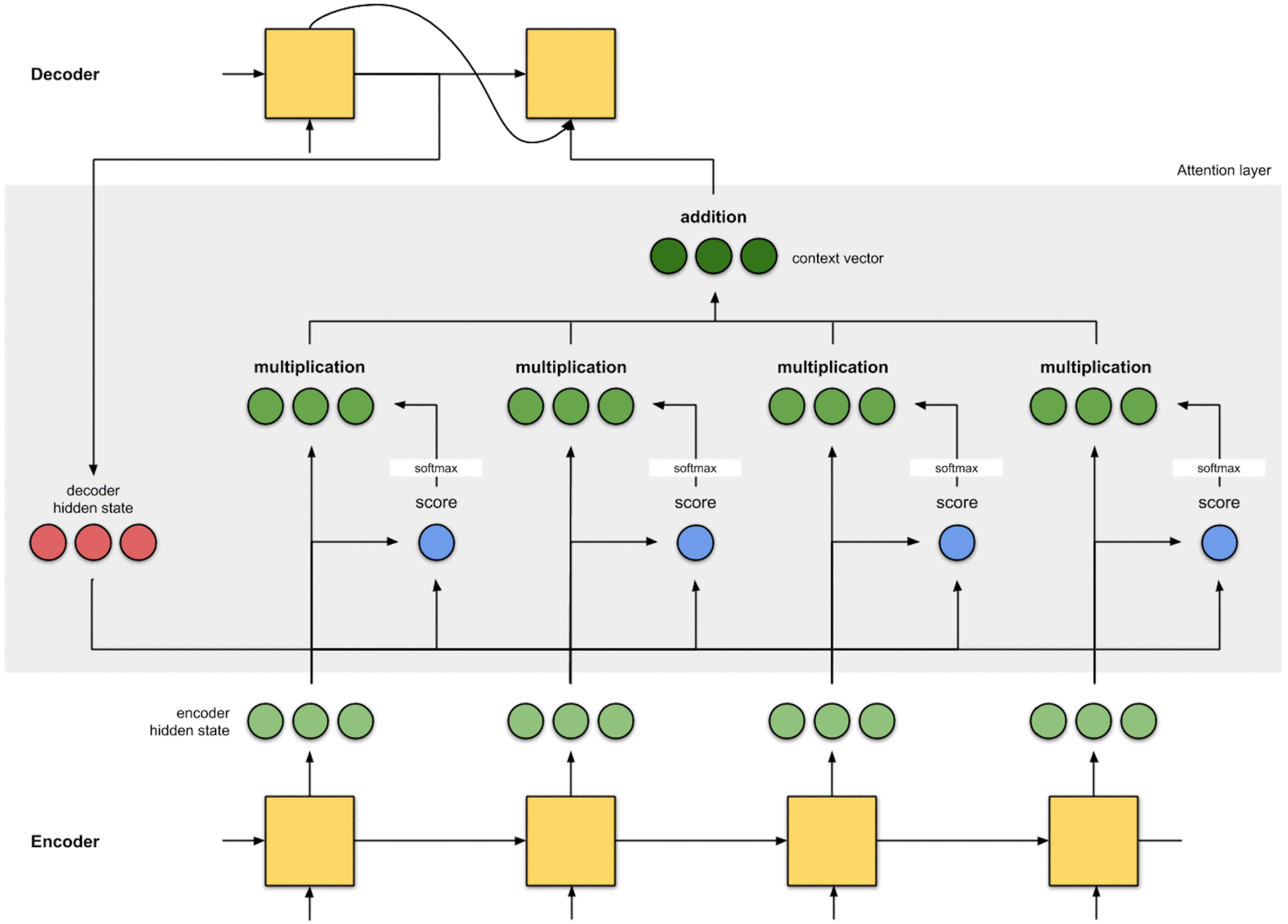
Recurrent Neural Network

Attention in NMT

- Usually, each output word is only related to a subset of input words (e.g., for machine translation)
- Let u be the current decoder latent state, $v_1, \ldots, v_n$ be the latent sate for each input word
- Compute the weight of each state by
  - $p = \text{Softmax}(u^T v_1, \ldots, u^T v_n)$
- Compute the context vector by $Vp = p_1 v_1 + \ldots + p_n v_n$

Recurrent Neural Network

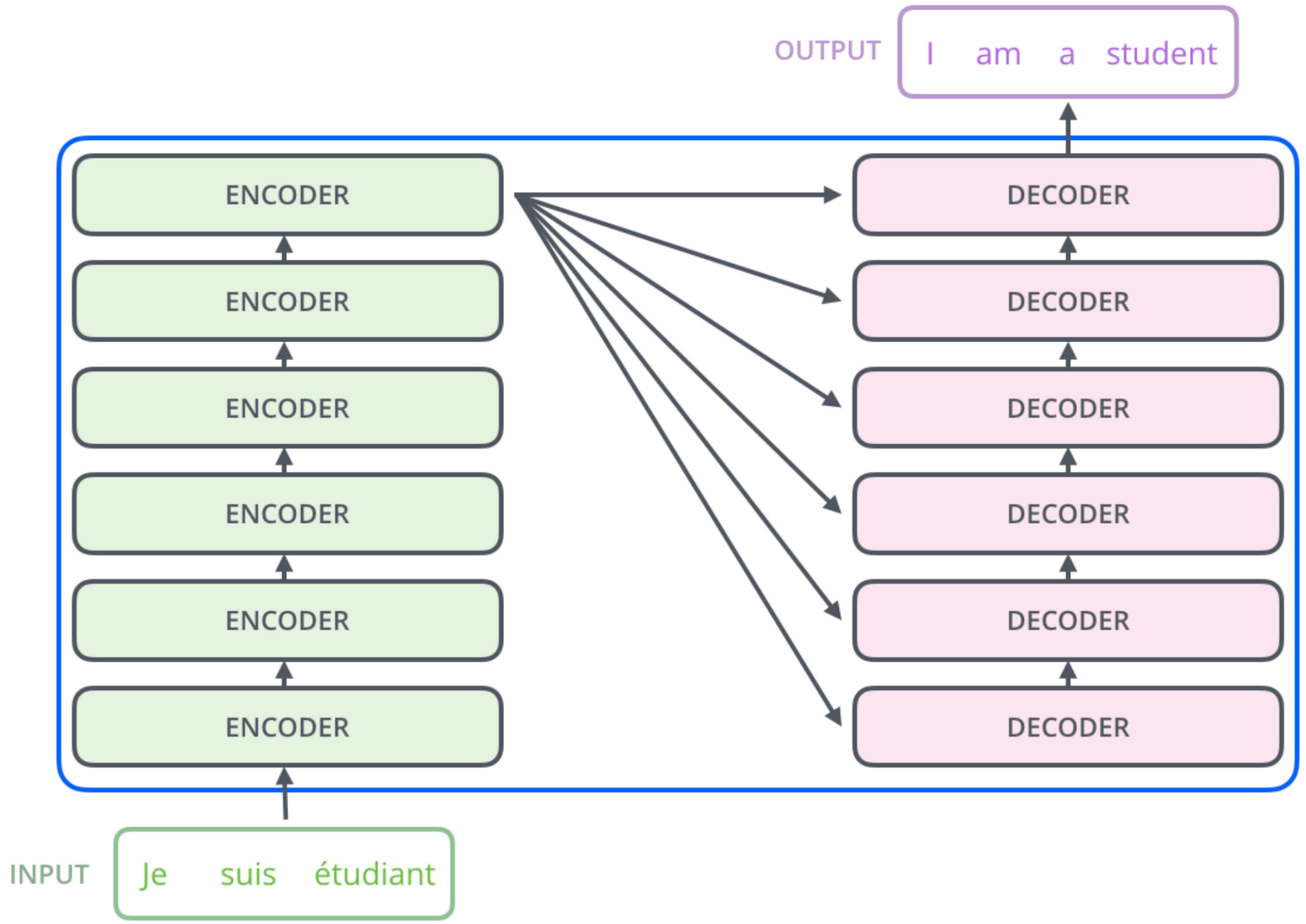
Attention in NMT



Transformer

Transformer

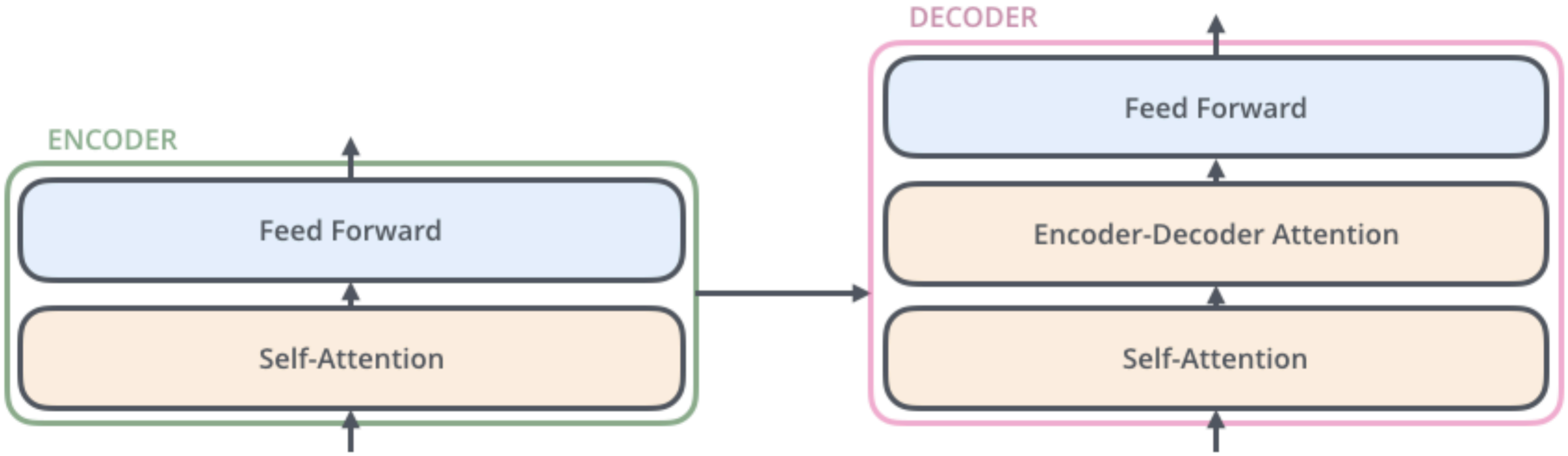
- An architecture that replies entirely on attention without using CNN/RNN
- Proposed in ``Attention Is All You Need'' (Vaswani et al., 2017)
- Initially used for neural machine translation



Transformer

Encoder and Decoder

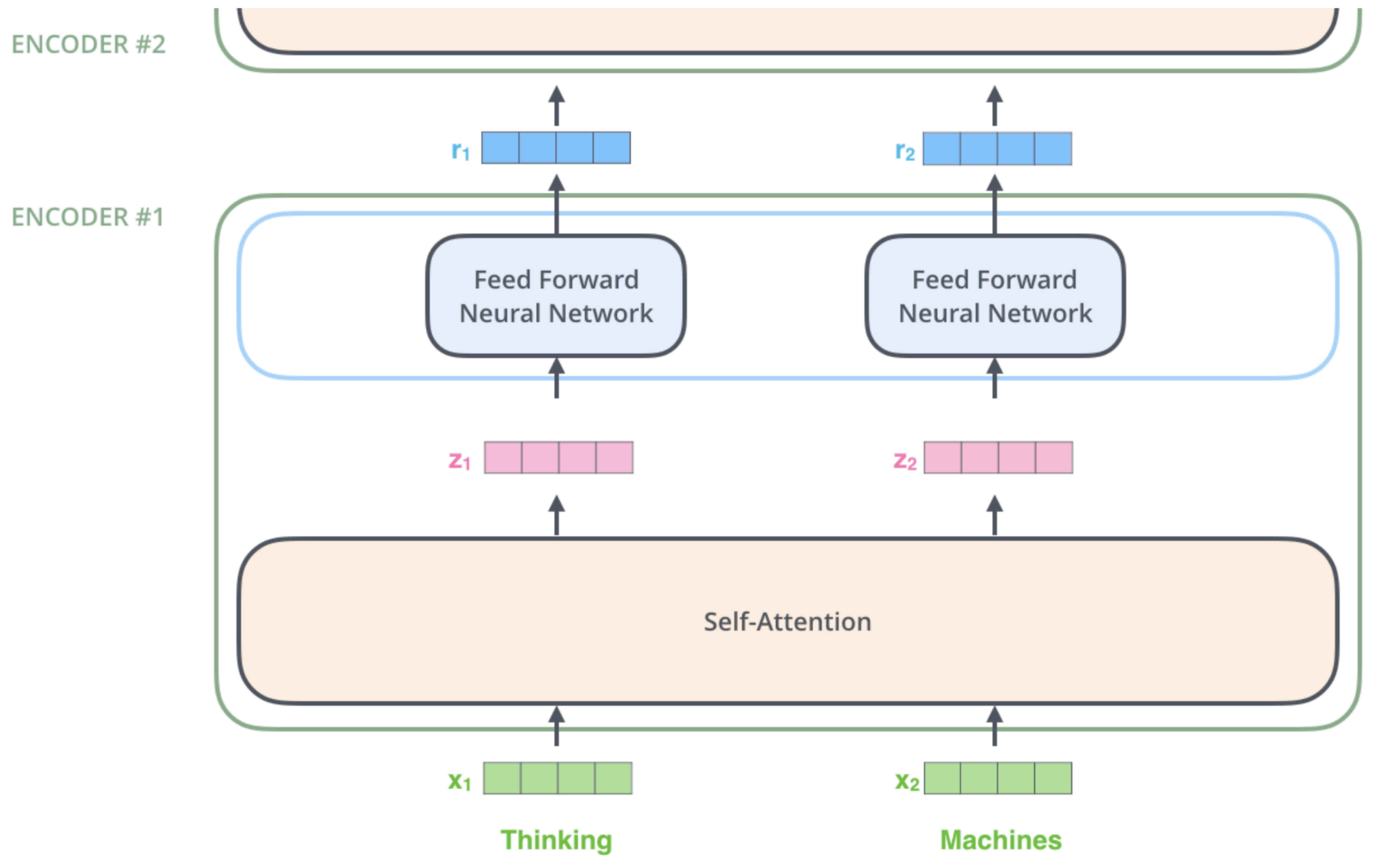
- Self attention layer: the main architecture used in Transformer
- Decoder: will have another attention layer to help it focuses on relevant parts of input sentences.



Transformer

Encoder

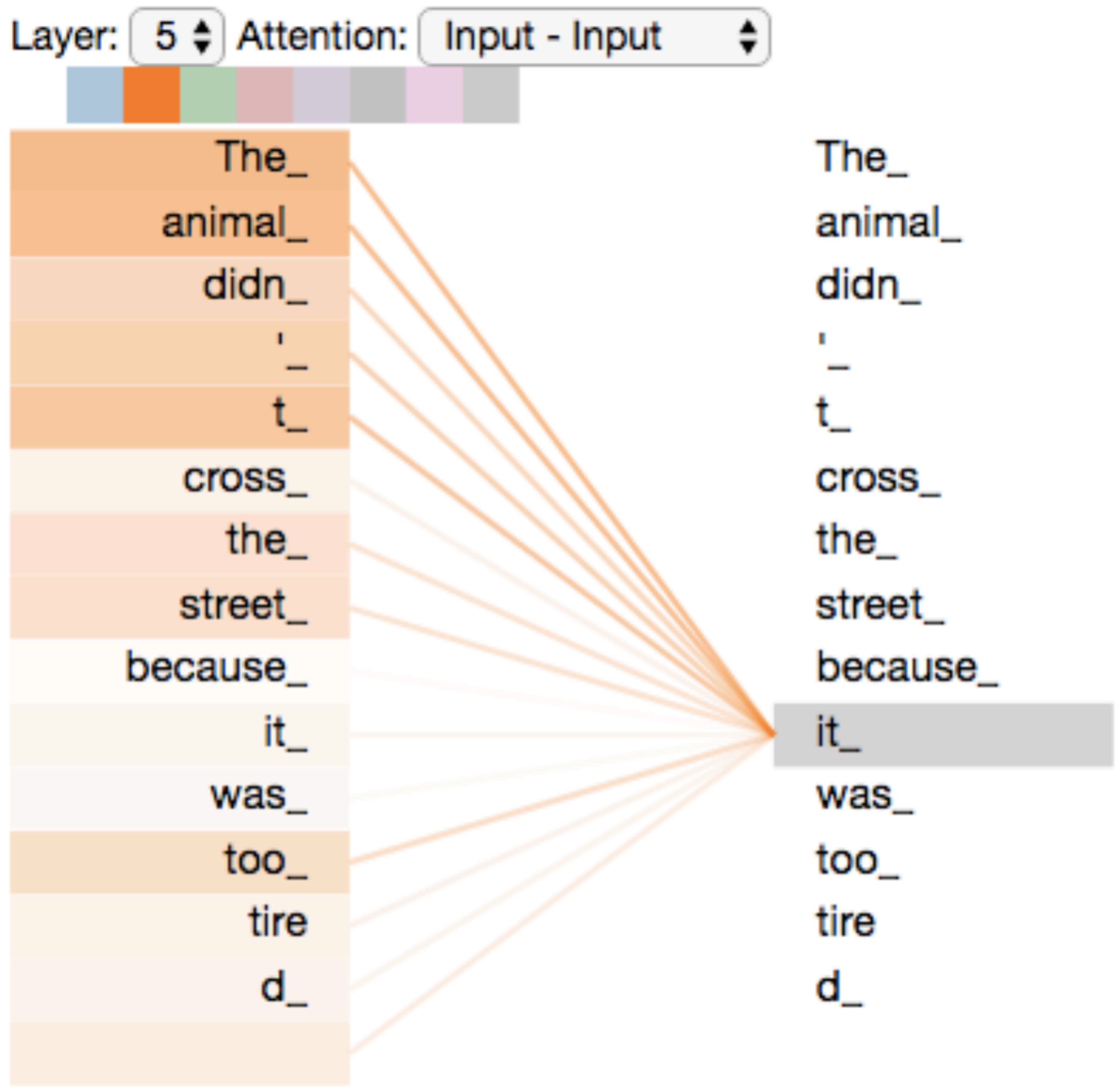
- Each word has a corresponding ``latent vector'' (initially the word embedding for each word)
- Each layer of encoder:
    - Receive a list of vectors as input
    - Passing these vectors to a self-attention layer
    - Then passing them into a feed-foward layer
    - Output a list of vectors



Transformer

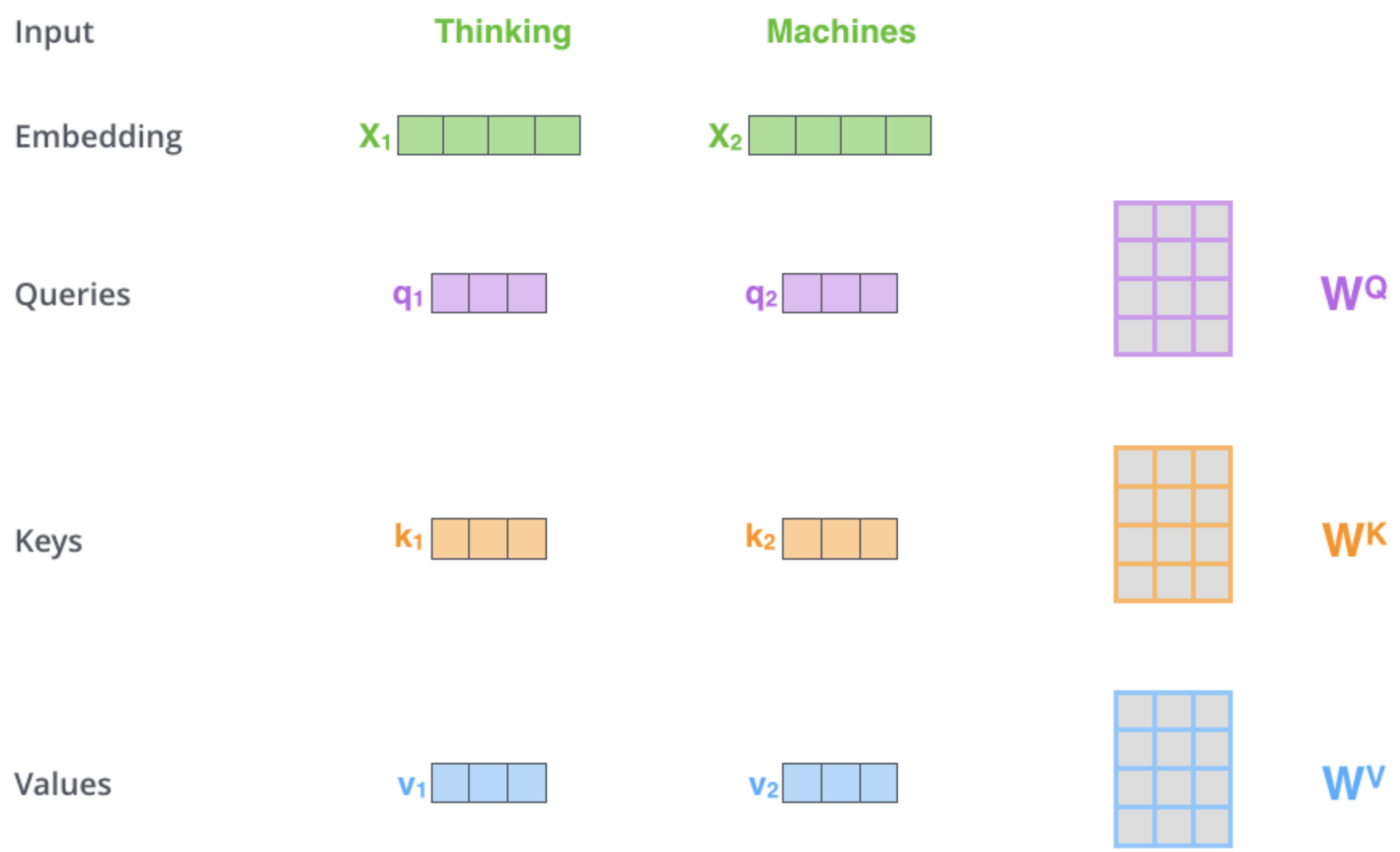
Self-attention layer

- Main idea: The actual meaning of each word may be related to other words in the sentence
- The actual meaning (latent vector) of each word is a weighted (attention) combination of other words (latent vectors) in the sentences



Transformer
Self-attention layer

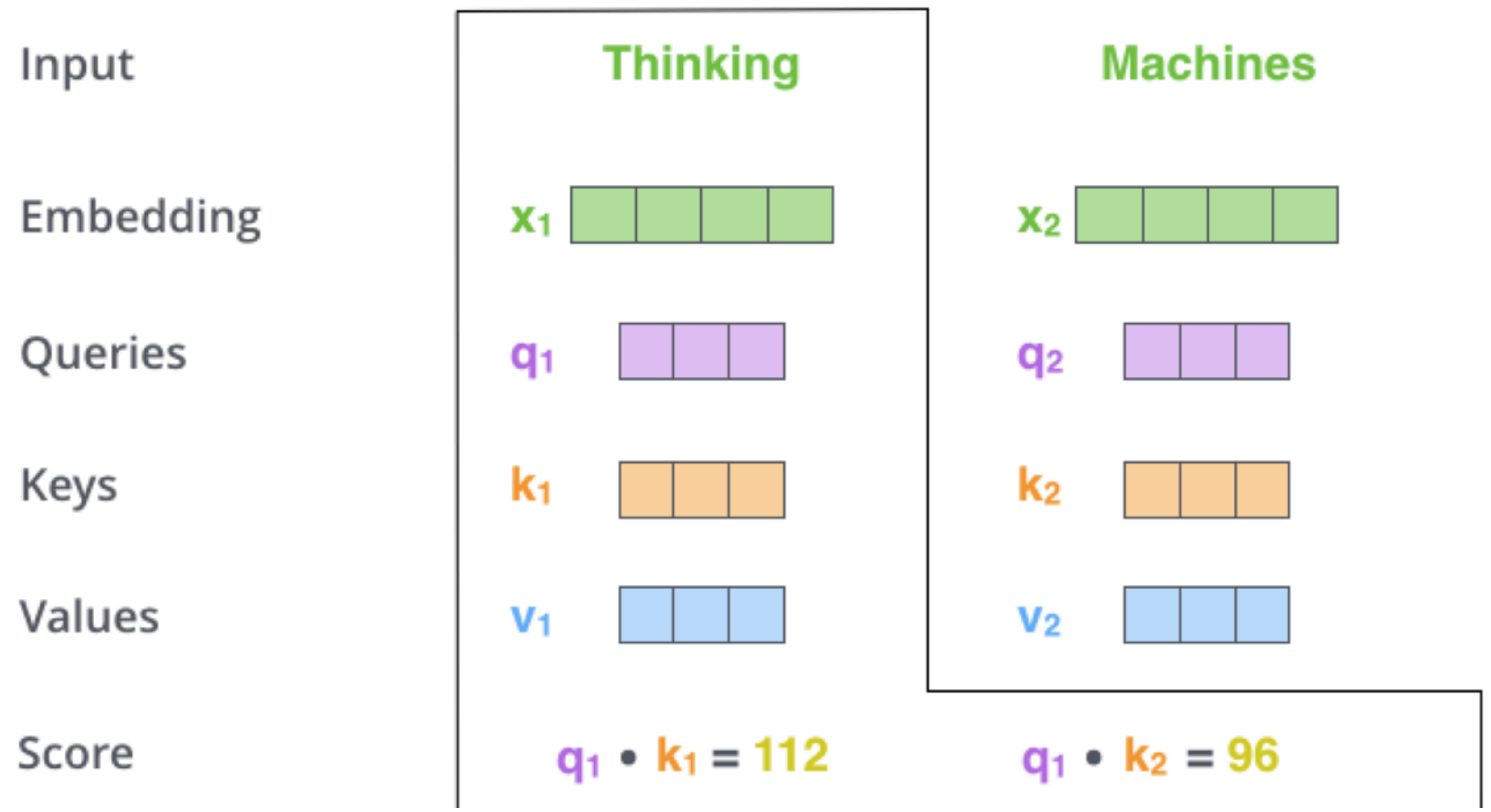
- Input latent vectors: $x_1, \ldots, x_n$
- Self-attention parameters: W^Q, W^K, W^V (weights for query, key, value)
- For each word i, compute
    - Query vector: $q_i = x_i W^Q$
    - Key vector: $k_i = x_i W^K$
    - Value vector: $v_i = x_i W^V$



Transformer

Self-attention layer

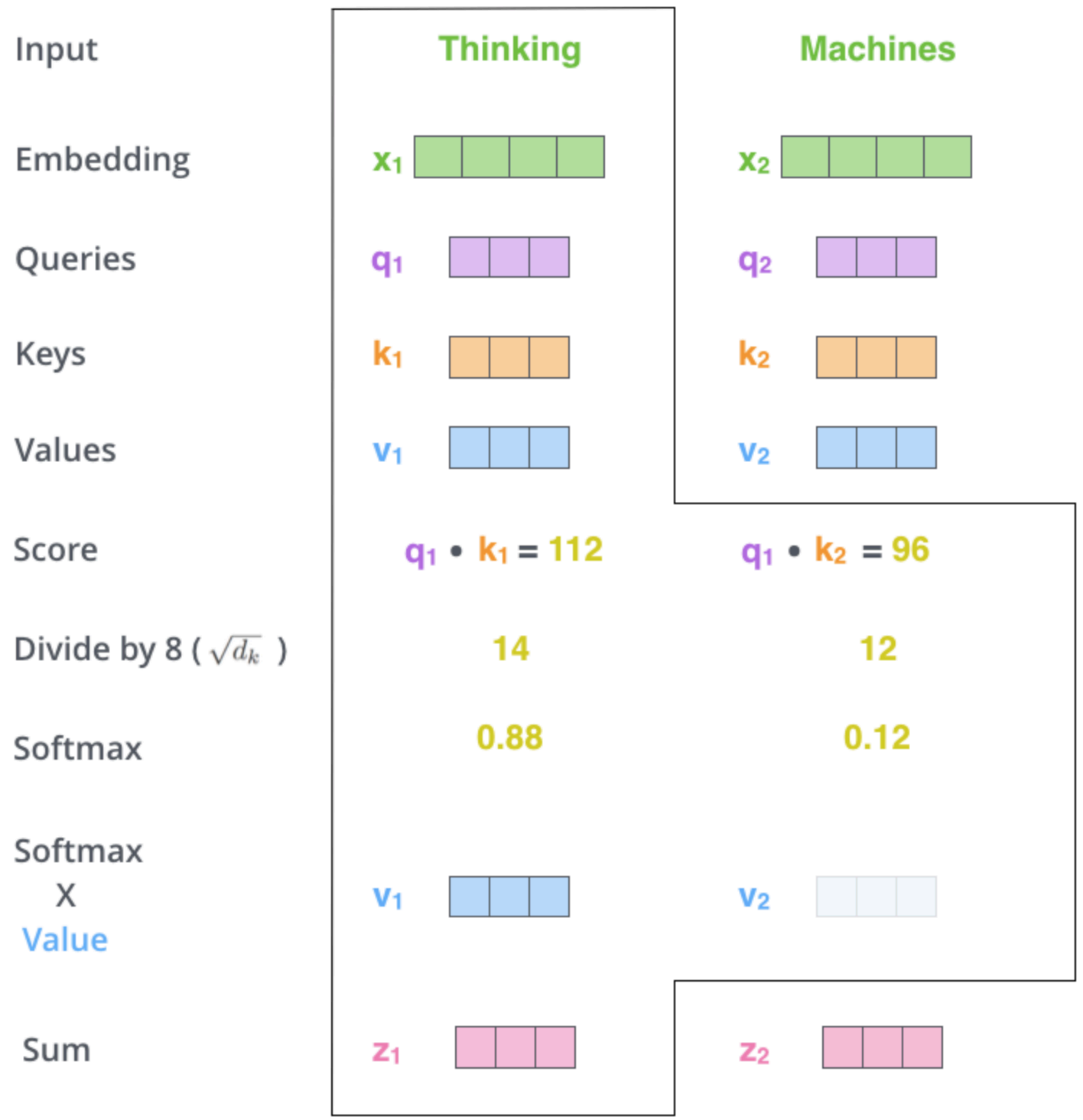
- For each word i, compute the scores to determine how much focus to place on other input words
  - The attention score for word j to word i: $q_i^T k_j$



Transformer

Self-attention layer

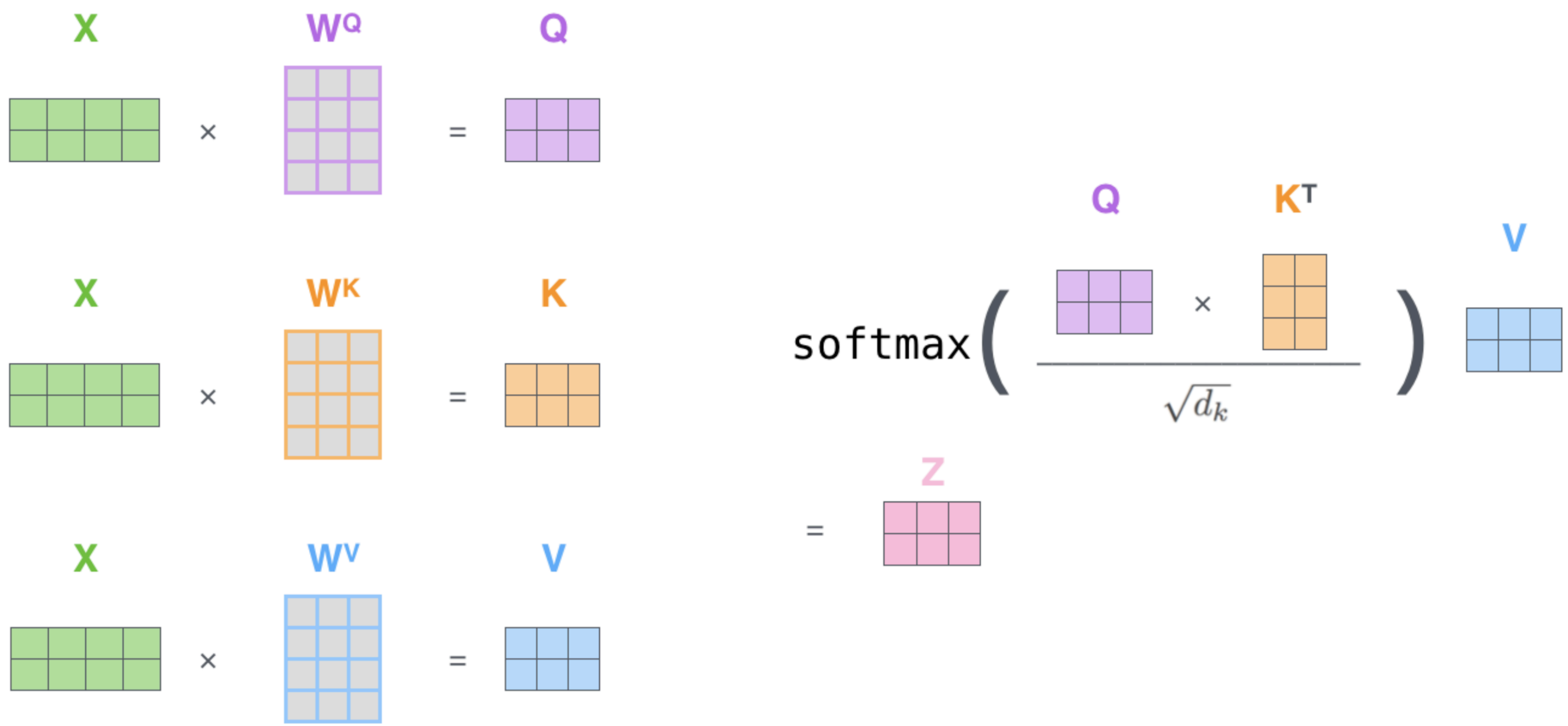
- For each word i, the output vector
  - $\sum_j s_{ij} v_j, \quad s_i = \text{softmax}(q_i^T k_1, \ldots, q_i^T k_n)$



Transformer

Matrix form

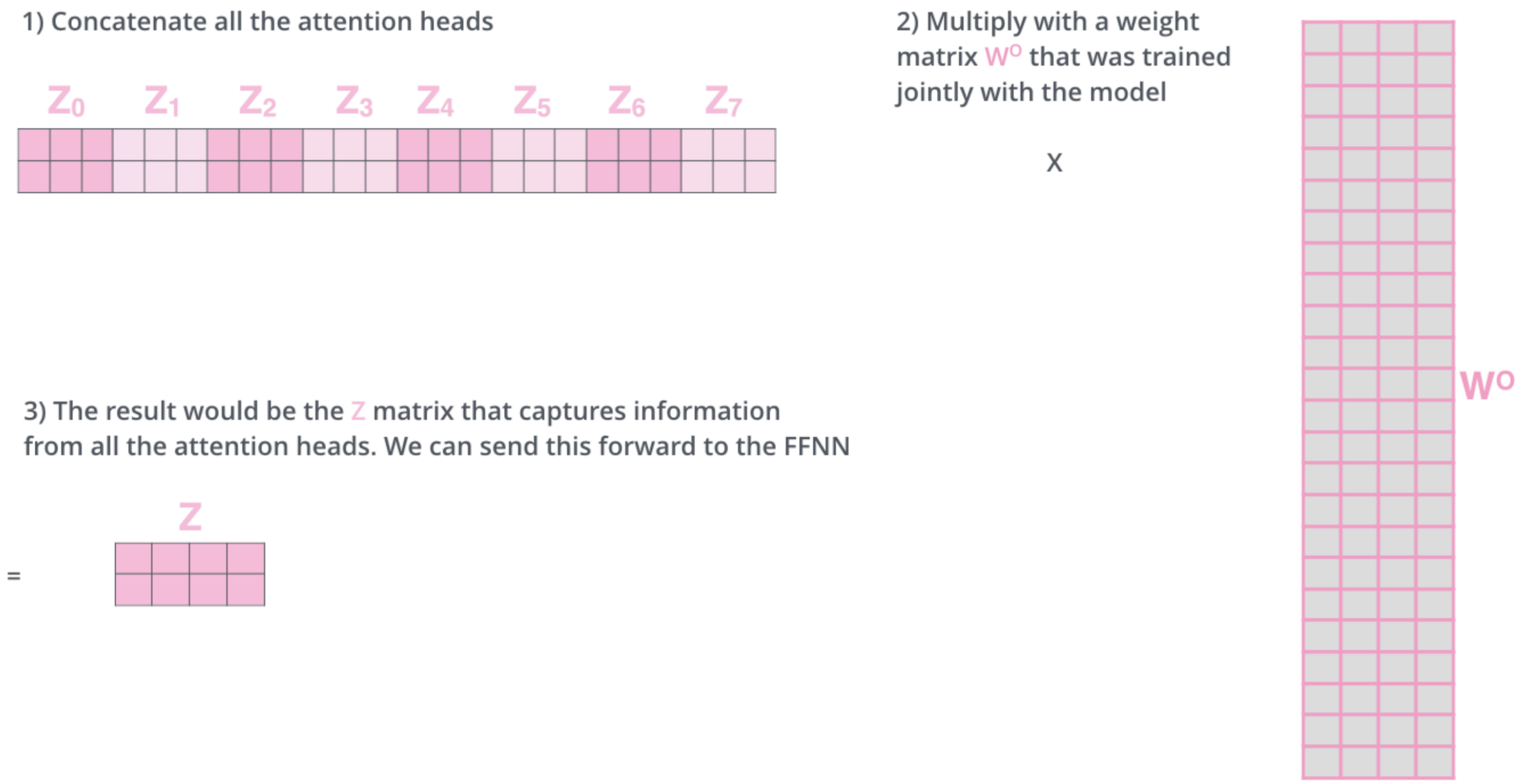
- $Q = XW^Q,\ K = XW^K,\ V = XW^V,\ \ Z = \text{softmax}(QK^T)V$



Transformer

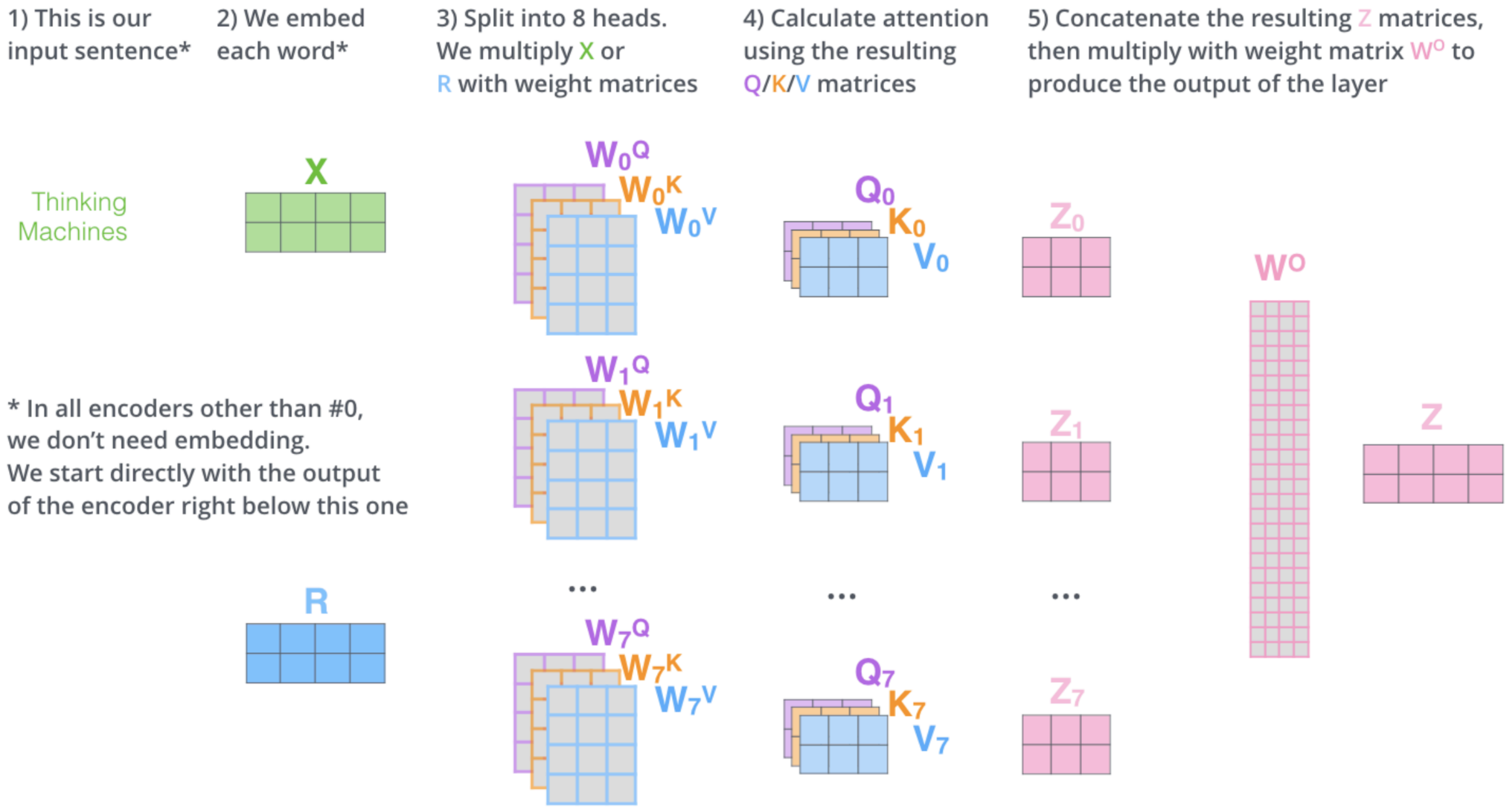
Multiply with weight matrix to reshape

- Gather all the outputs $Z_1, \ldots, Z_k$
- Multiply with a weight matrix to reshape
- Then pass to the next fully connected layer



Transformer

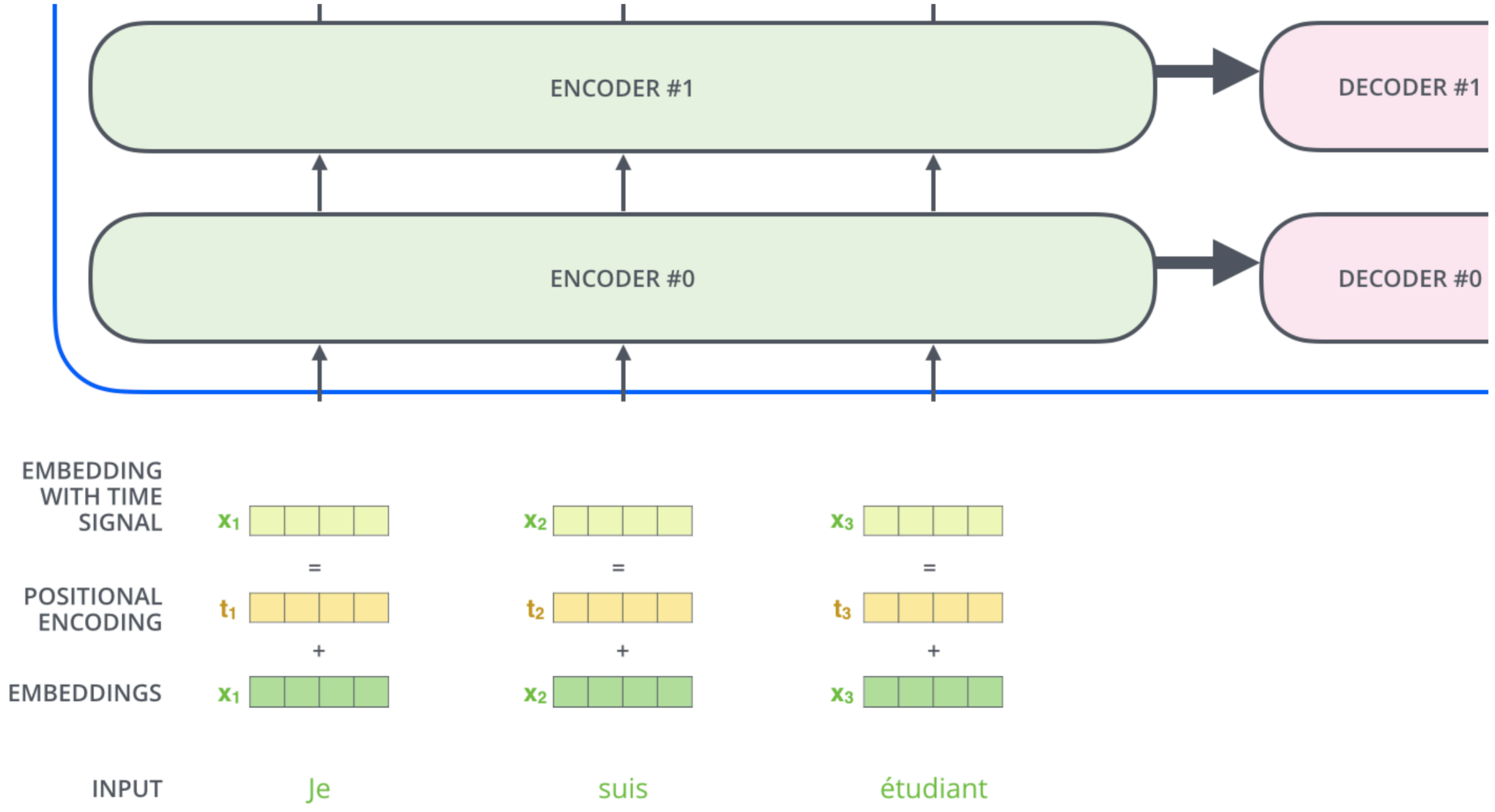
Overall architecture



Transformer

Sinusoidal Position Encoding

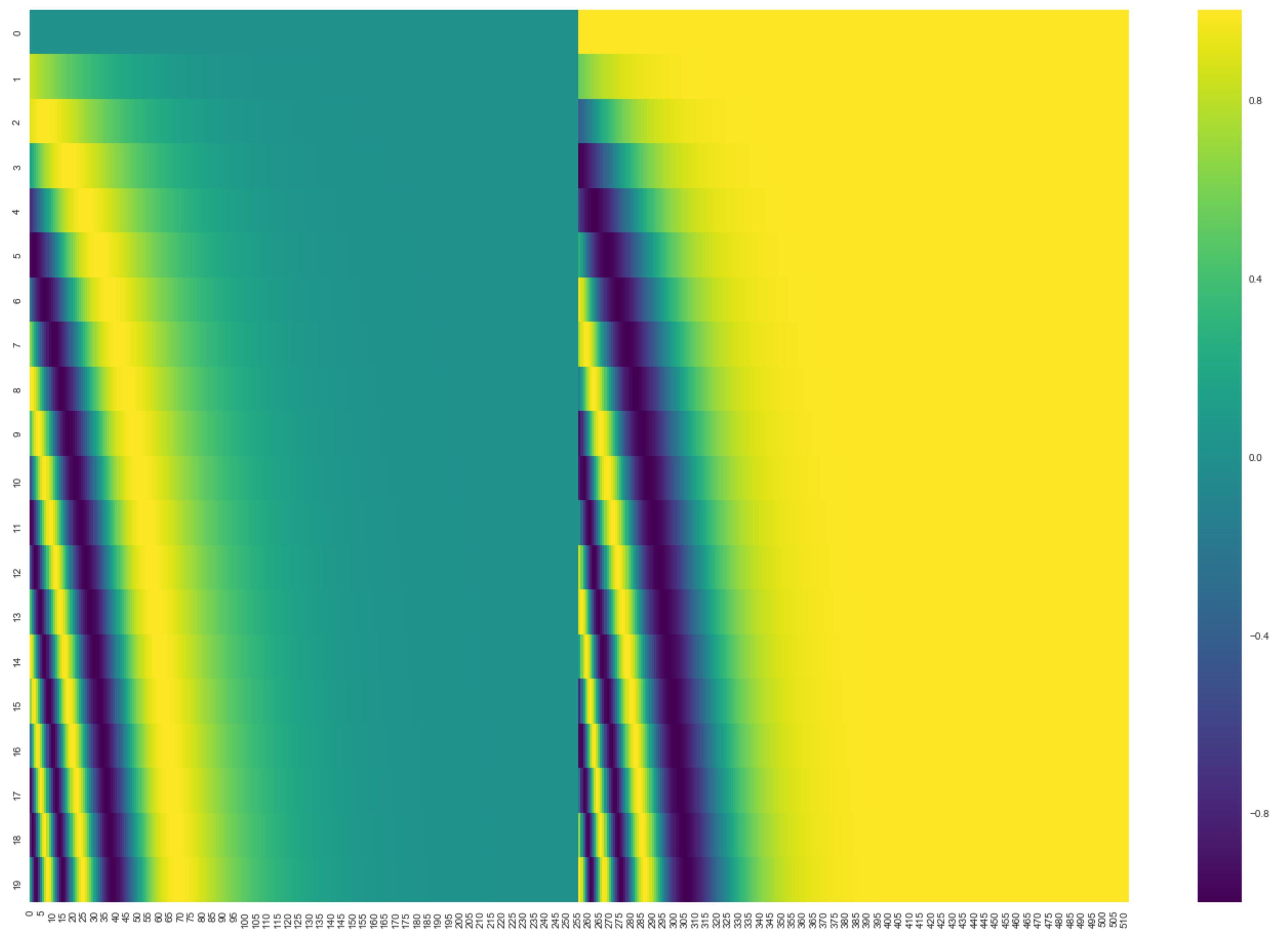
- The above architecture ignores the sequential information
- Add a positional encoding vector to each x_i (according to i)



Transformer

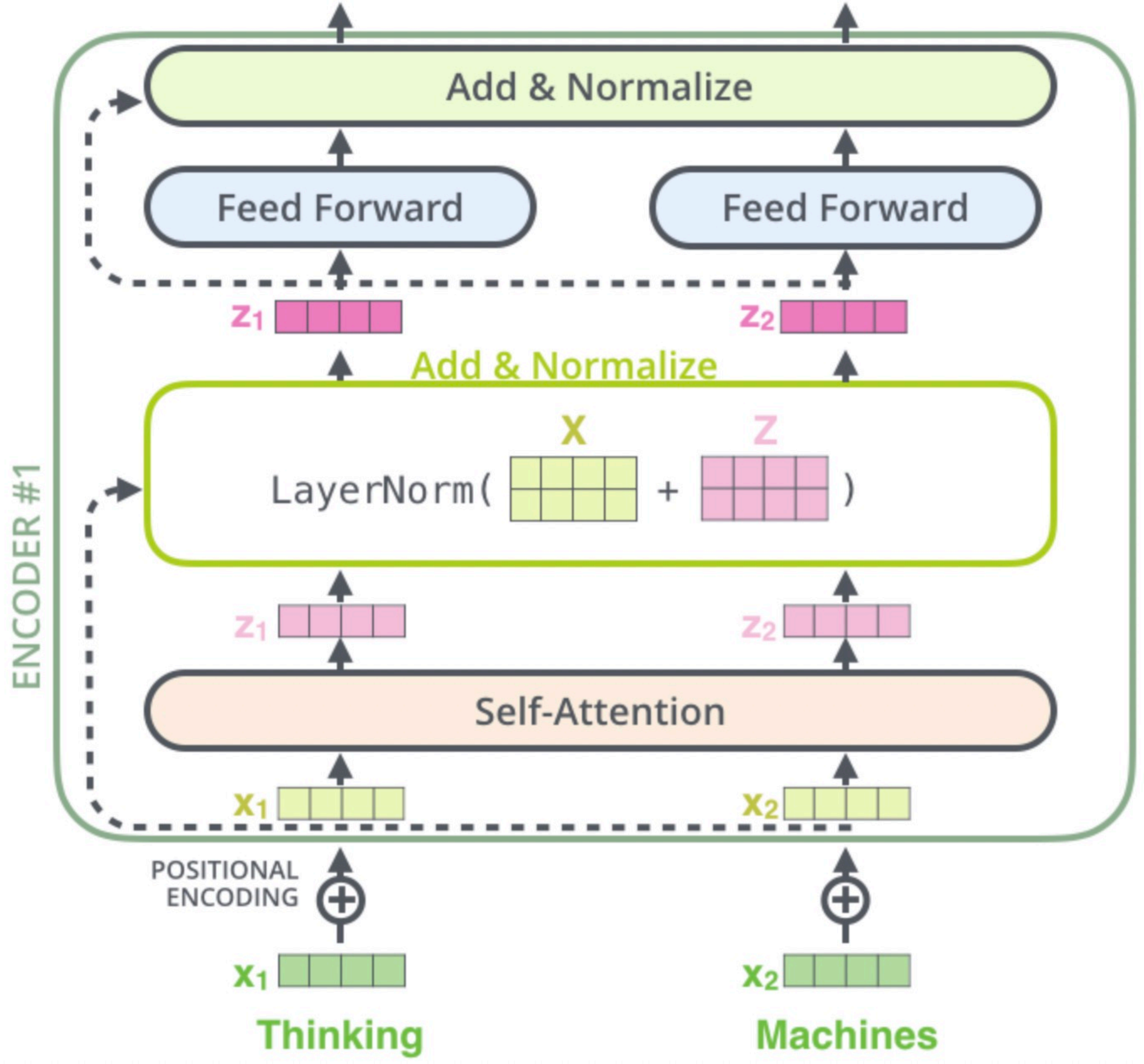
Positional Embedding

- Sin/cosine functions with different wavelengths (used in the original Transformer)
- The jth dimension of ith token $p_i[j] = \begin{cases} \sin(i \cdot c^{\frac{j}{d}}) \text{ if j is even} \\ \cos(i \cdot c^{\frac{j-1}{d}}) \text{ if j is odd} \end{cases}$
- smooth, parameter-free, inductive

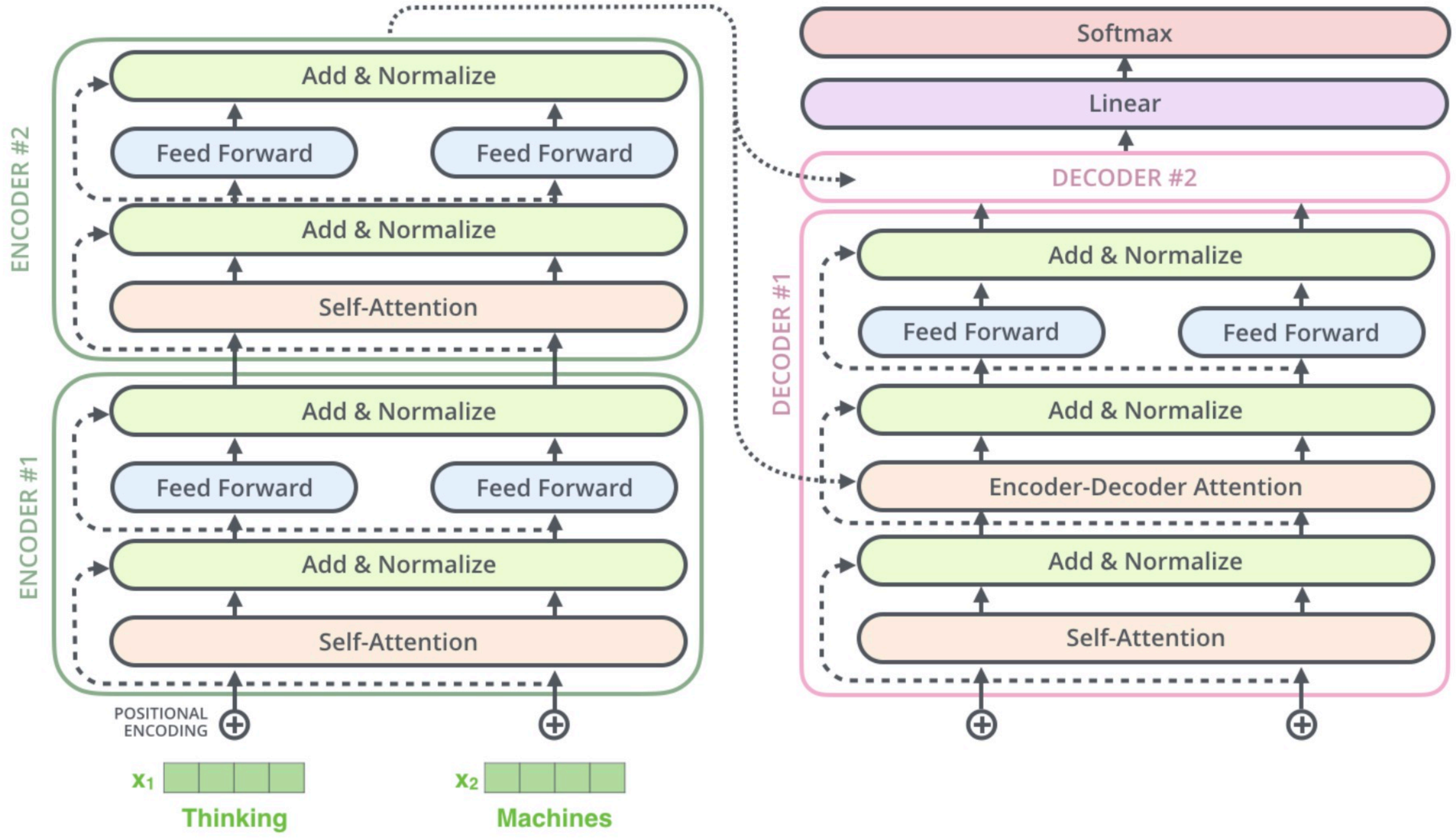


Transformer

Residual



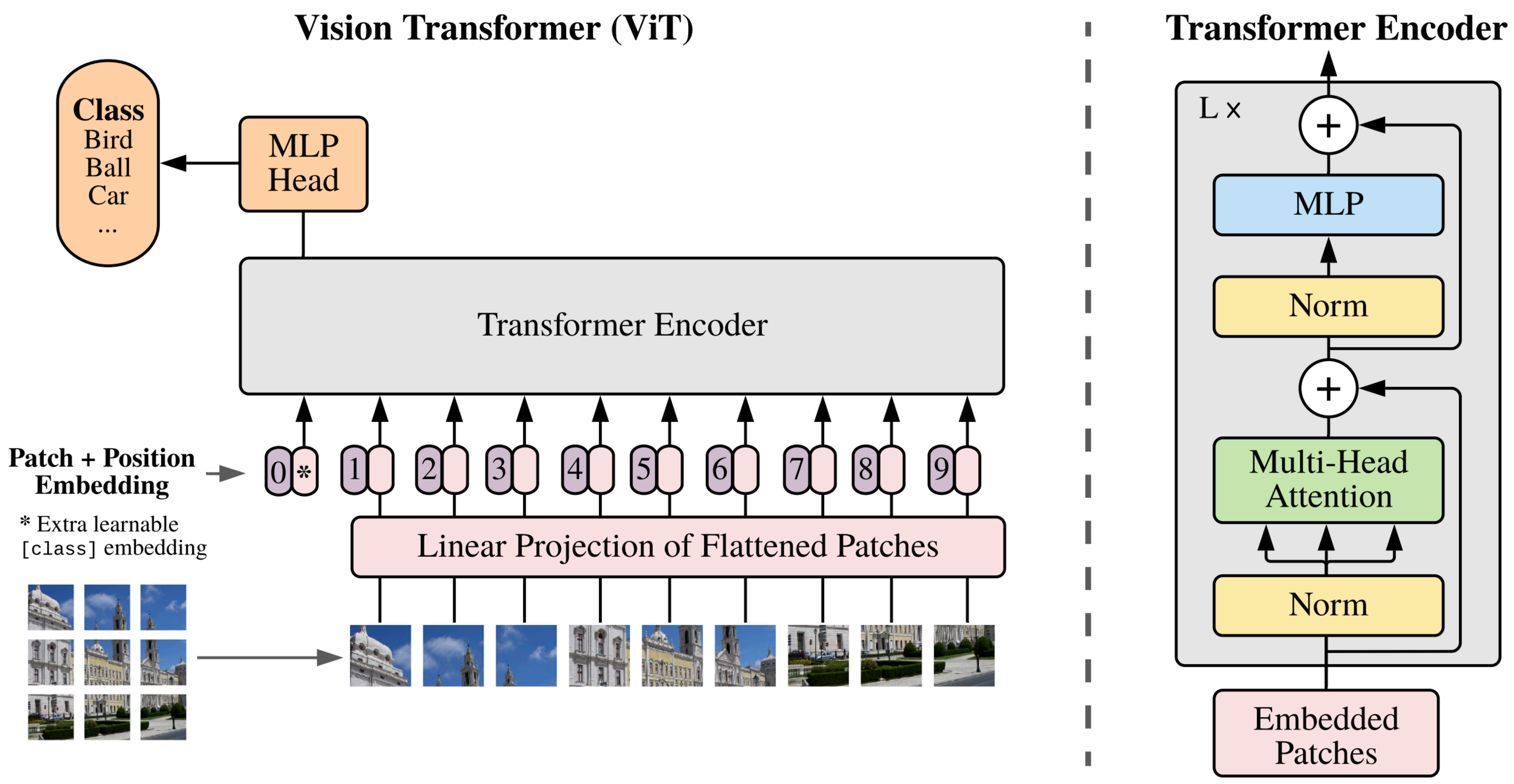
Transformer
Whole framework



Vision Transformer (ViT)

Vision Transformer (ViT)

- Partition input image into $K \times K$ patches
- A linear projection to transform each patch to feature (no convolution)
- Pass tokens into Transformer



Vision Transformer (ViT)

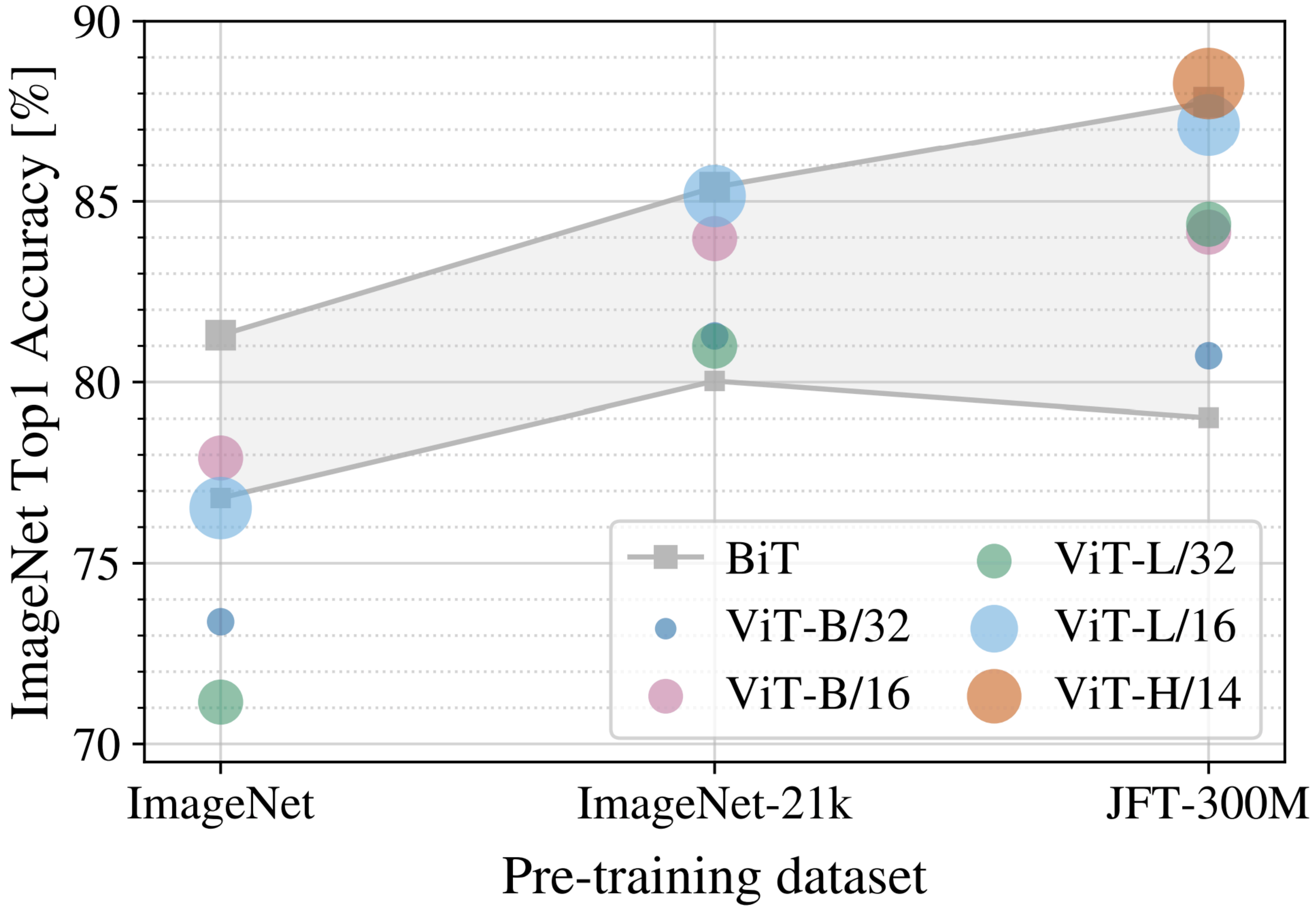
Vision Transformer (ViT)

- Patches are non-overlapping in the original ViT
- $N \times N$ image $\Rightarrow (N/K)^2$ tokens
- Smaller patch size $\Rightarrow$ more input tokens
    - Higher computation (memory) cost, (usually) higher accuracy
- Use 1D (learnable) positional embedding
- Inference with higher resolution:
    - Keep the same patch size, which leads to longer sequence
    - Interpolation for positional embedding

Vision Transformer (ViT)

ViT Performance

- ViT outperforms CNN with large pretraining



Vision Transformer (ViT)

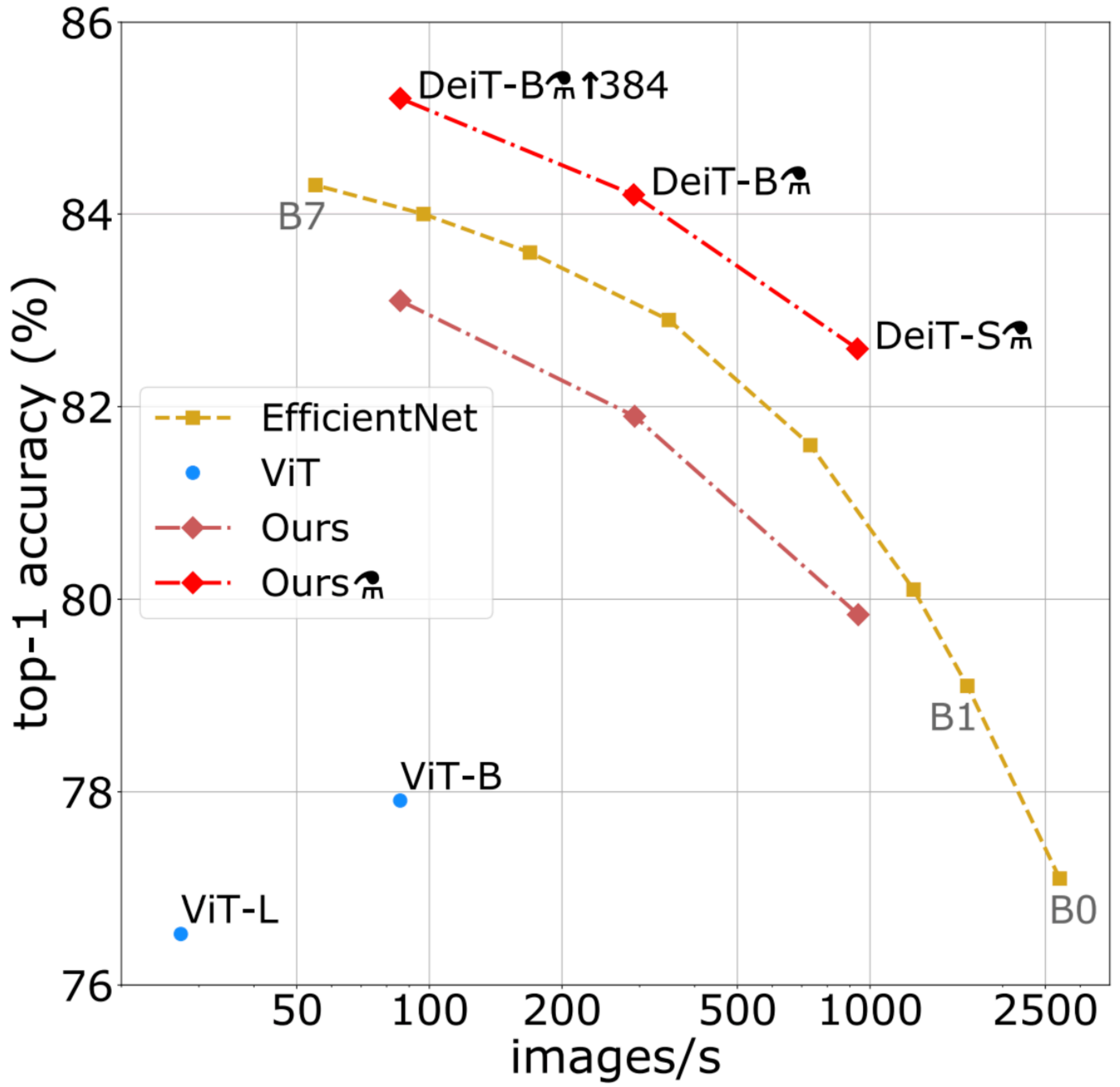
ViT Performance

- Attention maps of ViT (to input)

Vision Transformer (ViT)

ViT v.s. ResNet

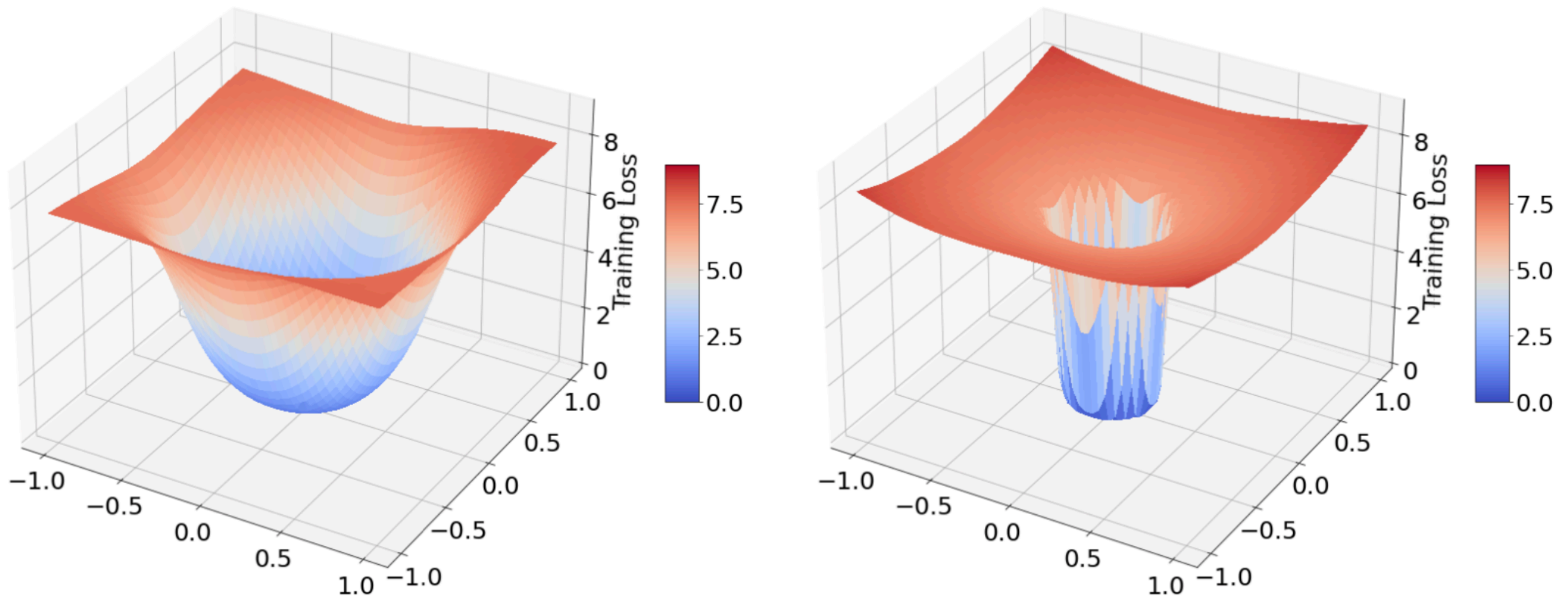
- Can ViT outperform ResNet on ImageNet without pretraining?
- Deit (Touvron et al., 2021):
  - Use very strong data augmentation
  - Use a ResNet teacher and distill to ViT



Vision Transformer (ViT)

ViT v.s. ResNet

- ViT tends to converge to sharper regions than ResNet



(a) ResNet

Leading eigenvalue of Hessian: 179.8

(b) ViT

Leading eigenvalue of Hessian: 738.8

Vision Transformer (ViT)

``Sharpness'' is related to generalization

- Testing can be viewed as a slightly perturbed training distribution
- Sharp minimum ⇒ performance degrades significantly from training to testing

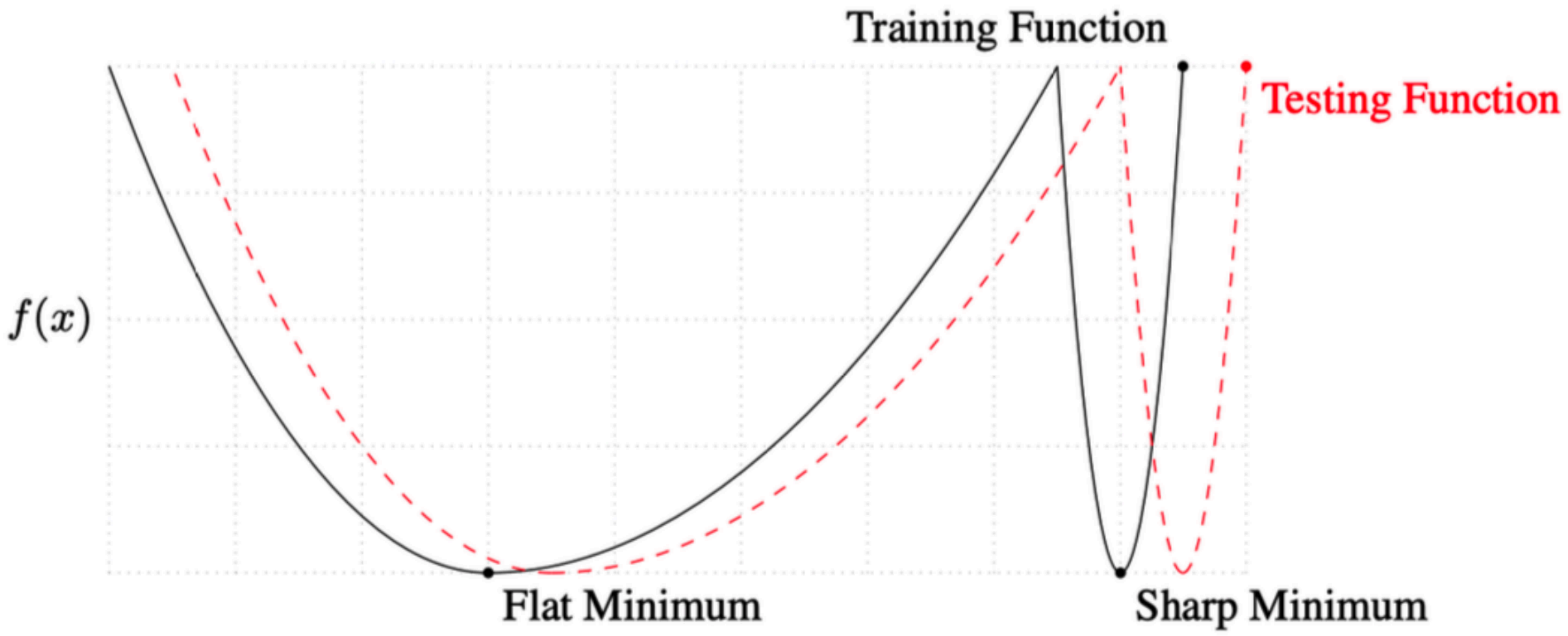


Figure from (Keskar et al., 2017)

Vision Transformer (ViT)

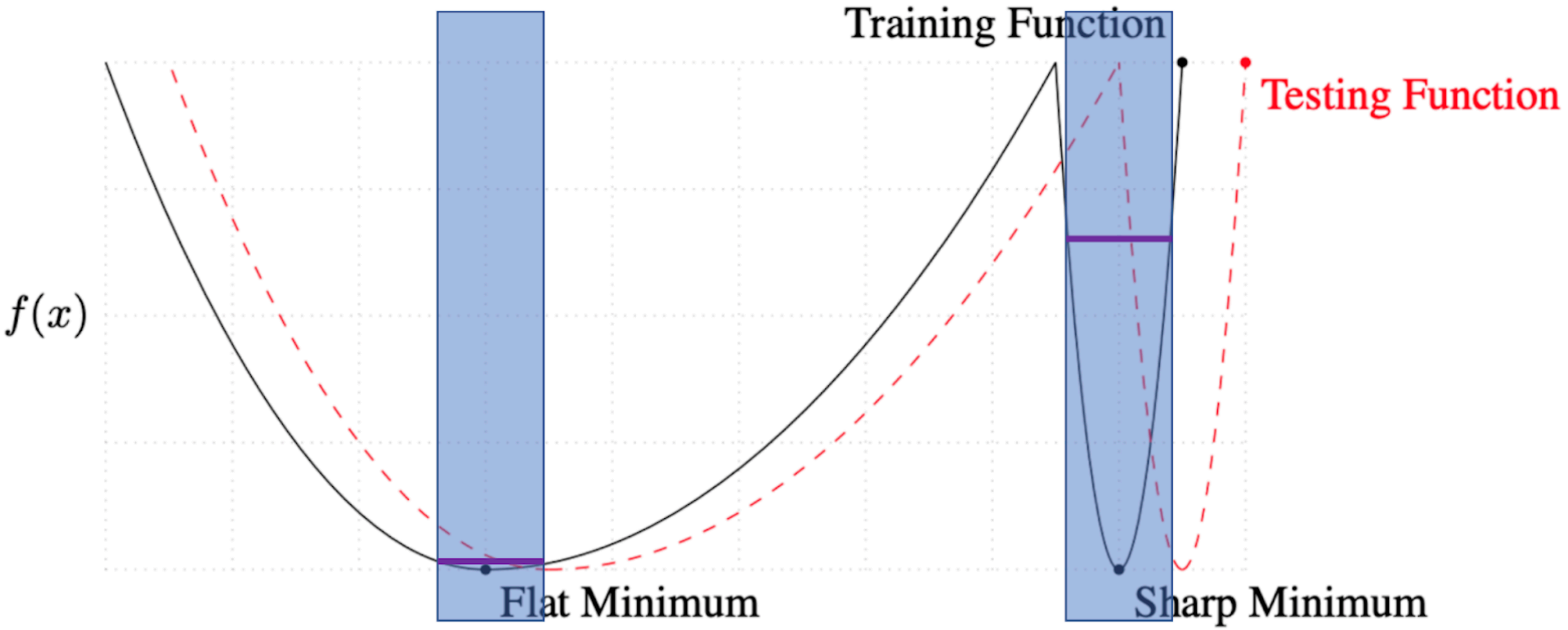
Sharpness Aware Minimization (SAM)

- Optimize the worst-case loss within a small neighborhood
    - $\min_{w} \max_{\|\delta\|_2 \leq \epsilon} L(w + \delta)$
    - ϵ is a small constant (hyper-parameter)
- Use 1-step gradient ascent to approximate inner max:
    - $\hat{\delta} = \arg \max_{\|\delta\|_2 \leq \epsilon} L(w) + \nabla L(w)^T \delta = \epsilon \frac{\nabla L(w)}{\|\nabla L(w)\|}$
- Conduct the following update for each iteration:
    - $w \leftarrow w - \alpha \nabla L(w + \hat{\delta})$

Vision Transformer (ViT)

Sharpness Aware Minimization (SAM)

- SAM is a natural way to penalize sharpness region (but requires some computational overhead)



Unsupervised pertaining for NLP

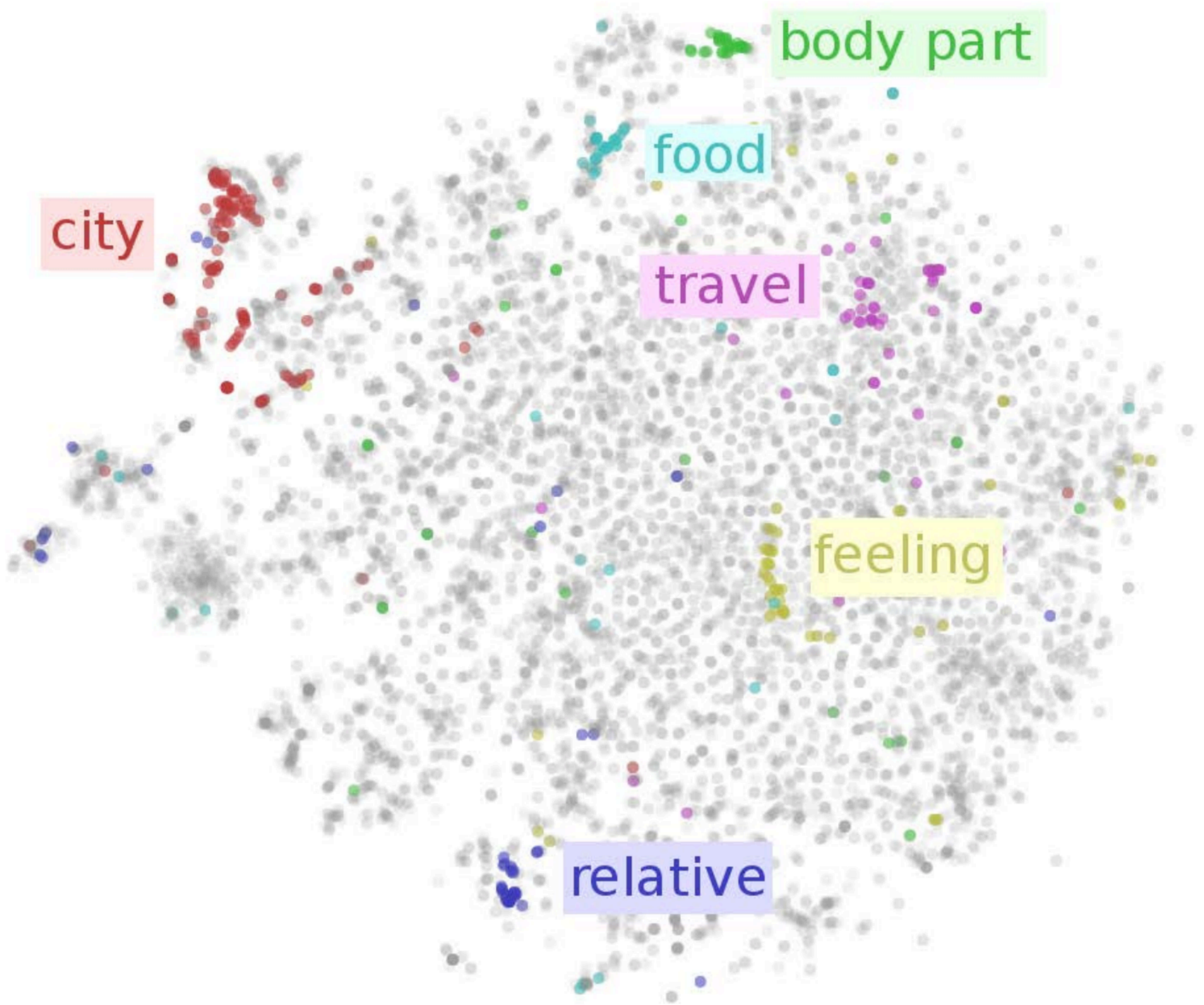
Motivation

- Many unlabeled NLP data but very few labeled data
- Can we use large amount of unlabeled data to obtain meaningful representations of words/sentences?

Unsupervised pertaining for NLP

Learning word embeddings

- Use large (unlabeled) corpus to learn a useful word representation
  - Learn a vector for each word based on the corpus
  - Hopefully the vector represents some semantic meaning
  - Can be used for many tasks
    - Replace the word embedding matrix for DNN models for classification/translation
  - Two different perspectives but led to similar results:
    - Glove (Pennington et al., 2014)
    - Word2vec (Mikolov et al., 2013)



Unsupervised pertaining for NLP

Context information

- Given a large text corpus, how to learn low-dimensional features to represent a word?

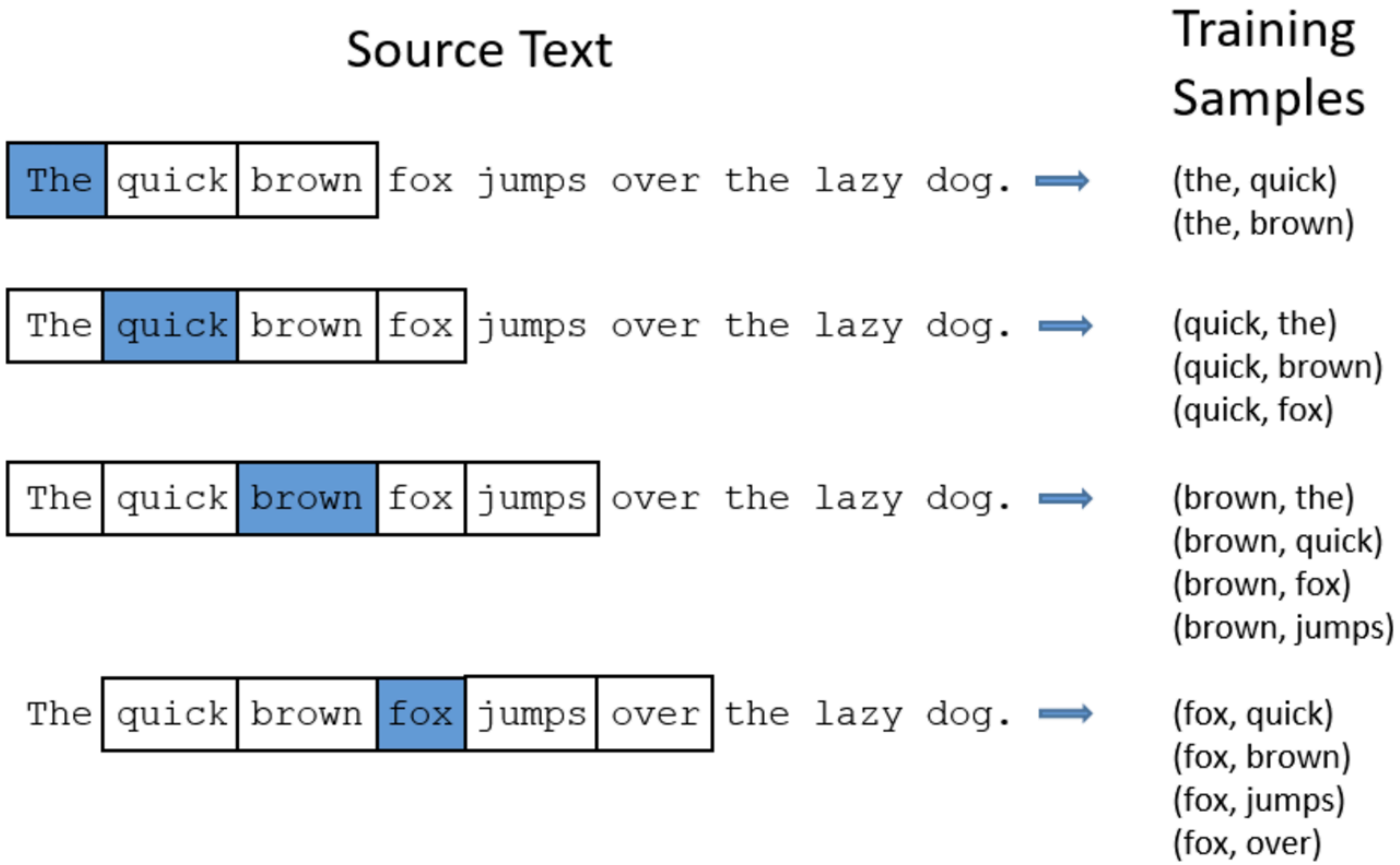
- For each word w_i, define the ``contexts'' of the word as the words surrounding it in an L-sized window:

- $$w_{i-L-2}, w_{i-L-1}, \underbrace{w_{i-L}, \cdots, w_{i-1}}_{\text{contexts of } w_i}, w_i, \underbrace{w_{i+1}, \cdots, w_{i+L}}_{\text{contexts of } w_i}, w_{i+L+1}, \cdots$$

- Get a collection of (word, context) pairs, denoted by D.

Unsupervised pertaining for NLP

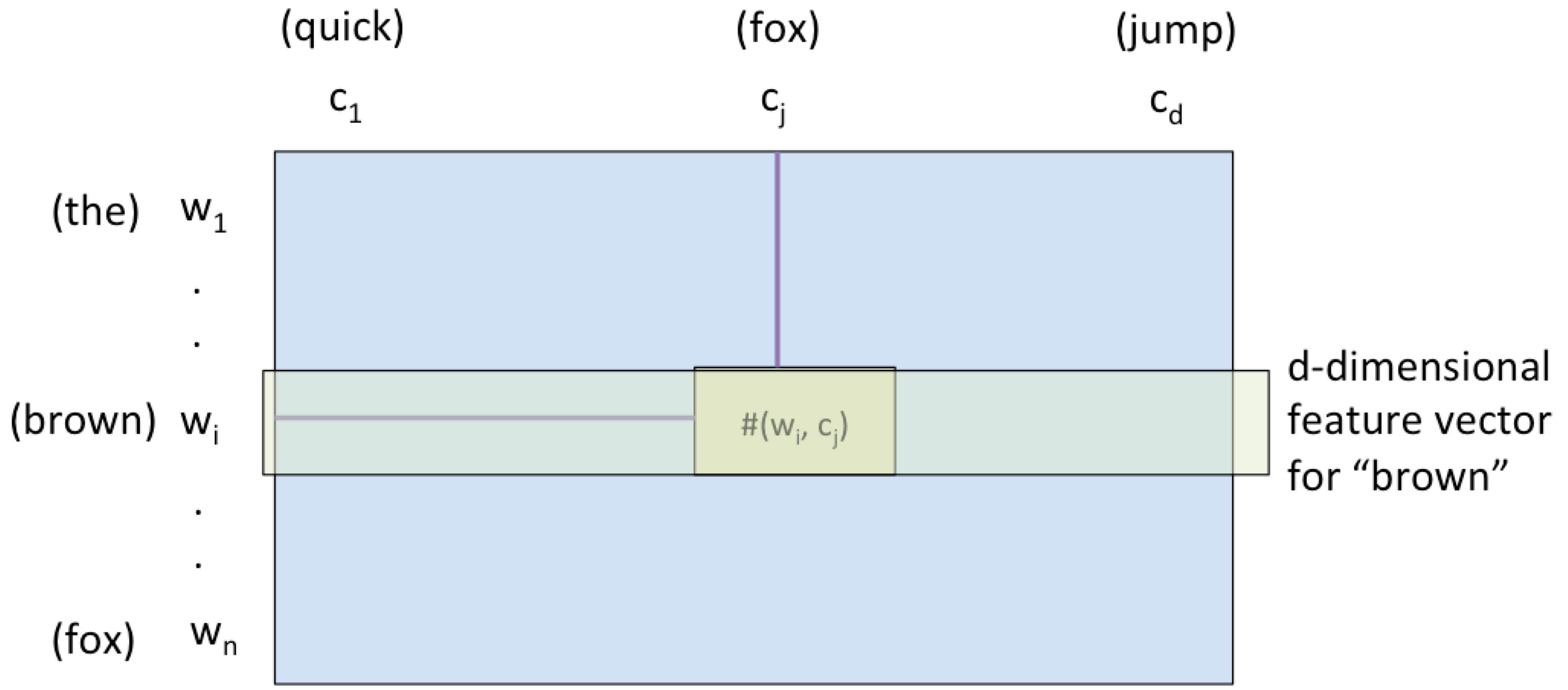
Examples



Unsupervised pertaining for NLP

Use bag-of-word model

- Idea 1: Use the bag-of-word model to ``describe'' each word
- Assume we have context words $c_1, \cdots, c_d$ in the corpus, compute
  - $\#(w, c_i) :=$ number of times the pair(w, c_i) appears in D
- For each word w, form a d-dimensional (sparse) vector to describe w
  - $\#(w, c_1), \cdots, \#(w, c_d),$

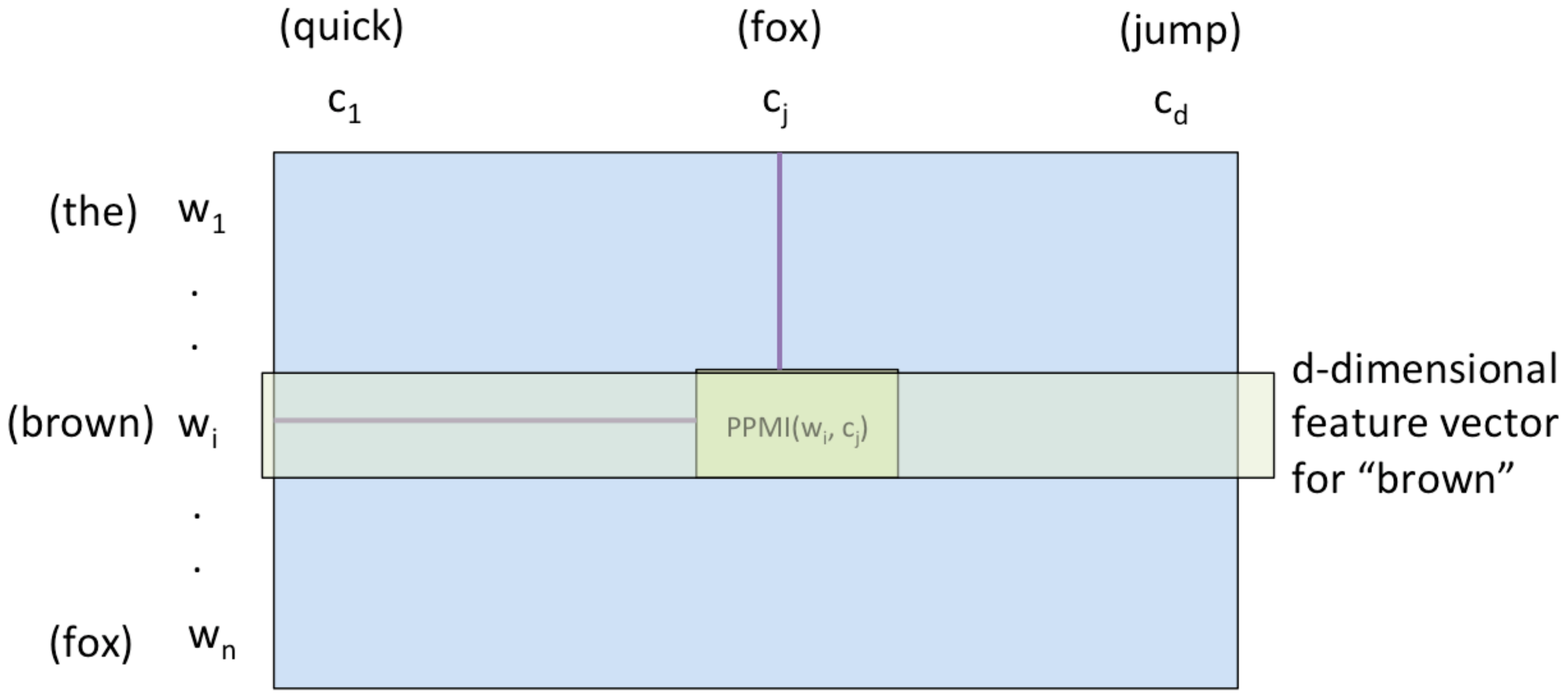


Unsupervised pertaining for NLP

PMI/PPMI Representation

- Similar to TF-IDF: Need to consider the frequency of each word and each context
- Instead of using co-ocurrent count $\#(w, c)$, we can define pointwise mutual information:
  - PMI$(w, c) = \log(\frac{\hat{P}(w, c)}{\hat{P}(w)\hat{P}(c)}) = \log \frac{\#(w, c)|D|}{\#(w)\#(c)}$,
  - $\#(w) = \sum_c \#(w, c)$: number of times word w occurred in D
  - $\#(c) = \sum_w \#(w, c)$: number of times context c occurred
  - $|D|$: number of pairs in D
- Positive PMI (PPMI) usually achieves better performance:
  - PPMI$(w, c) = \max($PMI$(w, c), 0)$
- M^{PPMI}: a n by d word feature matrix, each row is a word and each column is a context

Unsupervised pertaining for NLP
PPMI Matrix



Unsupervised pertaining for NLP

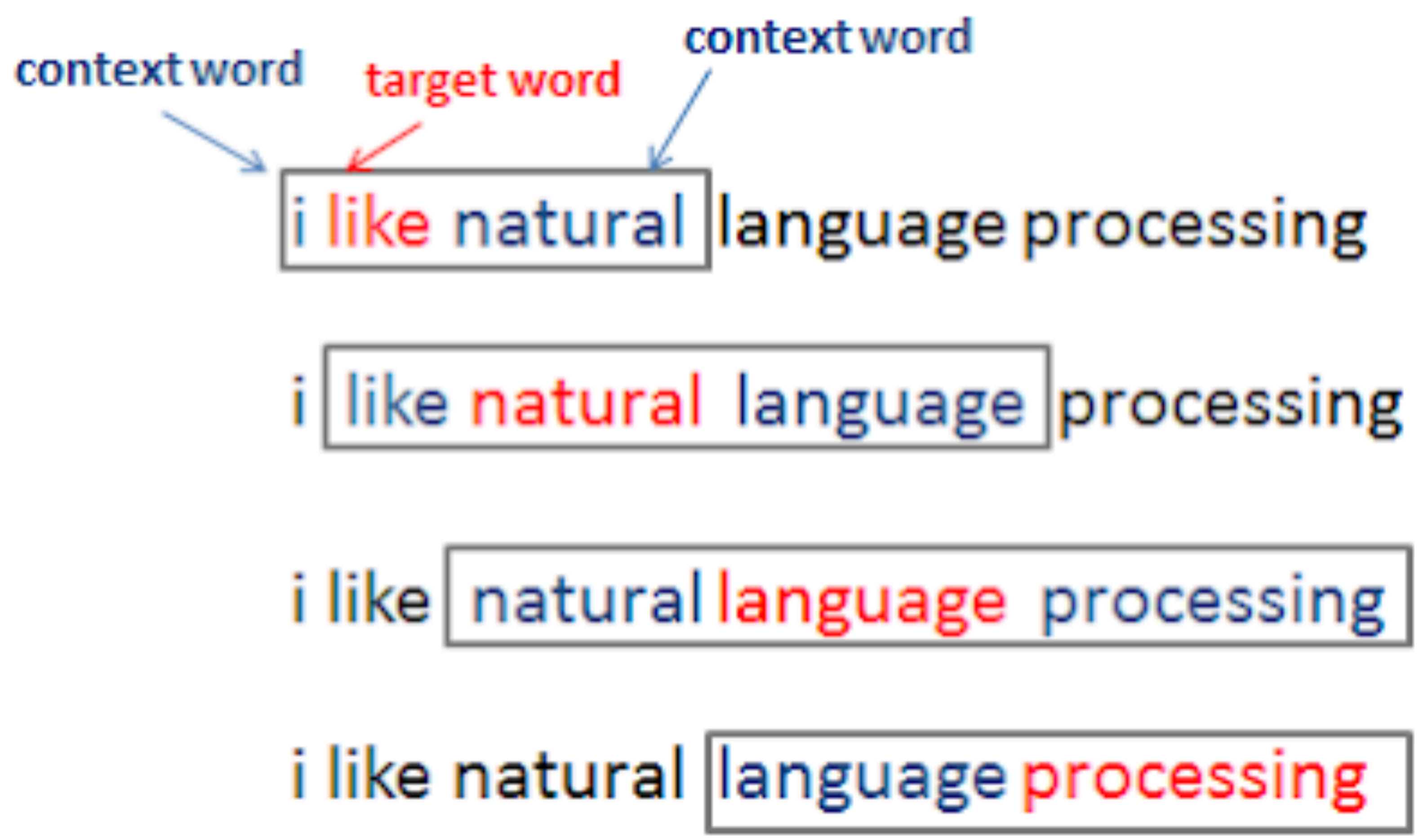
Generalized Low-rank Embedding

- SVD basis will minimize
  - $\min_{W,V} \|M^{\text{PPMI}} - WV^T\|_F^2$
- Glove (Pennington et al., 2014)
  - Negative sampling (less weights to 0s in M^{PPMI})
  - Adding bias term:
    - $M^{\text{PPMI}} \approx WV^T + b_w e^T + e b_c^T$
- Use W or V as the word embedding matrix

Unsupervised pertaining for NLP

Word2vec (Mikolov et al., 2013)

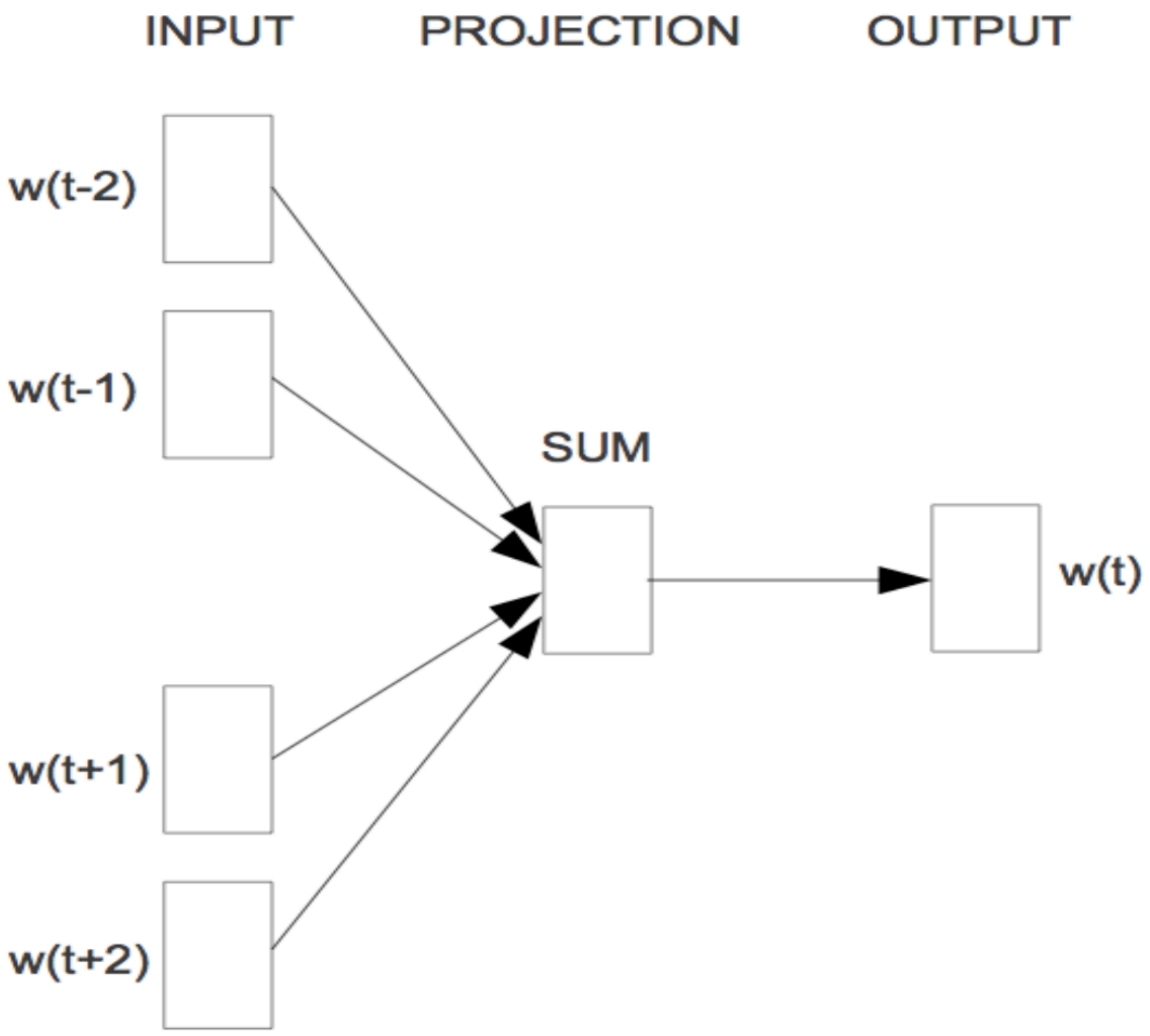
- A neural network model for learning word embeddings
- Main idea:
    - Predict the target words based on the neighbors (CBOW)
    - Predict neighbors given the target words (Skip-gram)



Unsupervised pertaining for NLP

CBOW (Continuous Bag-of-Word model)

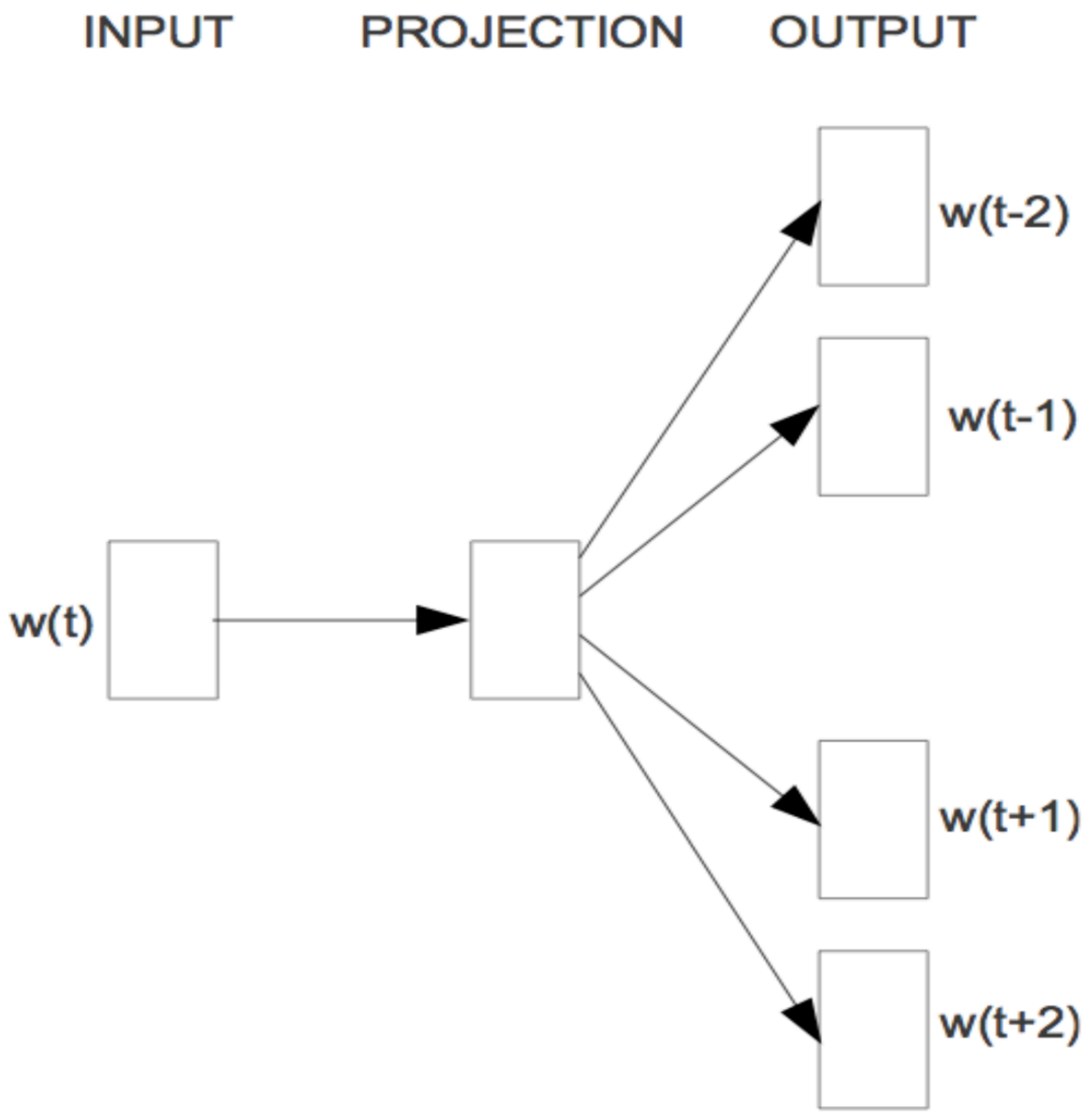
- Predict the target words based on the neighbors



Unsupervised pertaining for NLP

Skip-gram

- Predict neighbors using target word



Unsupervised pertaining for NLP

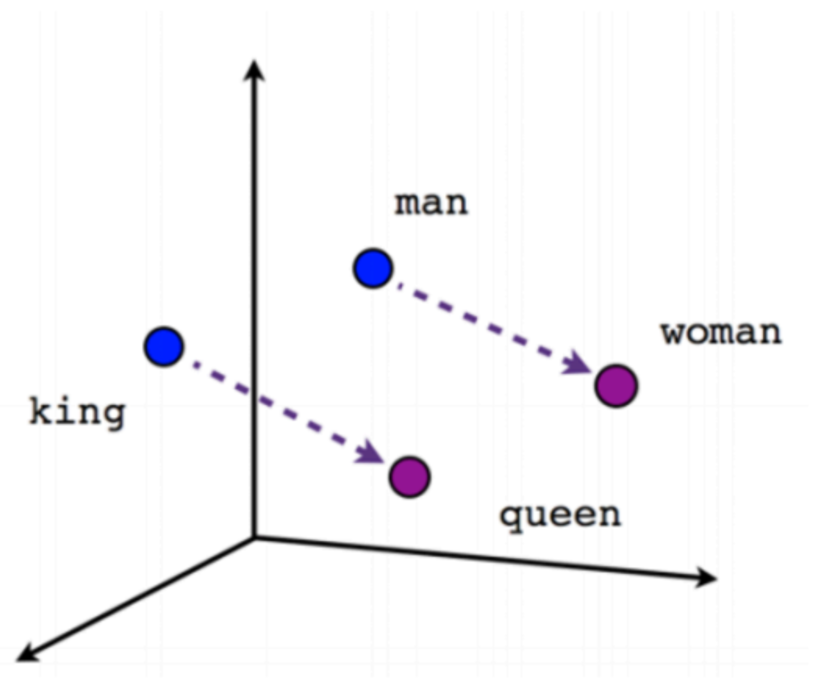
More on skip-gram

- Learn the probability $P(w_{t+j} | w_t)$: the probability to see w_{t+j} in target word w_t's neighborhood
- Every word has two embeddings:
  - v_i serves as the role of target
  - u_i serves as the role of context
- Model probability as softmax:
  - $$P(o | c) = \frac{e^{u_o^T v_c}}{\sum_{w=1}^{W} e^{u_w^T v_c}}$$

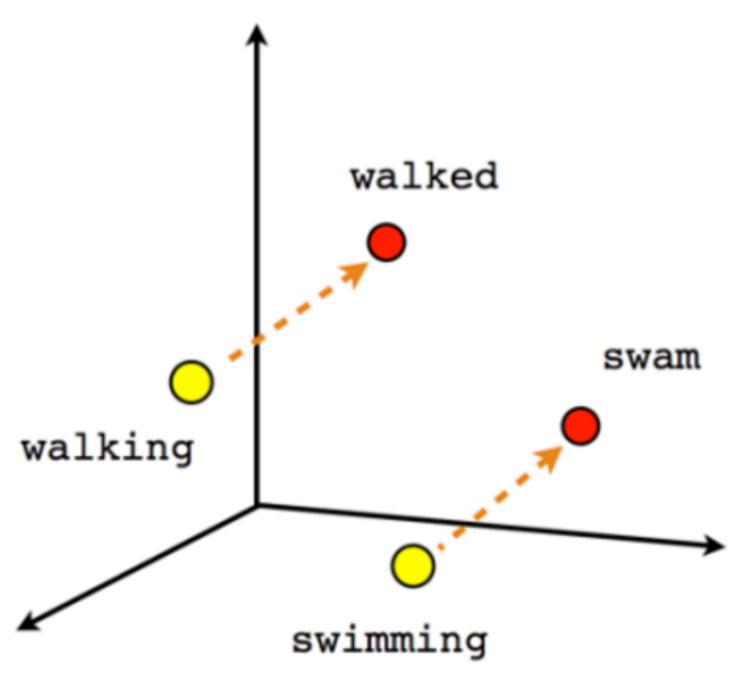
Unsupervised pertaining for NLP

Results

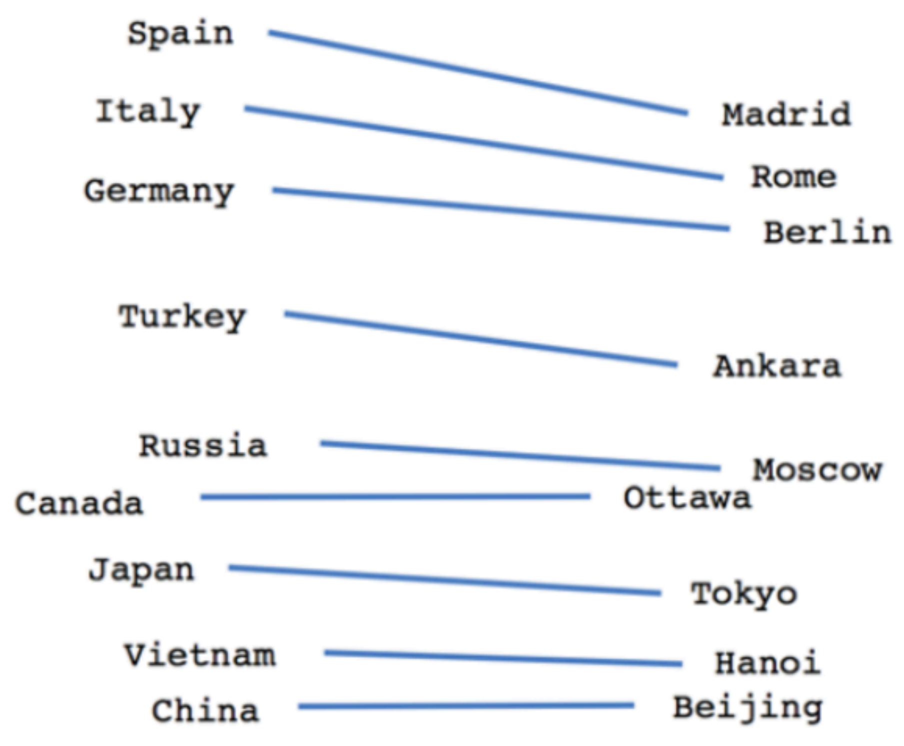
- The low-dimensional embeddings are (often) meaningful:



Male-Female



Verb tense



Country-Capital

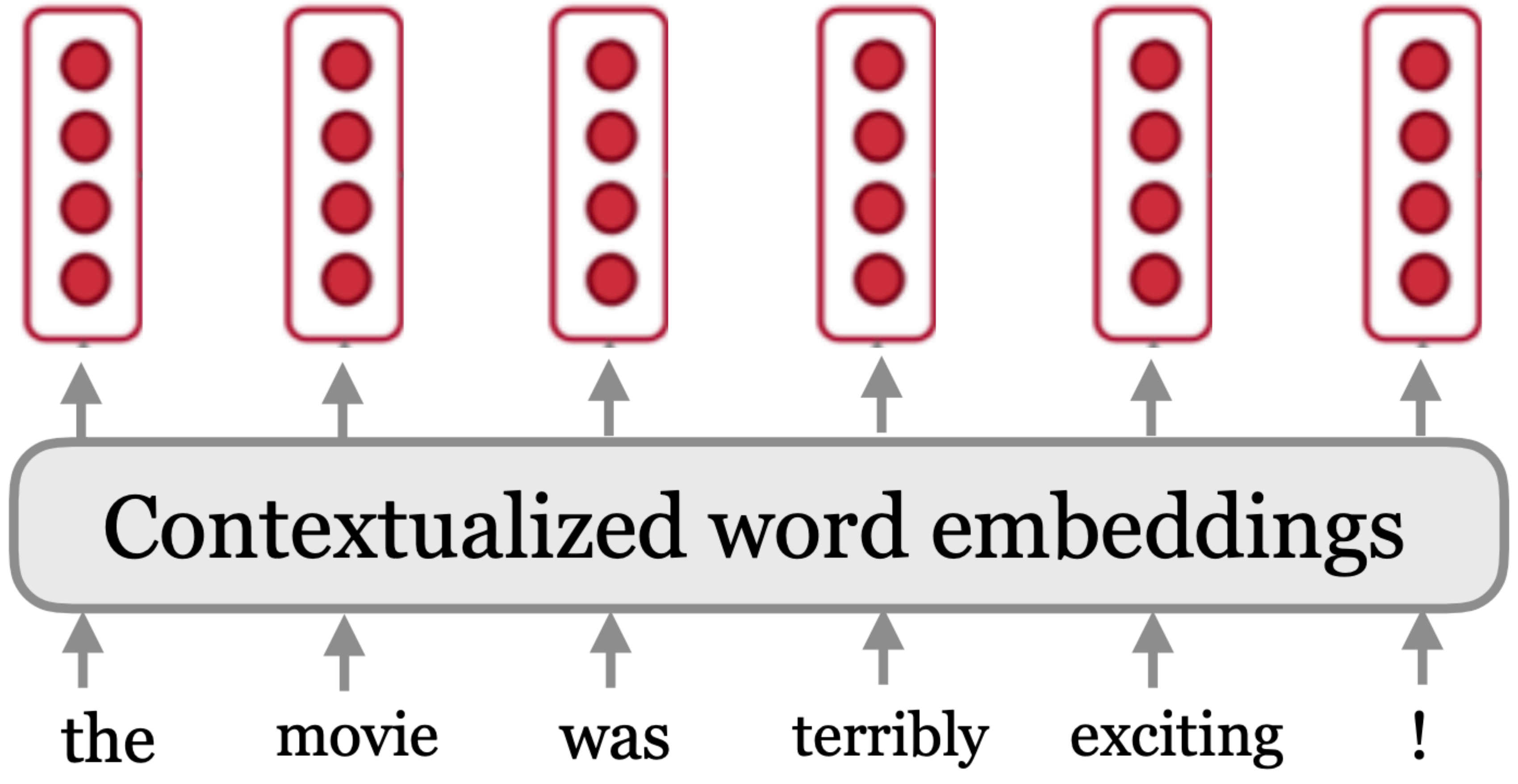
Contextual embedding

Contextual world representation

- The semantic meaning of a word should depend on its context

```
  [0.9, -0.2, 1.6, …]                [-1.9, -0.4, 0.1, …]
          ↑                                     ↑
open a bank account               on the river bank
```

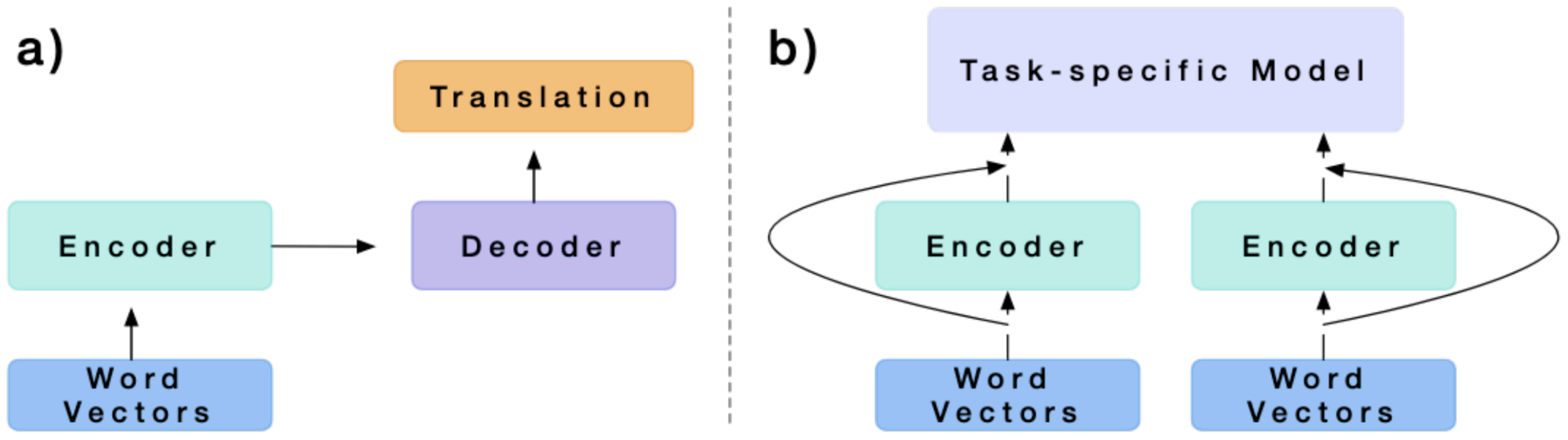
- Solution: Train a model to extract contextual representations on text corpus



Contextual embedding

CoVe (McCann et al., 2017)

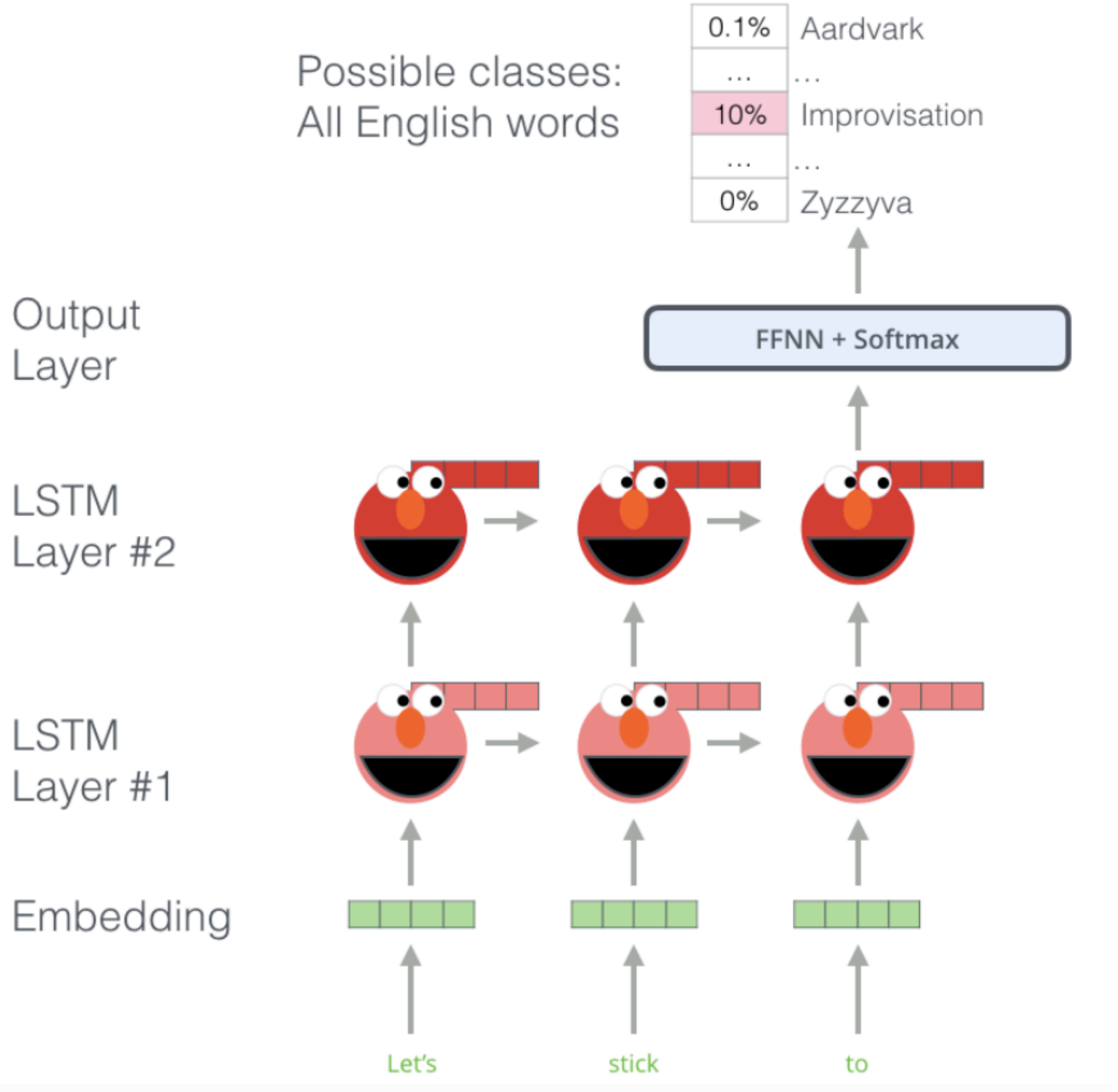
- Key idea: Train a standard neural machine translation model
- Take the encoder directly as contextualized word embeddings
- Problems:
  - Translation requires paired (labeled) data
  - The embeddings are tailored to particular translation corpuses



Contextual embedding

Language model pretraining task

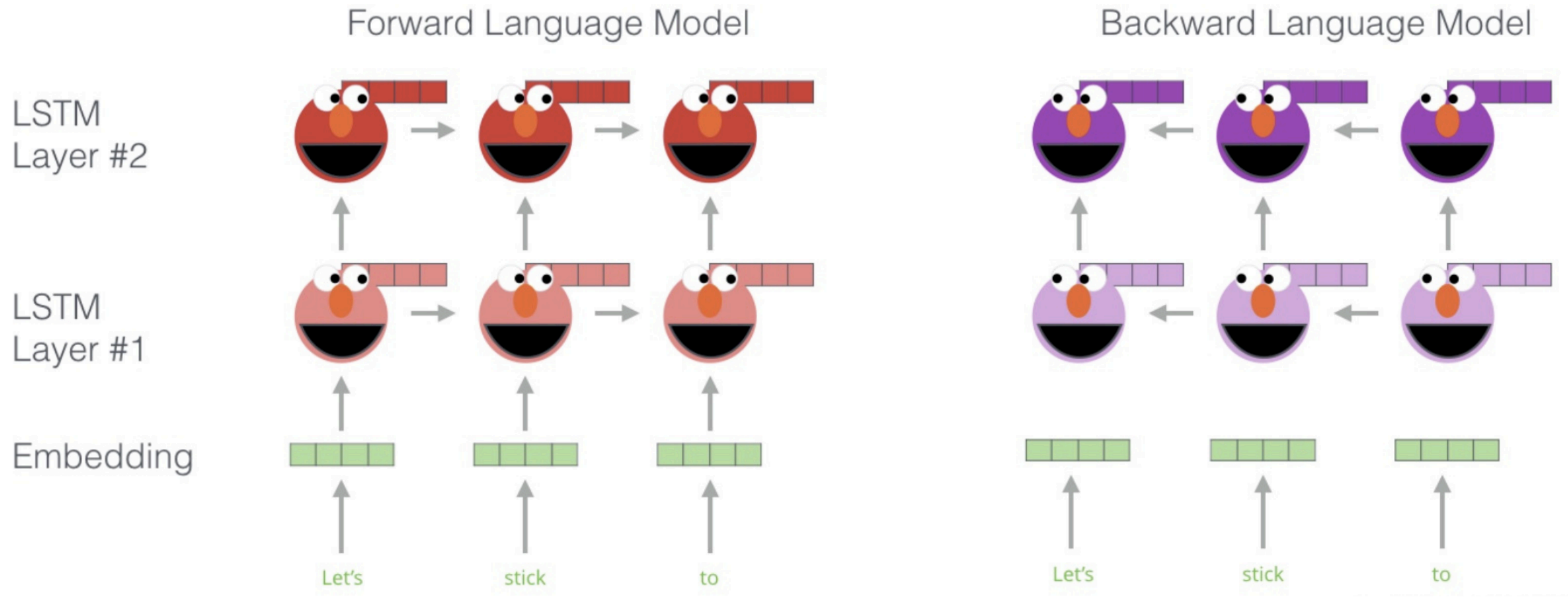
- Predict the next word given the prefix
- Can be defined on any unlabeled document



Contextual embedding

ELMo (Peter et al., 2018)

- Key ideas:
  - Train a foward and backward LSTM language model on large corpus
  - Use the hidden states for each token to compute a vector representation of each word
  - Replace the word embedding by Elmo's embedding (with fixed Elmo's LSTM weights)



Contextual embedding

ELMo results

Task	Previous SOTA		Our baseline	ELMo + baseline	Increase (absolute/ relative)
SQuAD	Liu et al. (2017)	84.4	81.1	85.8	4.7 / 24.9%
SNLI	Chen et al. (2017)	88.6	88.0	88.7 $\pm$ 0.17	0.7 / 5.8%
SRL	He et al. (2017)	81.7	81.4	84.6	3.2 / 17.2%
Coref	Lee et al. (2017)	67.2	67.2	70.4	3.2 / 9.8%
NER	Peters et al. (2017)	91.93 $\pm$ 0.19	90.15	92.22 $\pm$ 0.10	2.06 / 21%
SST-5	McCann et al. (2017)	53.7	51.4	54.7 $\pm$ 0.5	3.3 / 6.8%

Contextual embedding

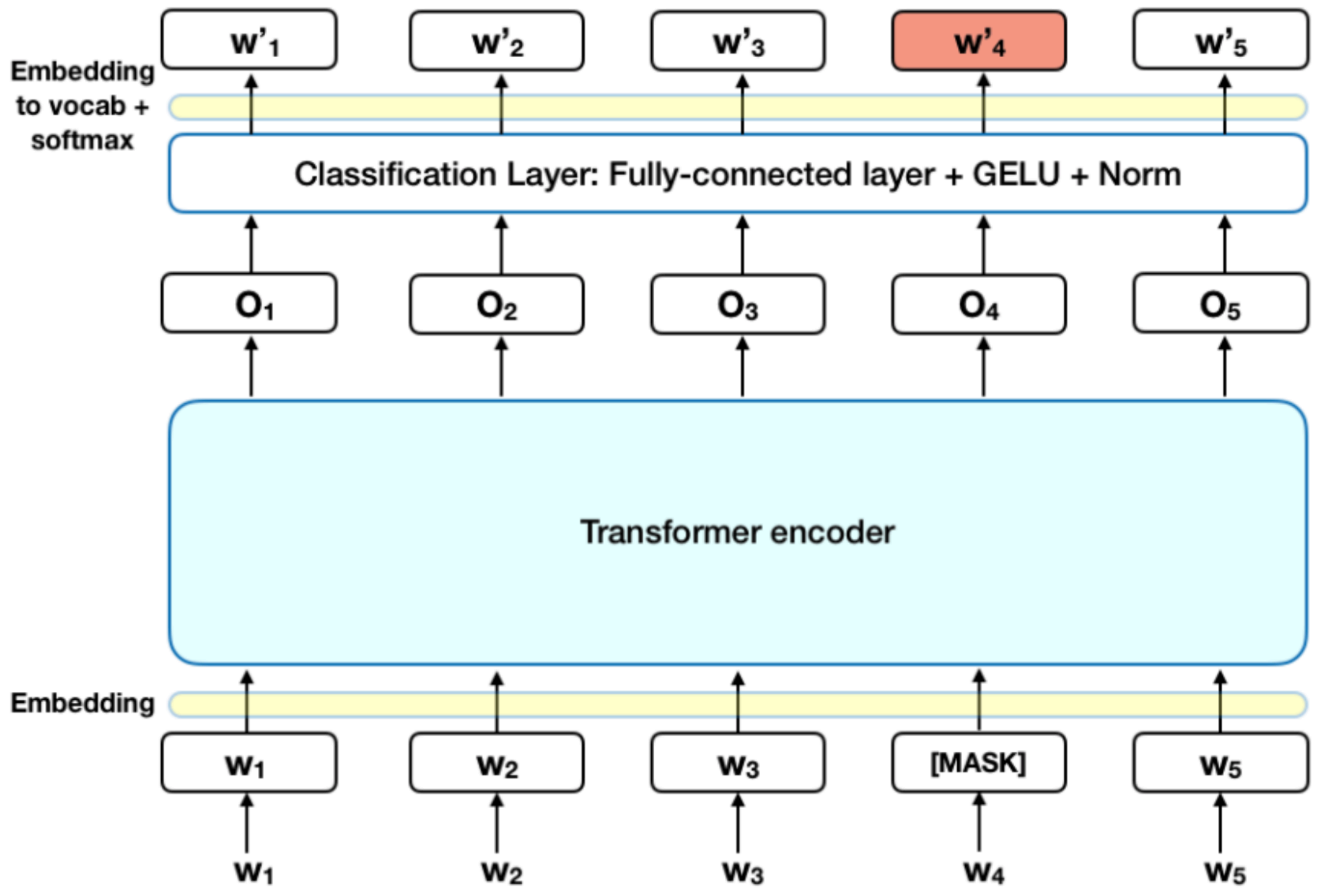
BERT

- Key idea: replace LSTM by Transformer
- Define the generated pretraining task by masked language model
- Two pretraining tasks
- Finetune both BERT weights and task-dependent model weights for each task

Contextual embedding

BERT pretraining loss

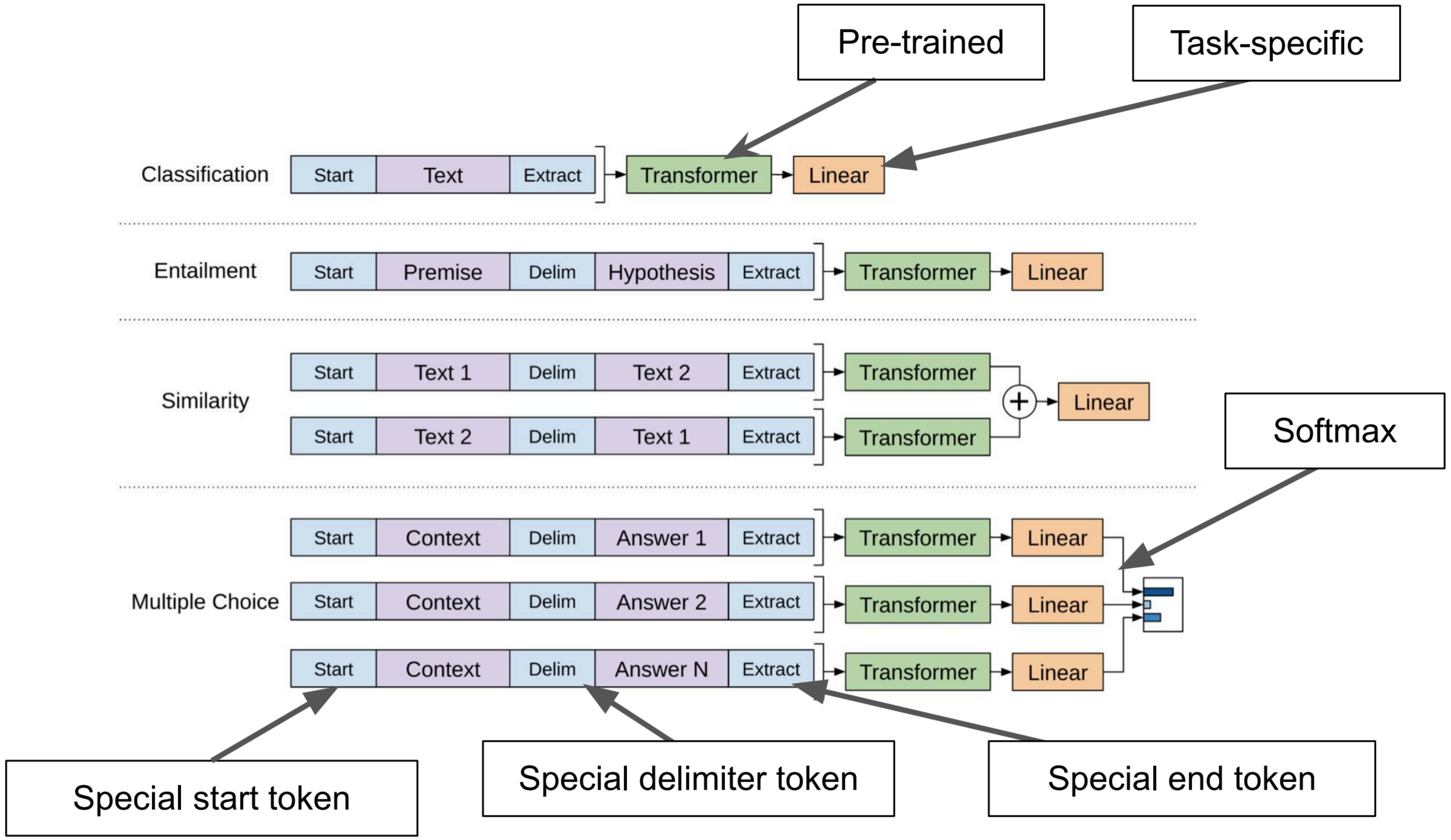
- Masked language model: predicting each word by the rest of sentence
- Next sentence prediction: the model receives pairs of sentences as input and learns to predict if the second sentence is the subsequent sentence in the original document.



Contextual embedding

BERT finetuning

- Keep the pretrained Transformers
- Replace or append a layer for the final task
- Train the whole model based on the task-dependent loss



Contextual embedding

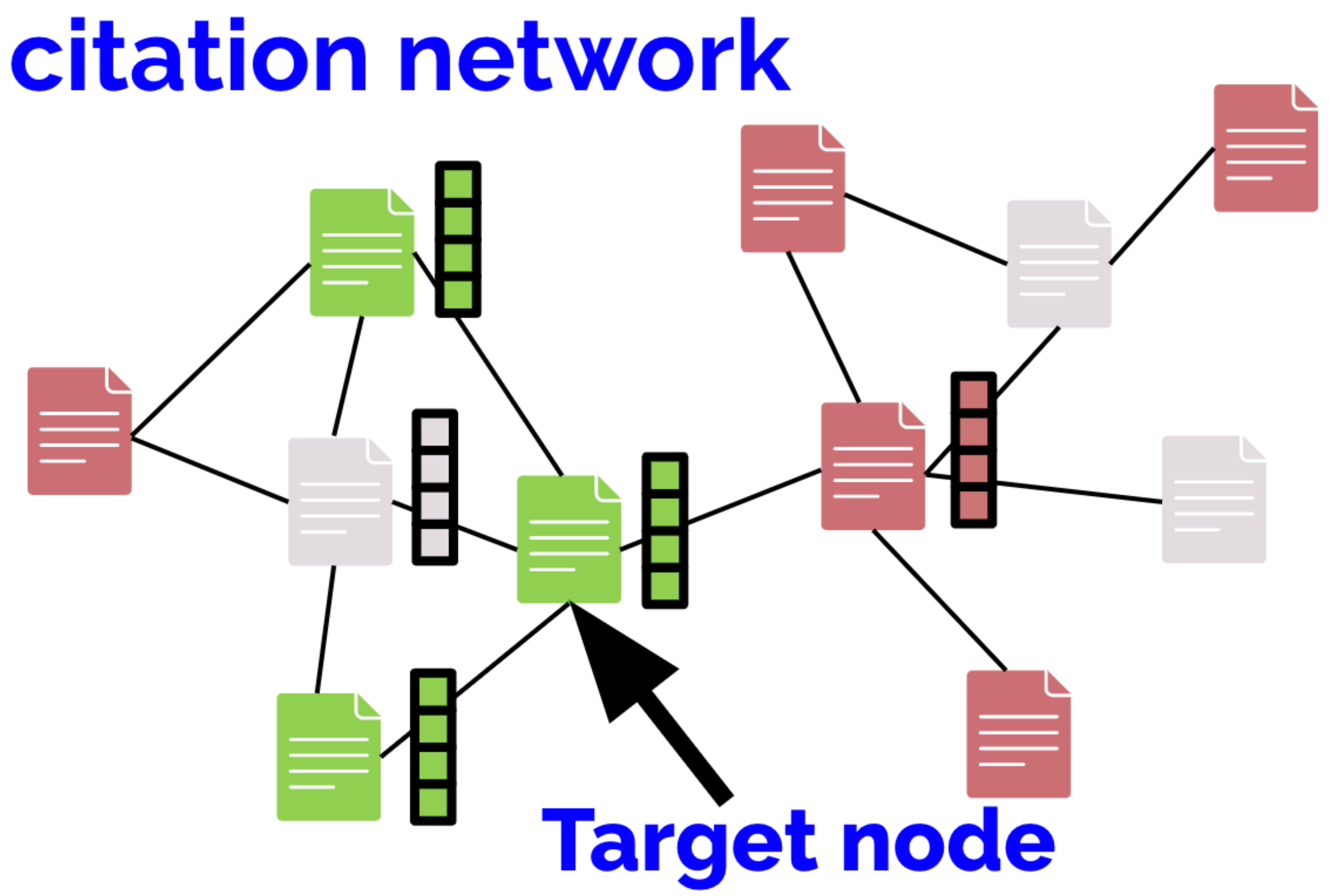
BERT results

System	MNLI-(m/mm)	QQP	QNLI	SST-2	CoLA	STS-B	MRPC	RTE	**Average**
	392k	363k	108k	67k	8.5k	5.7k	3.5k	2.5k	-
Pre-OpenAI SOTA	80.6/80.1	66.1	82.3	93.2	35.0	81.0	86.0	61.7	74.0
BiLSTM+ELMo+Attn	76.4/76.1	64.8	79.8	90.4	36.0	73.3	84.9	56.8	71.0
OpenAI GPT	82.1/81.4	70.3	87.4	91.3	45.4	80.0	82.3	56.0	75.1
$\text{BERT}_{\text{BASE}}$	84.6/83.4	71.2	90.5	93.5	52.1	85.8	88.9	66.4	79.6
$\text{BERT}_{\text{LARGE}}$	**86.7/85.9**	**72.1**	**92.7**	**94.9**	**60.5**	**86.5**	**89.3**	**70.1**	**82.1**

Graph Convolutional Neural Network

Node classification problem

- Given a graph of N nodes, with adjacency matrix $A \in \mathbb{R}^{N \times N}$
- Each node is associated with a D-dimensional feature vector.
- $X \in \mathbb{R}^{N \times D}$: each row corresponds to the feature vector of a node
- Observe labels for a subset of nodes: $Y \in \mathbb{R}^{N \times L}$, only observe a subset of rows, denoted by Y_S
- Goal: Predict labels for unlabeled nodes (transductive setting) or
- test nodes (inductive setting) or test graphs (inductive setting)



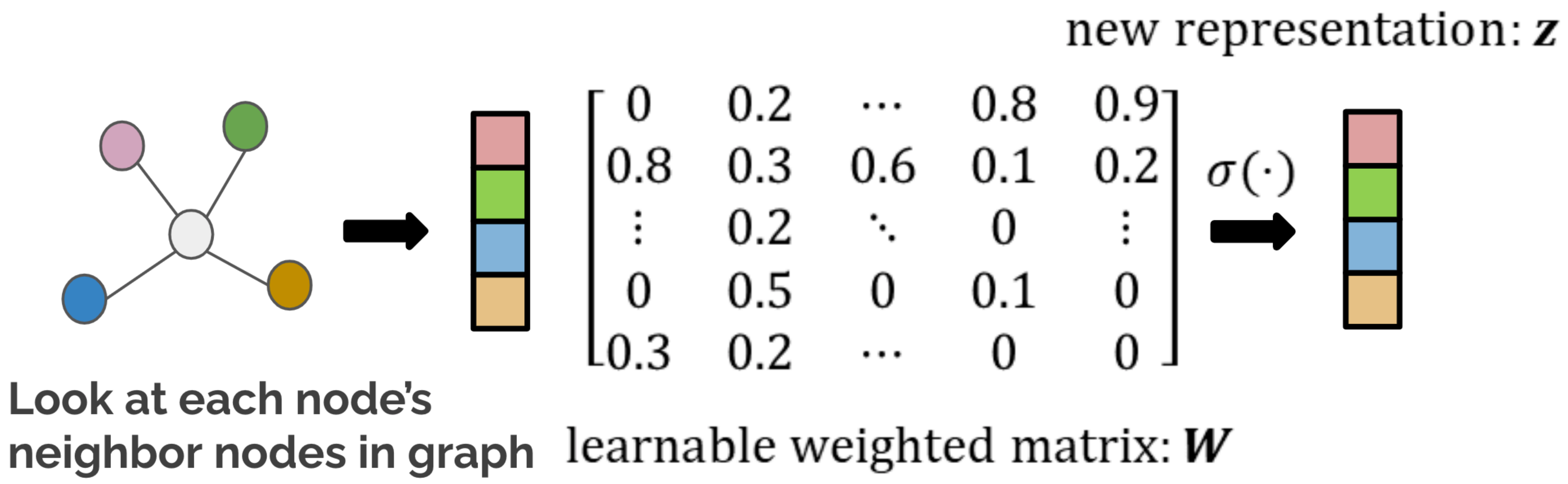
Graph Convolutional Neural Network

Graph Convolution Layer

- GCN: multiple graph convolution layers
- $\hat{A}$: normalized version of A:
  - $\tilde{A} = A + I, \quad \tilde{D}_{uv} = \sum_{v} \tilde{A}_{uv}, \quad P = \tilde{D}^{-1}\hat{A}$
- Graph convolution:
  - Input: features for each node $H^{(l)} \in \mathbb{R}^{n \times D}$
  - Output: features for each node $H^{(l+1)}$ after gathering neighborhood information
  - Convolution: $PH^{(l)}$: Aggregate features from neighbors
  - Convolution + fully-connected layer + nonlinear activation:
    - $H^{(l+1)} = \sigma(PH^{(l)}W^{(l)})$,
    - $W^{(l)}$ is the weights for the linear layer
    - $\sigma(\cdot)$: usually ReLU function

Graph Convolutional Neural Network

Graph convolutional network



Graph Convolutional Neural Network

Graph convolutional network

- Initial features $H^{(0)} := X$
- For layer $l = 0, \ldots, L$
  - $Z^{(l+1)} = PH^{(l)}W^{(l)}, \quad H^{(l+1)} = \sigma(Z^{(l+1)}),$
- Use final layer feature $H^{(L)} \in \mathbb{R}^{N \times K}$ for classification:
  - $\text{Loss} = \frac{1}{|S|} \sum_{s \in S} \text{loss}(y_s, Z_s^{(L)})$
  - Each row of $Z_s^{(L)}$ corresponds to the output score for each label
  - Cross-entropy loss for classification

Graph Convolutional Neural Network

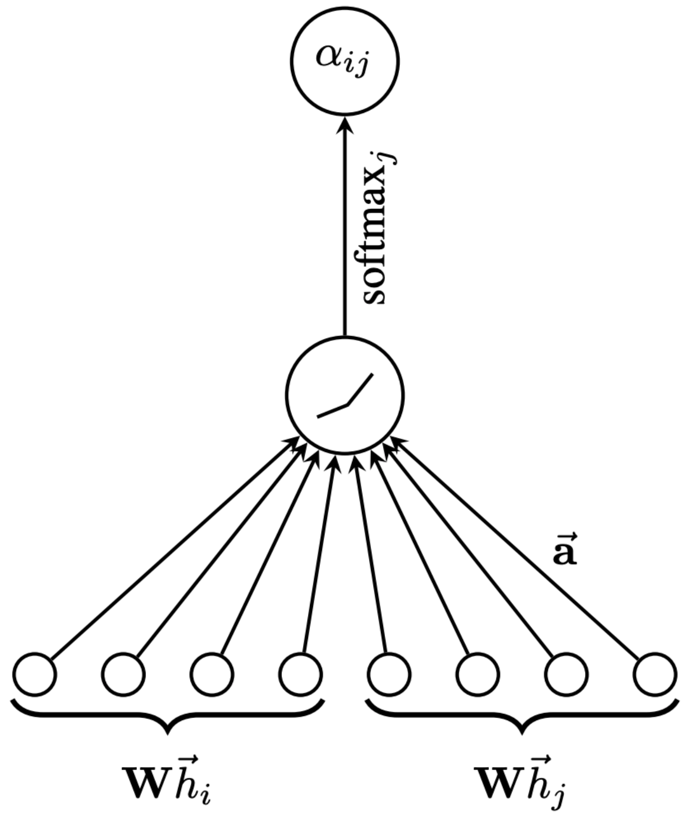
Graph convolutional network

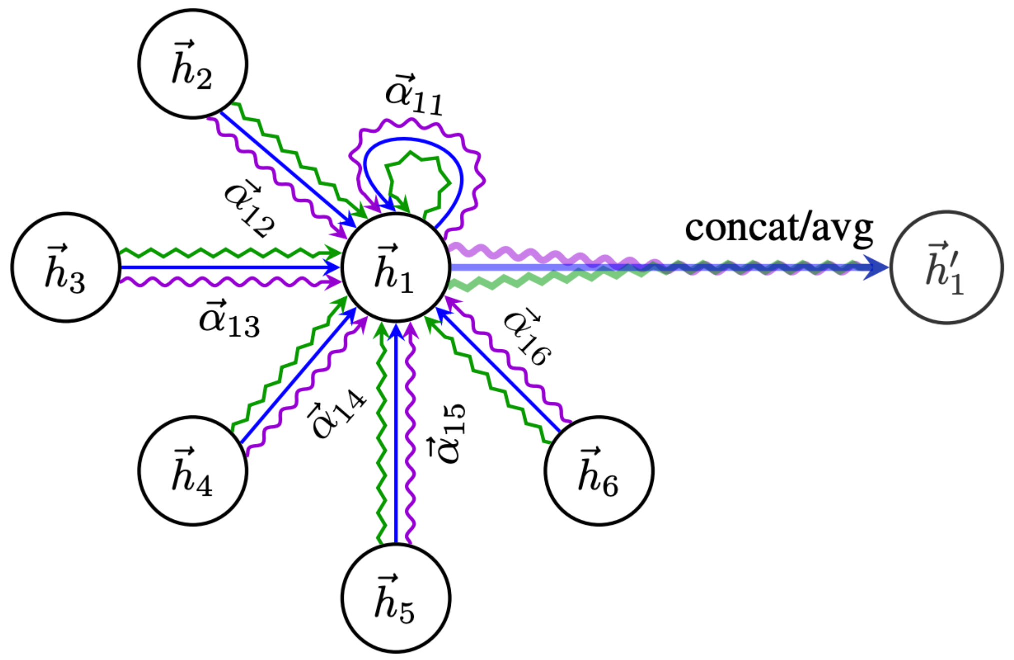
- Model parameters: $W^{(1)}, \cdots, W^{(L)}$
- Can be used to
  - Predict unlabeled nodes in the training set
  - Predict testing nodes (not in the training set)
  - Predict labels for a new graph
- Also, features extracted by GCN $H^{(L)}$ is usually very useful for other tasks

Graph Convolutional Neural Network

Graph Attention Networks

- Each edge may not contribute equally
- Using attention mechanism to automatically assign weights to each edge:
    - $\alpha_{i,j} = \dfrac{\exp(\text{LeakyReLU}(a^T[Wh_i \mid Wh_j]))}{\sum_{k \in N_i} \exp(\text{LeakyReLU}(a^T[Wh_i \mid Wh_k]))}$
    - where h_i, h_j are the features for node i and j at previous layer, W is the GNN weight, a is the additional learnable parameter for attention





Graph Convolutional Neural Network

GNN Pretraining

- Standard GNN pipeline:
    - Text features ⇒ BERT/Word2vec ⇒ GNN
- GIANT-XRT: pretrain the feature extractors (e.g., BERT) based on the graph information.