QUCK INTRODUCTION TO TRANSFORMERS S. Giagu - 3rd ML_INFN Hackathon: Advanced Level

INFN & Università di Bari - 23.11.2022



ATTENTION MECHANISM

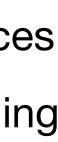
- the input:
 - RNN example: to translate each element of a sequence
 - CNN example: to classify each pixel in a image segmentation (eg classification pixel by pixel)
 - GNN example: to predict the target for each node in a graph
- to solve the sub-task in all these cases the model learns to form an internal representation of the input that acts as context for the sub-task
- ideally this context vector should contains information from the entire input, however:
 - fixed length vectors scales quite poorly with input size (number of subtasks grow), like in the analysis of long sequences
 - either the size of the context vector grows or it will not have the capacity to represent all the relevant information leading to a degradation in performance
- this clash with computational resources
- relevant than others. The attention mechanism provides a way to identify such parts ...

• Several examples in DNN in which the whole task to be learned is subdivided in sub-tasks which apply to local elements of

• idea: even if the model may need to draw upon information from the entire input, however some parts of it will be more

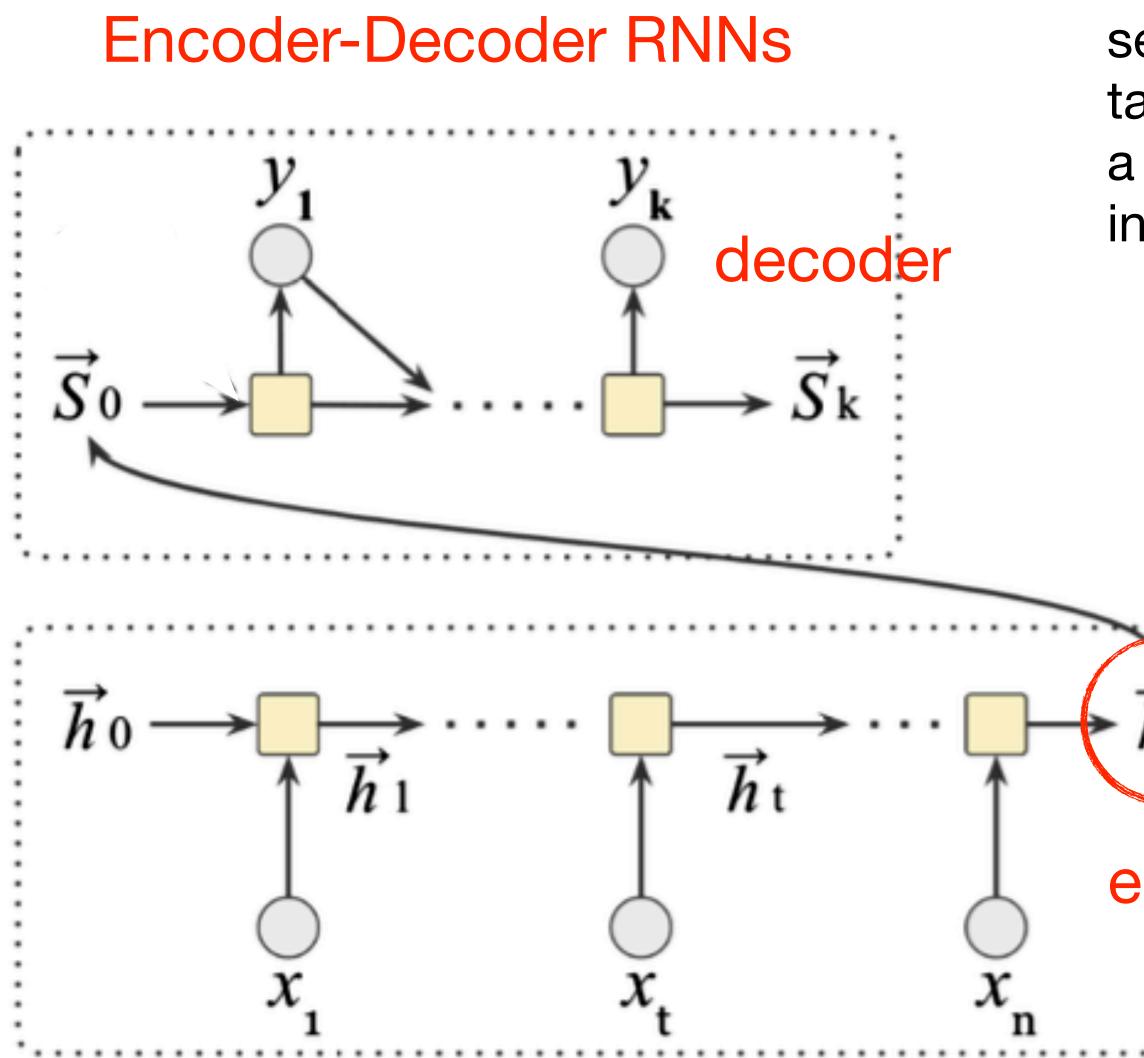








REMINDER: SEQ-TO-SEQ LSTM/GRU



seq2seq models (used for example in machine translation tasks) represents a first example of such attempt to create a context vector (the cell state of the LSTM/GRU) from the input

> use of LSTM o GRU cells allows to "memorise" relevant terms that are far from the current element in the sequence and that are crucial to solve the task

n n encoder limitation: LSTM/GRU becomes ineffective for very long sequence, unless implemented in complex StackedRNN architectures that are impossible to train in an acceptable time due to the recursive (i.e. non parrallelizable) intrinsic structure of a RNN





ATTENTION

- network can learn to attend to the relevant parts of the input
- example: in a NLP translation task, attention will works by aligning each words in the output take into account that words order may be for example different in different languages ...

context vector for the i-th output word (or sequence element in general)

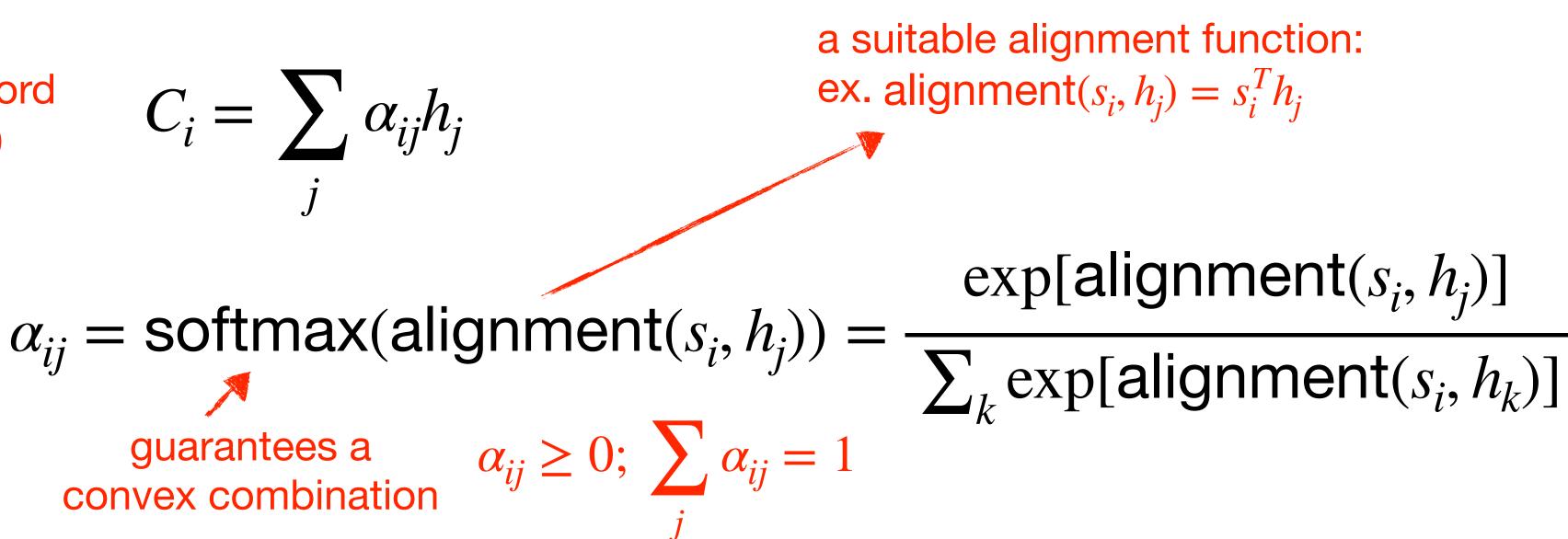
 $C_i = \sum \alpha_{ij} h_j$

alignment weight between input encoding h_i and output encoding s_i

guarantees a convex combination

• intuitive idea: one forms a representation for the entire input, but different parts of the input are weighted differently according to the task at hand. By making the weights a learnable component, the

sequence (translated text) with some words in the input sequence that give context to the translation. These words are not necessarily aligned in the original order, they can aligned in different order to

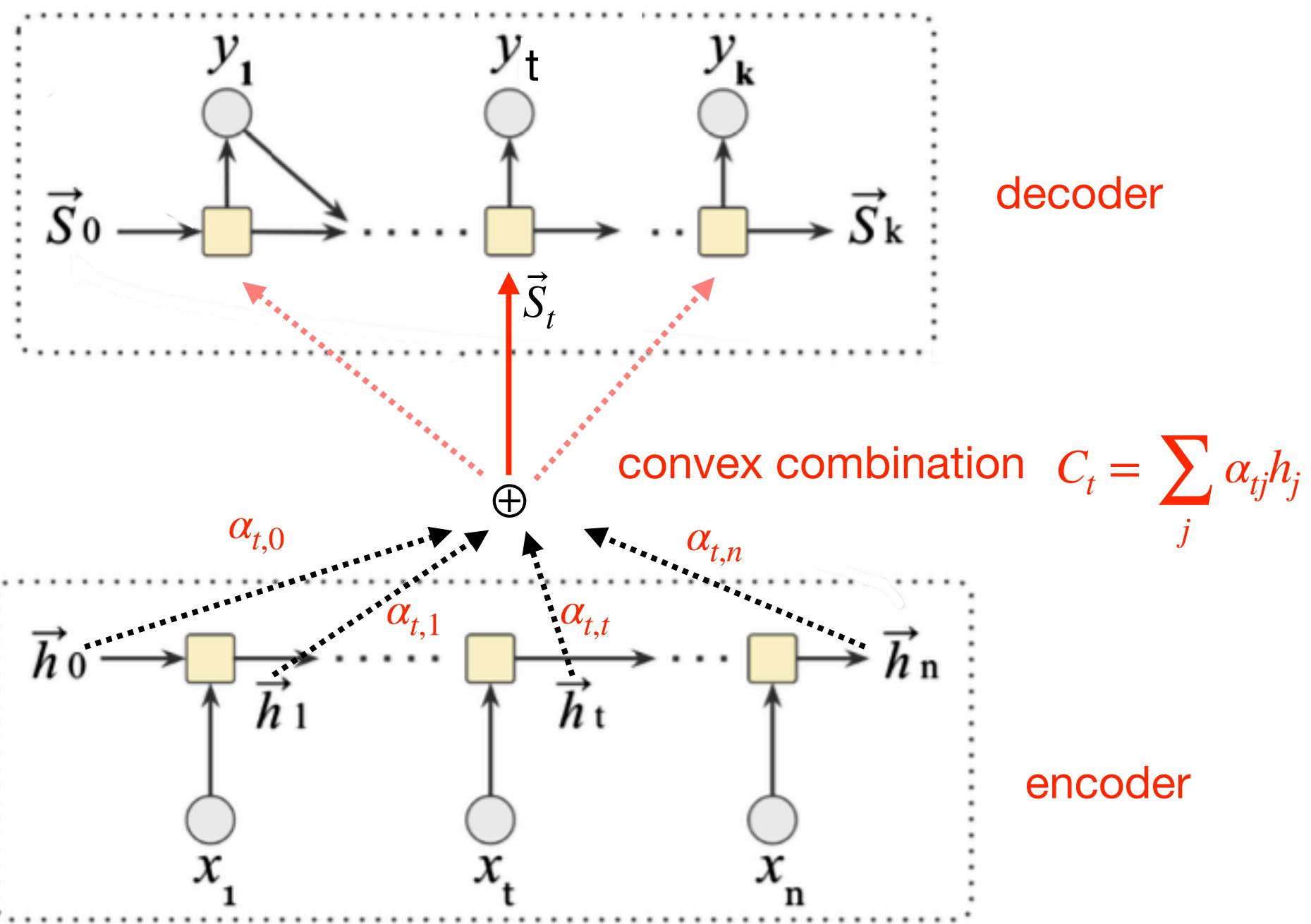






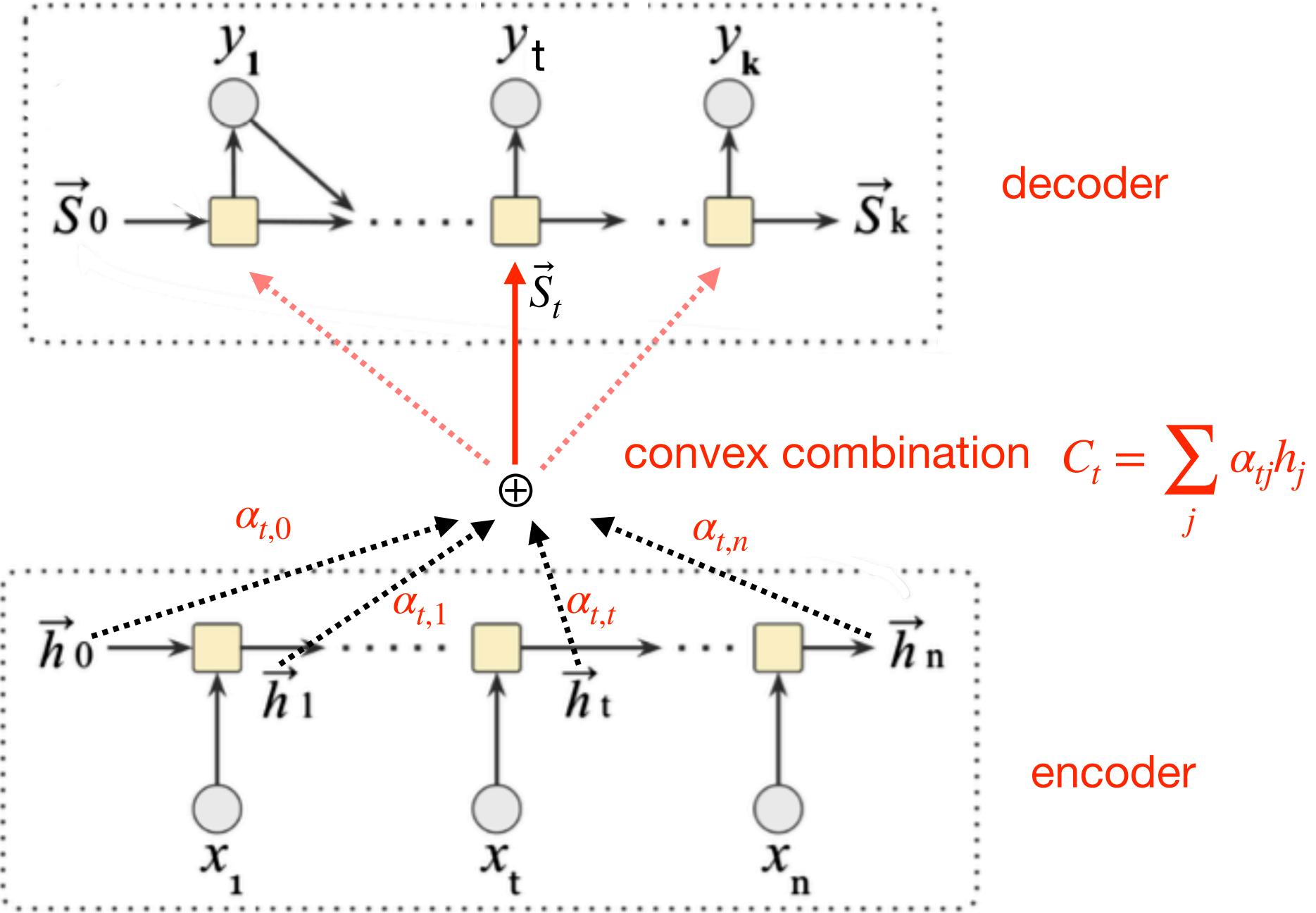


output



hidden states

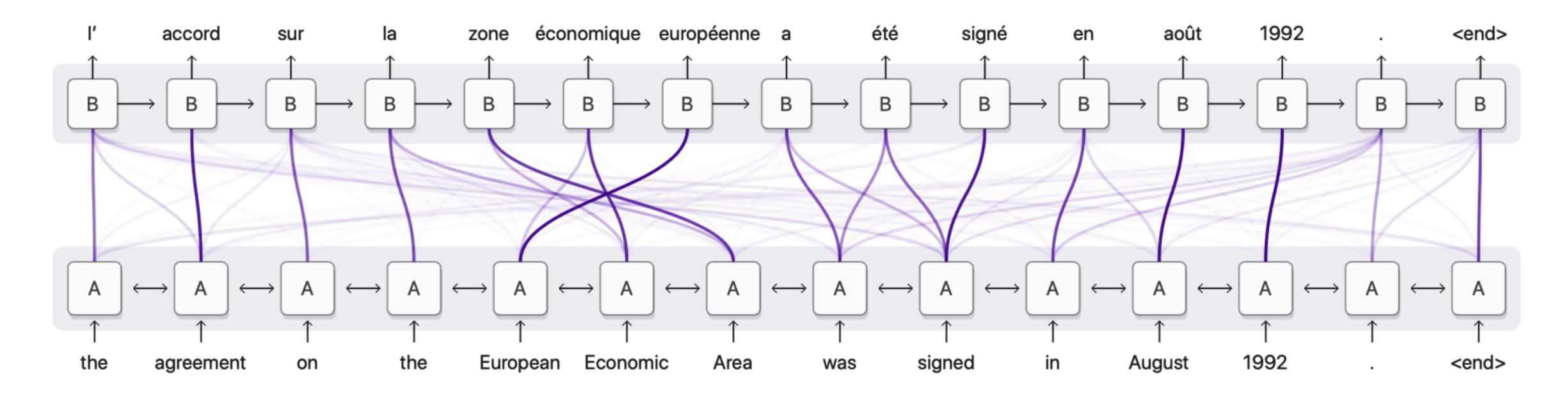
input





RNNSearch: BIDIRECTIONAL RNN WITH ATTENTION

attention mechanism



attention weights in a seq-to-seq problem of translation from ENG to FR

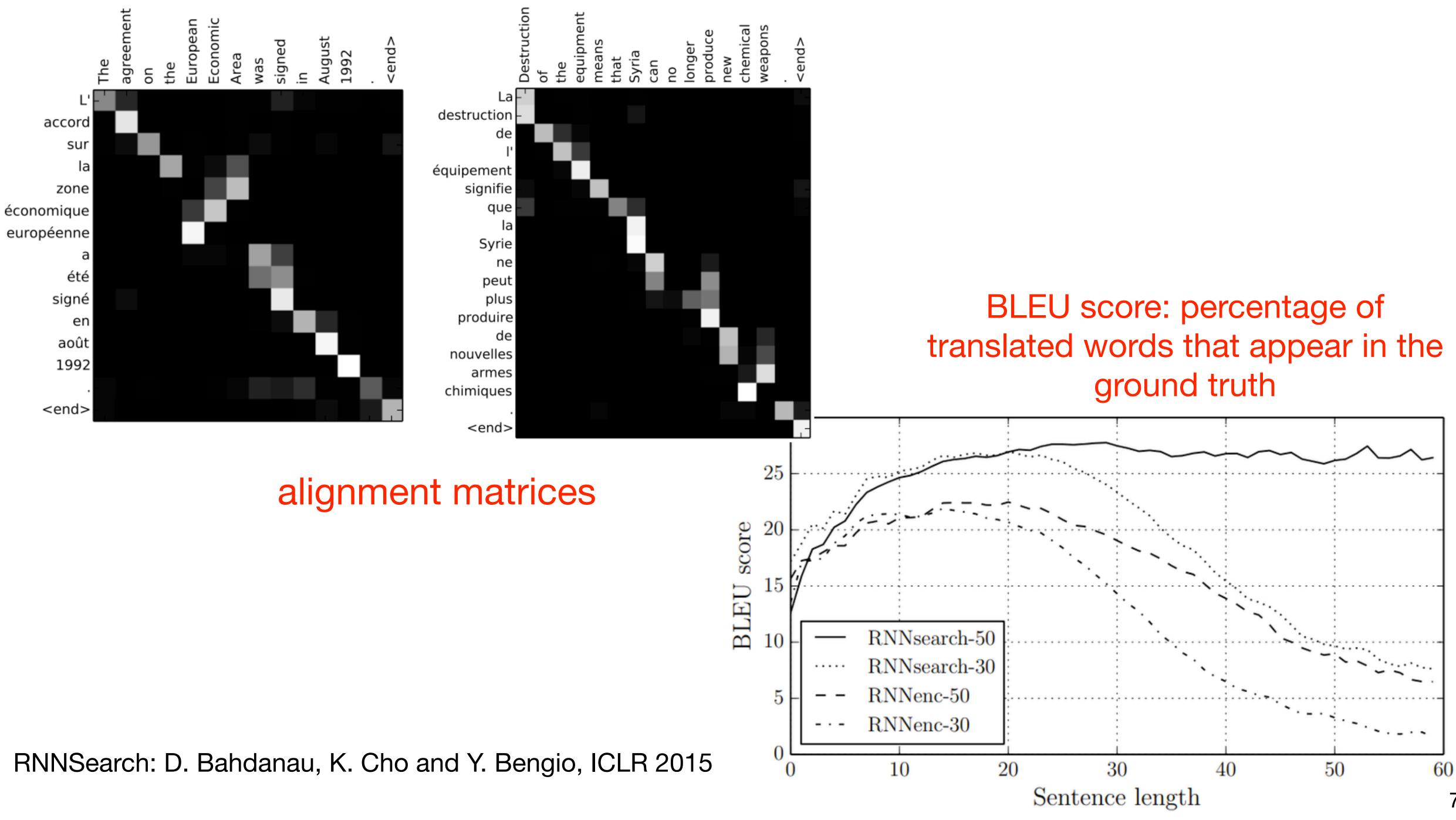
• attention idea implemented for the first time in a model (RNNSearch: D. Bahdanau, K. Cho and Y. Bengio, ICLR 2015) which made a breakthrough in machine translation by combining a bi-directional RNN with an additive

 $alignment(s_i, h_i) = U tanh(Ws_{i-1} + \tilde{W}h_i + b_i)$

 U, W, \tilde{W}, b_i learnable weights







DIGRESSION: ATTENTION AND NOTION OF SPARSITY OF INTERACTIONS

- the attention mechanism is a generalisation of the assumption of locality used in CNN with the concept of sparsity of interactions
- this can be intuitively understood by considering the k-NN algorithm:

$$g(x) = \frac{1}{k} \sum_{i \in k - nn(x)} y_i$$

- g(x) is considered "sparse" as only depends on k points of the entire dataset
- over all points and weighting them with the distance d:

$$g(x) = \sum_{i} d(x, x_i) y_i = \sum_{i}^{i} d(x$$

the attention mechanism makes this estimator a convex sum using the softmax

in a regression task returns the average of the values of the closest k-points according to a defined distance $d(x, x_i)$

• the attention makes the operation of selection the k-nn points differentiable and useable by summing

 $e^{-\beta \|x-x_i\|_2} v$

Nadaraya-Watson kernel estimator



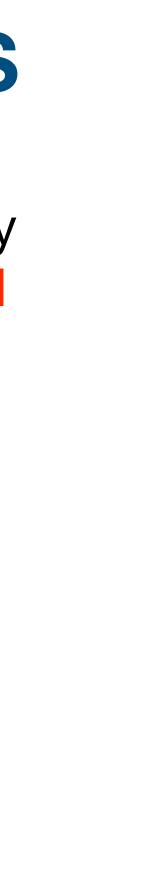


SCALED DOT-PRODUCT ATTENTION AND TRANSFORMERS

- with very large datasets) CNNs and RNNs in vision and in time-domain related tasks
- Compared to RNN, Transformers:
 - facilitate the learning of long range sequences
 - don't need recurrence:
 - no gradient vanishing or explosion problems
 - serial)
- The core ingredient of Transformers is the so called multi head (self) attention layers based on scaled doct-product alignment

• Transformers are recent DNN architectures based on the attention mechanism that have gradually replaced RNNs in mainstream NLP tasks, and that can also often compete/surpass (when trained

• typically need fewer training steps (contrarily to RNNs that due to recurrence when unrolled are very deep networks), and can be easily parallelised on GPUs (while recurrence is intrinsically

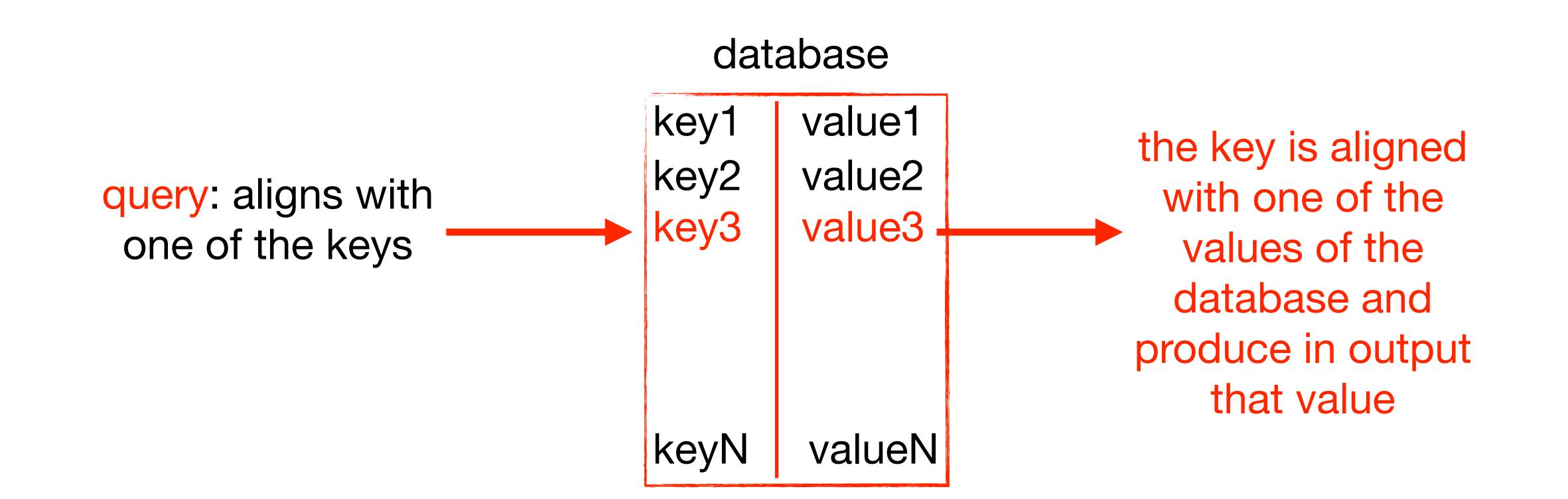






ATTENTION MECHANISM AS A DB RETRIEVAL TECHNIQUE

- retrieve a given value associated to that key:



• the attention mechanism can be also seen in a different way, as a technique that mimics the retrieval in a database of a value v based on a query q and on a key k

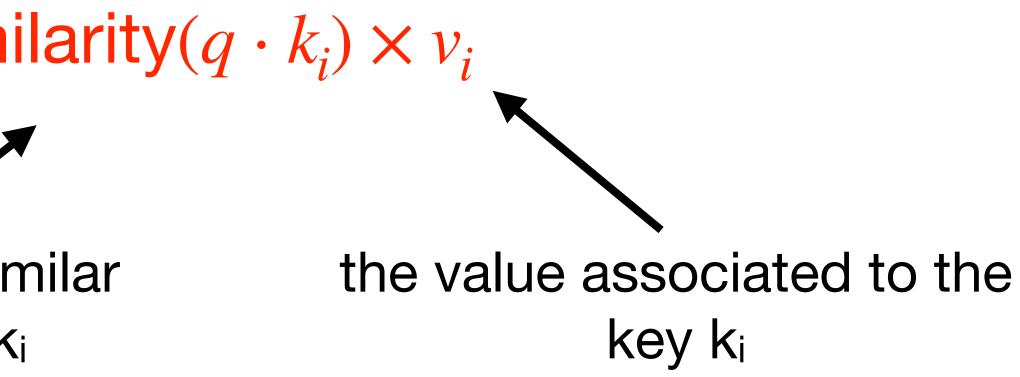
• in a database retrieval process the query is used to identify a key that allows to



attention(
$$q$$
, \mathbf{k} , \mathbf{v}) = $\sum_{i} sim_{i}$
a way to measure how sin
("aligned") are g and k

- in a db normally the query returns one value, and this corresponds to use a similarity value v_k

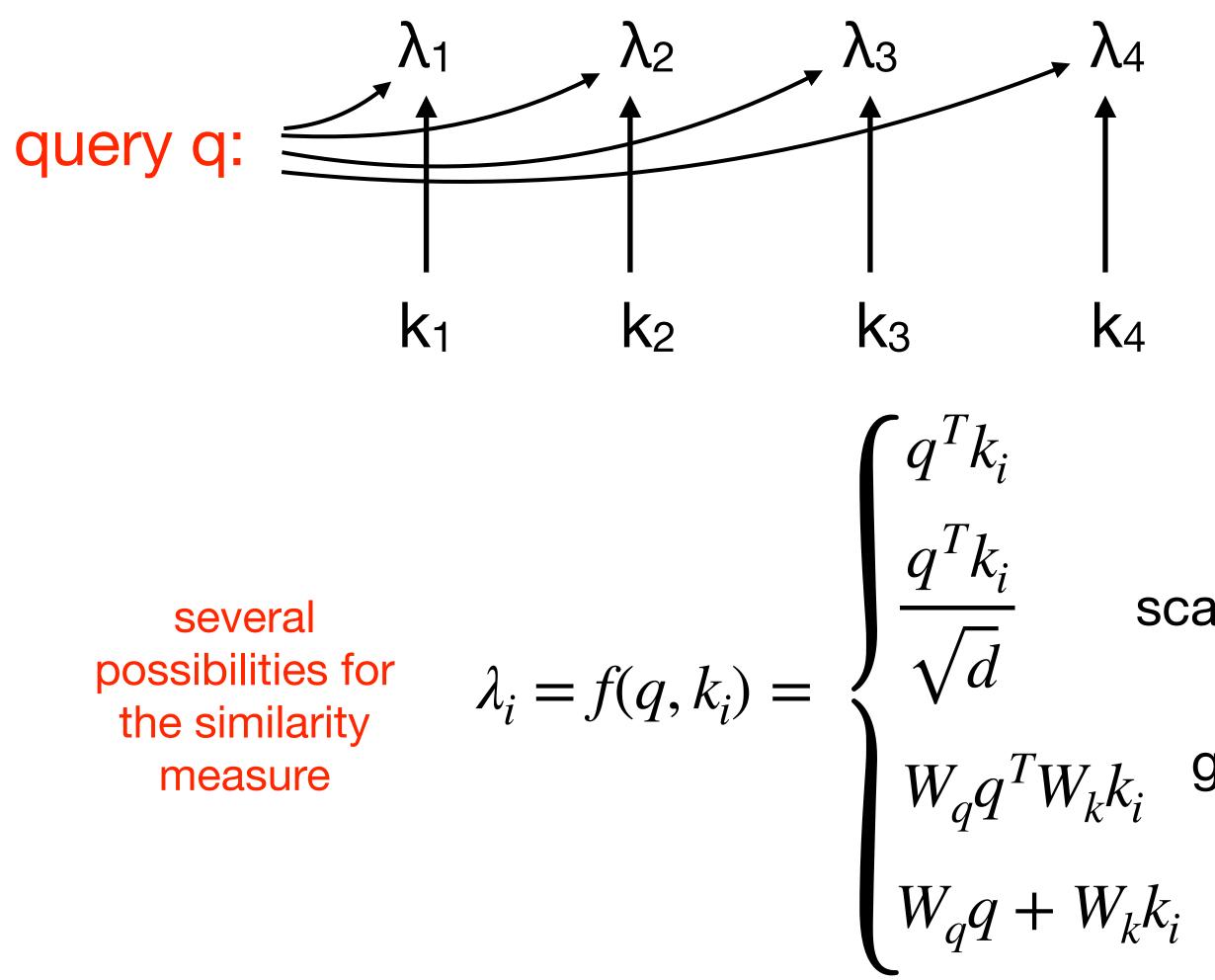
the dotted attention mechanism mimics this via a neural network architecture:



function that produce a one-hot encoding [0,0,0,...,1,0,...,0] that effectively return just one

• the dotted attention generalise this by using a distribution, e.g. weights $\in [0,1]$ that sum up to 1





- as example in a machine translation task we may have:
 - query i: hidden representation vector for the i-th output word: si
 - key j: hidden representation vector for the j-th input word: hi
 - value i: again the hidden representation vector for the j-th input word: hi

similarity measures

dot product

much more efficient than additive similarity

scaled dot product

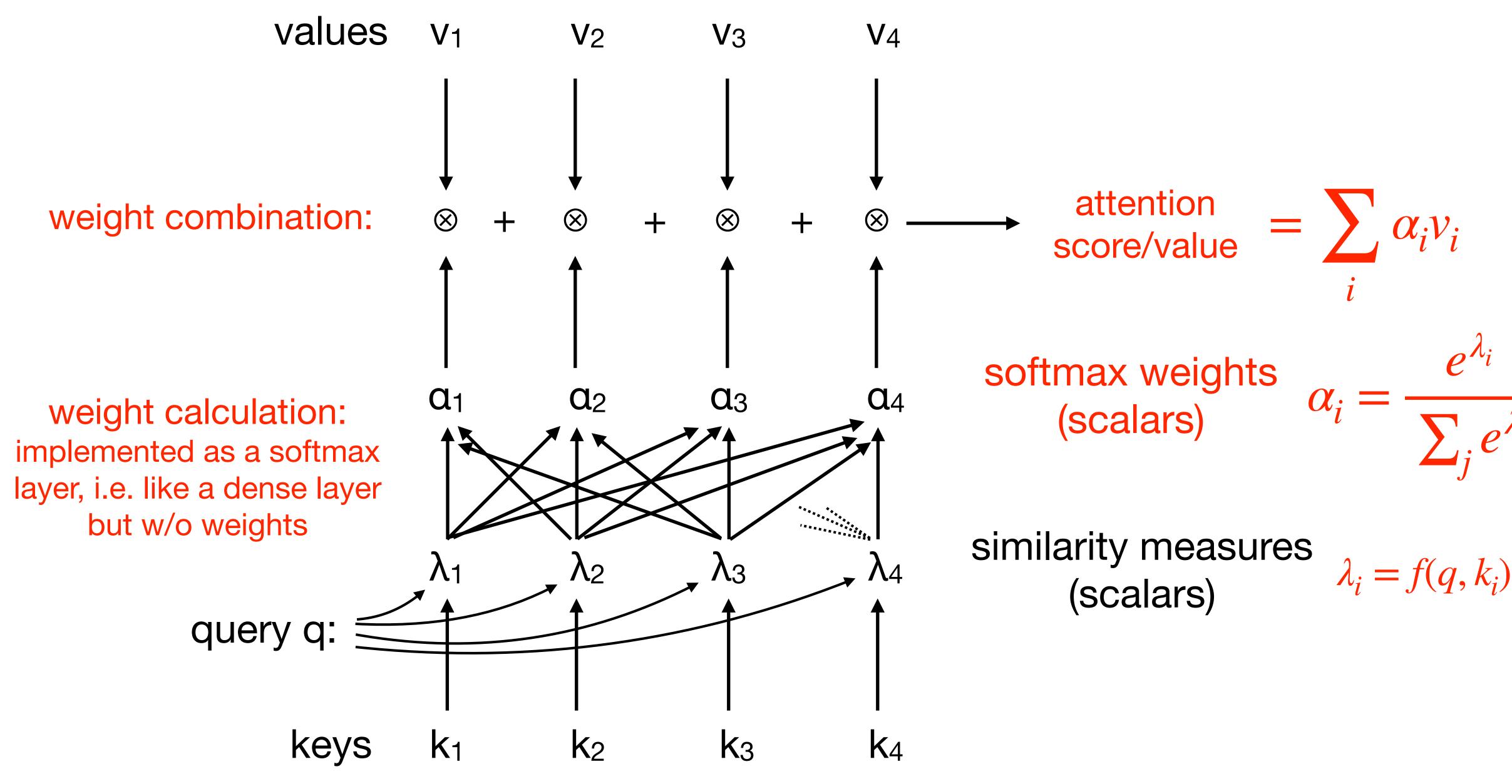
project the query on a new space (for example to be in the same space from $W_q q^T W_k k_i$ general (scaled) the point of view of the similation dot product the key) via a learnable transf $W_q q + W_k k_i$ additive similarity (as in the RNNSearch) the point of view of the similarity as the key) via a learnable transformation

general (scaled)

this way the attention allows to compare each output word with a context vector that takes into account all the input words







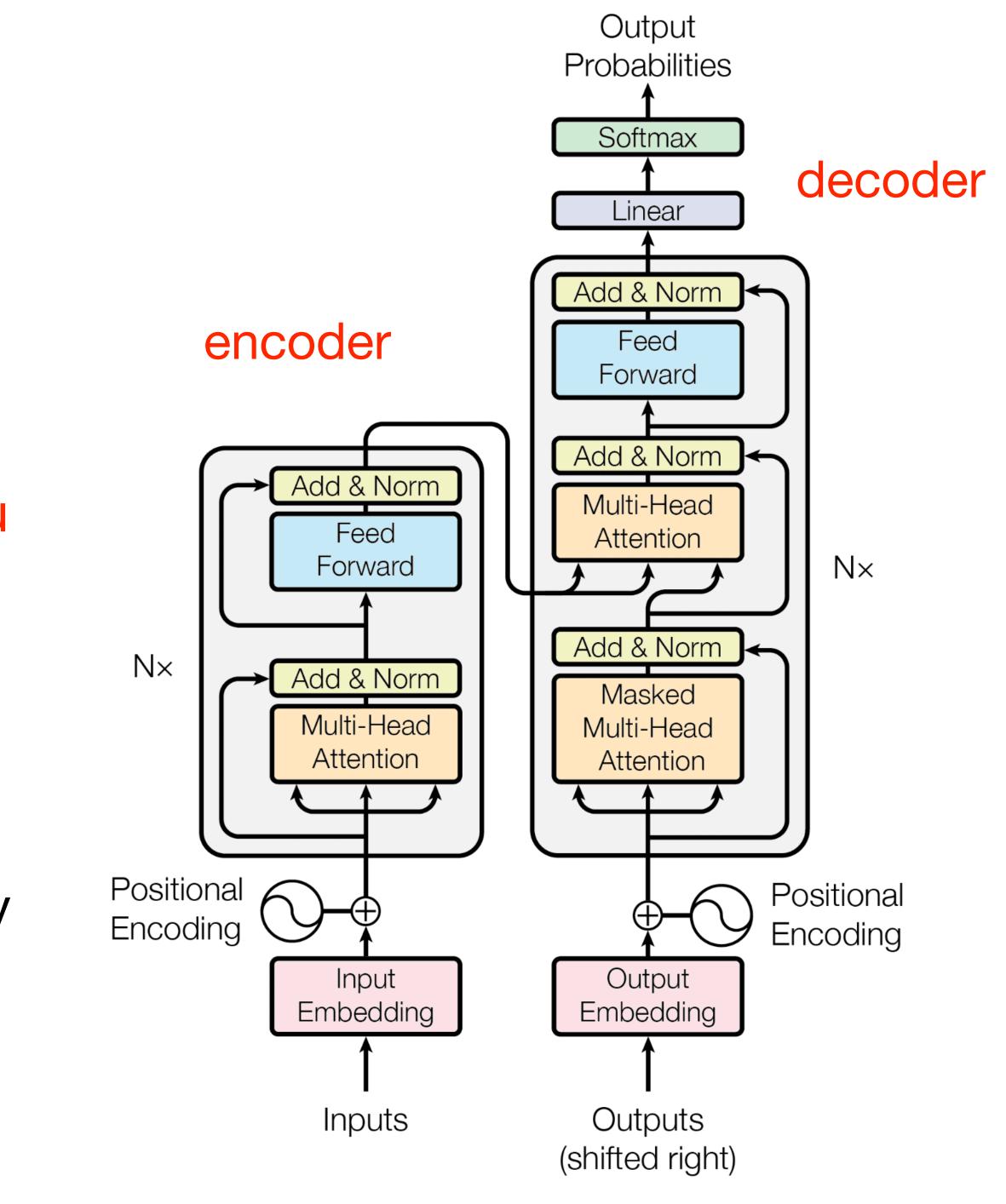


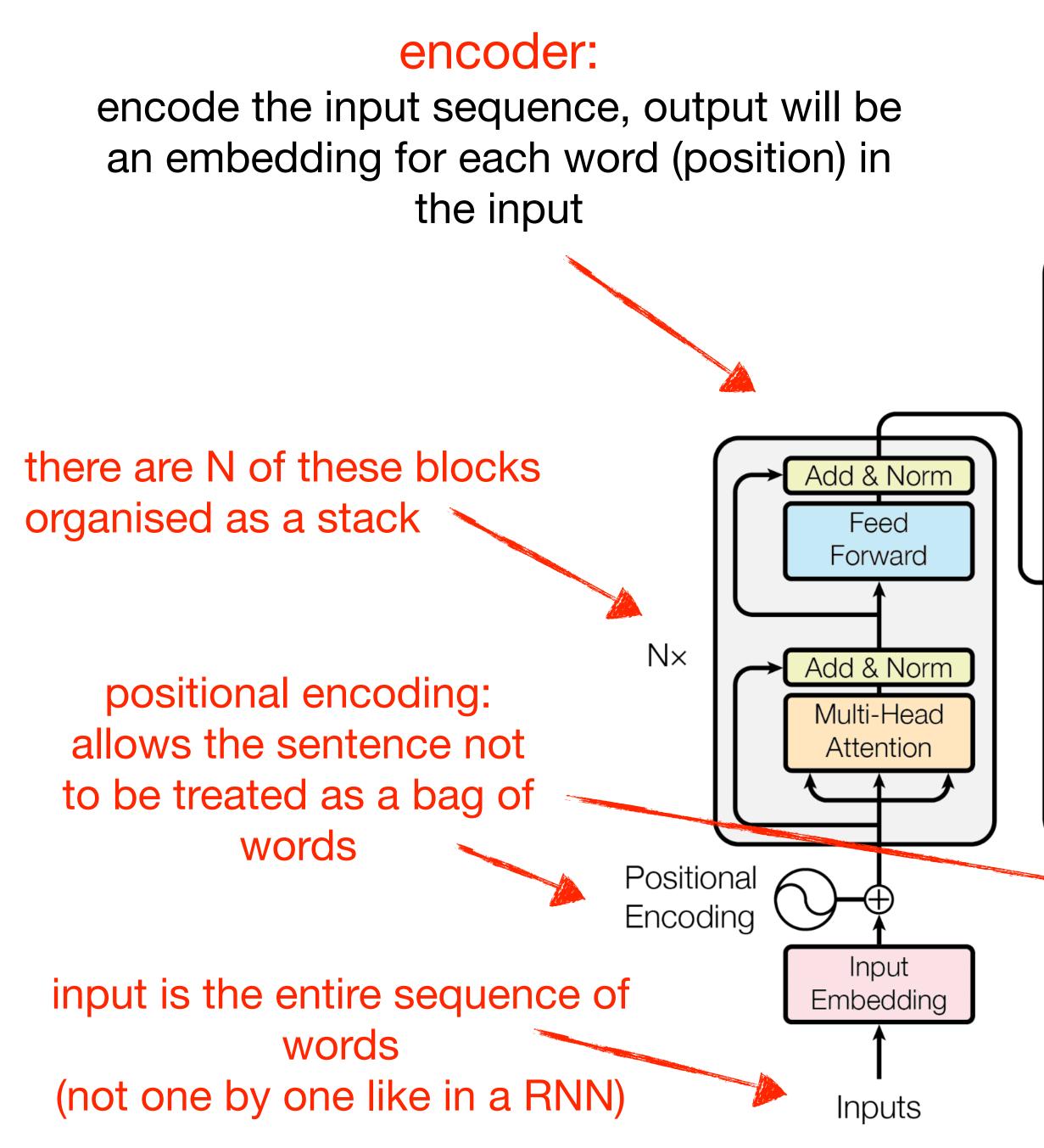




TRANSFORMER ARCHITECTURE

- A. Vaswani et al. "Attention is All You Need" (2017) <u>arXiv:1706.03762</u>
- Encoder-decoder architecture for sequence analysis fully based on attention w/o recurrence
- Today has substantially replaced any other DNN model for NLP tasks





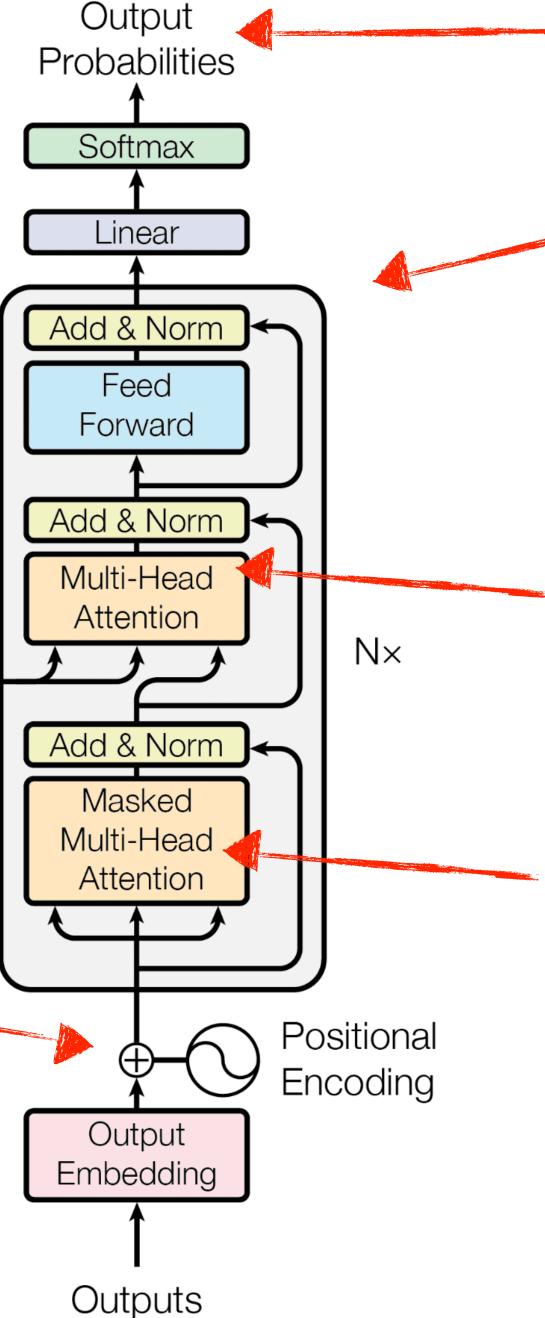


decoder:

looks at the correlations from the output words and between them and the encoded input to produce the translated text

attention layer that combines output words embedding with input words embeddings

self attention layer that combines output words with previous output words (w/ teacher forcing)



(shifted right)



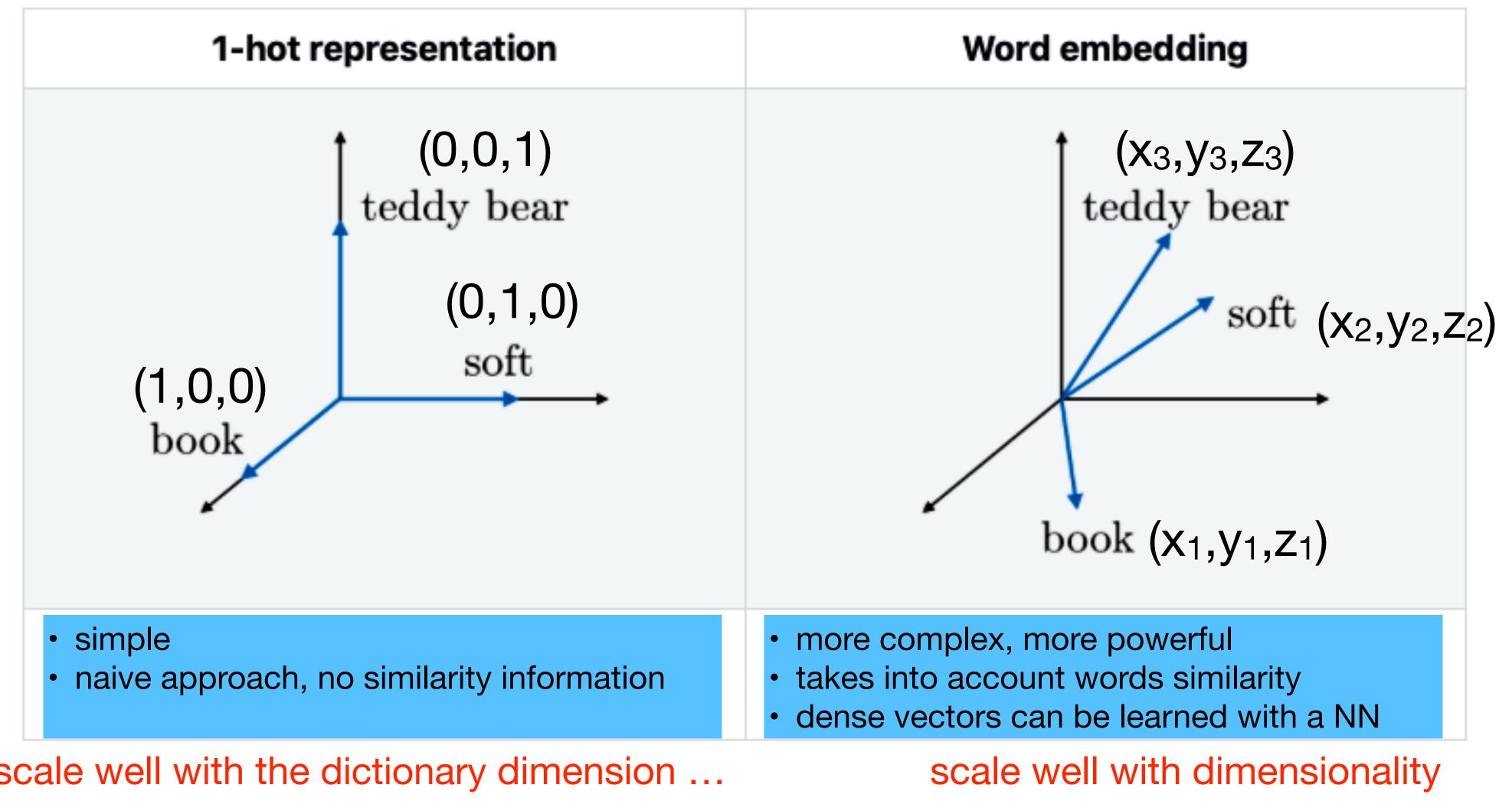






WORD EMBEDDING (I.E. LEARN REPRESENTATIONS OF WORDS)

to be understood by a NN a text must be vectorized + represented effectively two main techniques typically used:



example: a 3 words dictionary

doesn't scale well with the dictionary dimension ...



MULTI HEAD (SELF) ATTENTION

- it is the core of the Transformer architecture, the structure is the same of the attention layer we have just discussed:
 - feed with a vector made by the embedding vectors of every words in the sentence

 - and values are computed:

$$Q_{i} = XW_{q,i} \qquad K_{i} = XW_{k,i} \qquad V_{i} = XW_{v,i}$$

extention is computed: $h_{i}(Q_{i}, K_{i}, V_{i}) = \operatorname{attention}(Q_{i}, K_{i}, V_{i}) = \operatorname{softmax}\left(\frac{Q_{i}K_{i}^{T}}{\sqrt{d_{k}}}\right)V_{i}$

for each one a dot product a

and finally all of them are concatenated before to apply a final projection:

combined together ...

• the MH attention compute the self attention between every position and every other position in the input vector, treating each word as a query and find some keys that corresponds to the other words on the sentence and make a weighted convex sum of the values (taken to be equal to the keys) to produce a better embedding that merge informations from pair of words

• to increase the expressive power, in a way similar to the convolution filters in a CNN, multiple sets i=1,...,h of keys, querys,

 $MultiHead(Q, K, V) = concat[h_1, h_2, ..., h_h]W_0$

• NOTE: in the Transformer there are N of these multi head attention blocks organised in stacks, the first one capture correlations between pair of words, second between pair of pair of words, and so on so eventually all the words in the sentence will be









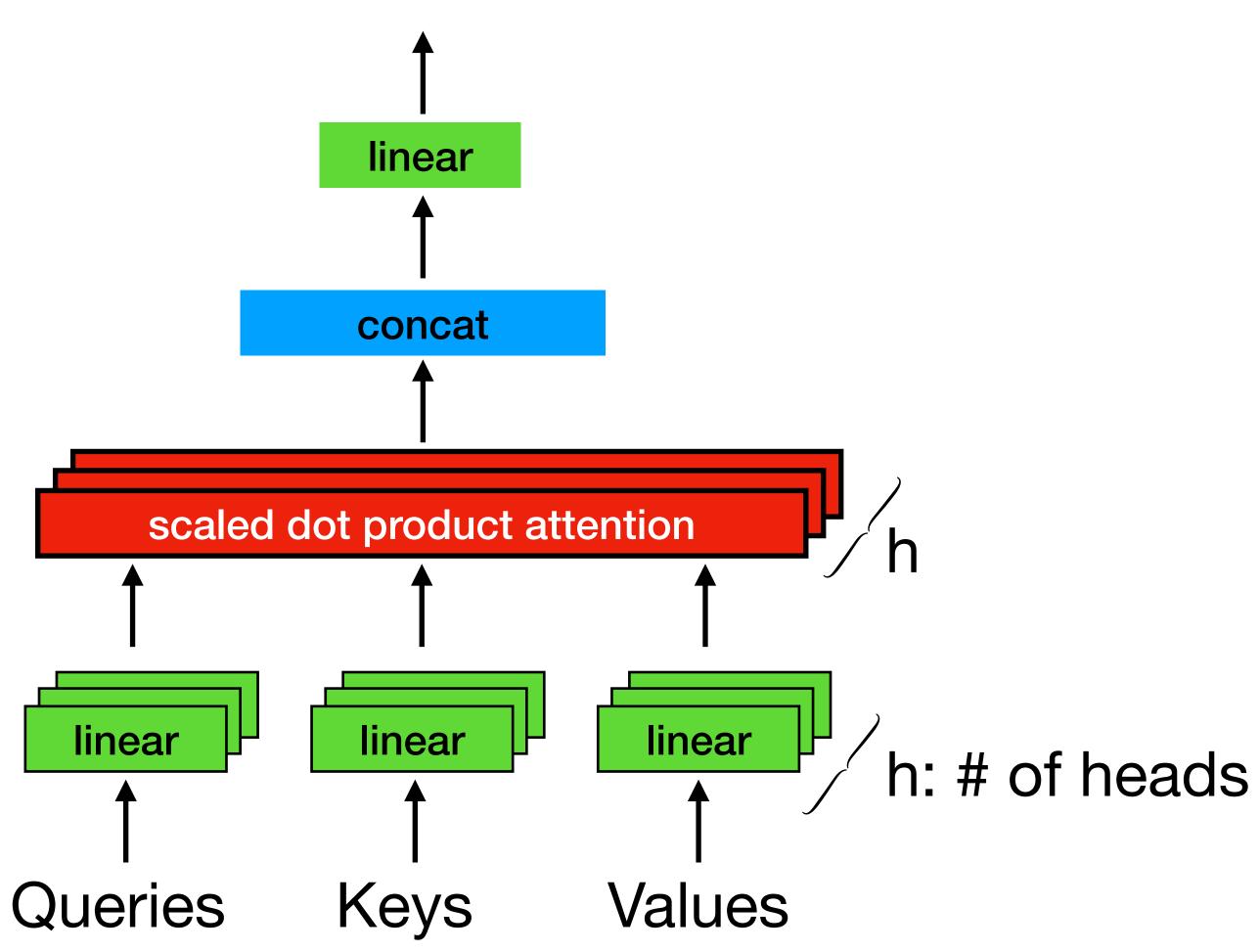
schema of a MH Attention layer

$concat[h_1, h_2, ..., h_h]$

$$\mathsf{H}_{i}(Q_{i}, K_{i}, V_{i}) = \operatorname{softmax}\left(\frac{Q_{i}K_{i}^{T}}{\sqrt{d_{k}}}\right)V_{i}$$

 $Q_i = XW_{q,i}$ $K_i = XW_{k,i}$ $V_i = XW_{v,i}$

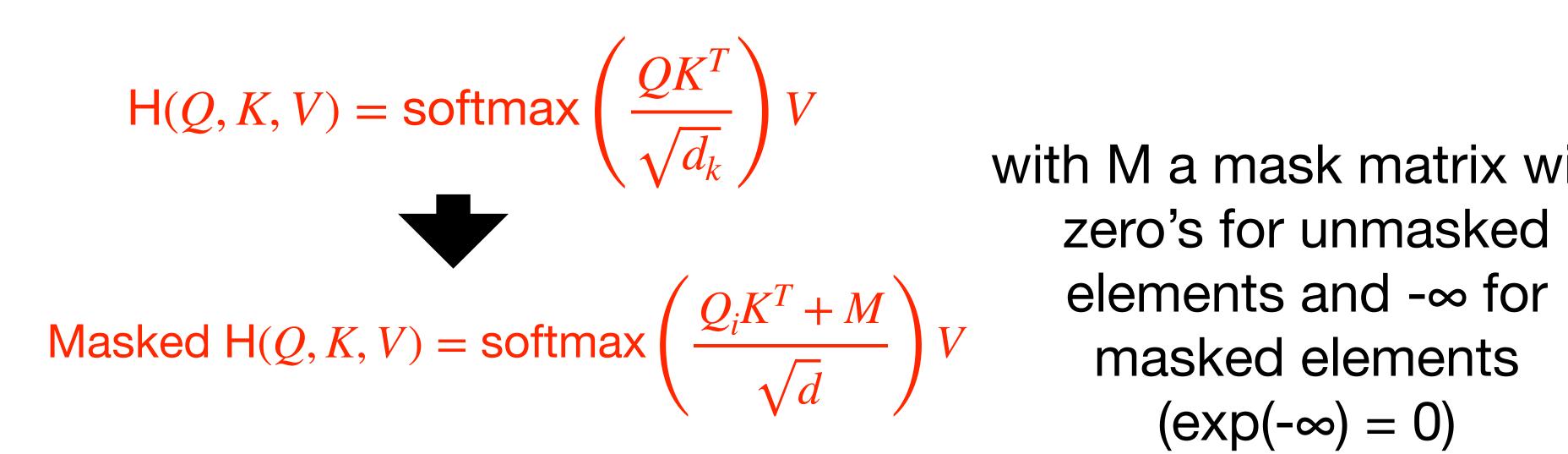






MASKED MH ATTENTION

- them to be selected





is a masked version of the MHA layer in which some values are masked to prevent

• in the decoder the first MHA combines output words with previous output words (a given output cannot depends on future outputs), so future outputs will be masked

> MatMu SoftMax with M a mask matrix with Mask (op MatMul $(\exp(-\infty) = 0)$







LAYER NORMALIZATION

- compensate for the fact that we are normalising:

$$\mu = \frac{1}{H} \sum_{i=1}^{H} h_i$$

• is very similar to a batch normalisation layer, with the difference that here the small batch sizes

 normalize values in each layer to have 0 mean and 1 variance to reduce covariate shifts (eg gradient correlations/dependences between each layer), making training faster

• for each hidden unit h substitute h with $\gamma(h-\mu)/\sigma$ with γ a "gain" hyper parameter that

$$\sigma = \sqrt{\frac{1}{H} \sum_{i=1}^{H} (h_i - \mu)^2}$$

normalisation is done at the level of the layer (normalising across hidden units) while in BN is done for each units normalising across batch elements, so it is no sensitive to







POSITIONAL EMBEDDING

- is used in both encoder and decoder modules just right after the input
- \bullet
- permutation equivariance in the transformer model)
- implemented with a trick:

 - \bullet always well, instead very good performances have been obtained using a sinusoidal embedding:

word position in the input embedding

for each position (scalar) a vector is produced E:

and added to the embedding (X \rightarrow X+E) instead of concatenating it to reduce the number of parameters (this is debatable)



allows the words in the sentence not to be treated as a bag of words, e.g. takes into account the position in the sentence of each word

• this is needed as the attention mechanism is equivariant to the ordering of the elements (e.g. MH(PX) = P MH(X) with P permutation matrix) and this is not what we want for an input that is a sequence in which order is important (PE can be omitted in case we want to retain

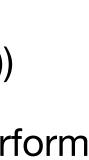
• use a vector that embed the position and add or concatenate this to the word embedding vector: $MH(Pconc(X,E)) \neq P MH(conc(X,E))$

empirically using as positional embedding vector a position integer or a one-hot encoding of the position has been shown to not perform

$$E_{pos,2i} = \sin(pos \times \omega_i) = \sin\left(\frac{pos}{10000^{2i/d}}\right)$$

i: from 0 to d-1
$$E_{pos,2i+1} = \cos\left(\frac{pos}{10000^{2i/d}}\right)$$
 d = dimension of the
embedding vector





PERFORMANCES

• original transformer

	Madal	BLEU		Training Cost (FLOPs)		
	Model	EN-DE	EN-FR	EN-DE	EN-FR	
	ByteNet [18]	23.75				
	Deep-Att + PosUnk [39]		39.2		$1.0 \cdot 10^{20}$	
	GNMT + RL [38]	24.6	39.92	$2.3\cdot 10^{19}$	$1.4\cdot10^{20}$	
	ConvS2S [9]	25.16	40.46	$9.6\cdot10^{18}$	$1.5\cdot 10^{20}$	
	MoE [32]	26.03	40.56	$2.0\cdot10^{19}$	$1.2\cdot10^{20}$	
	Deep-Att + PosUnk Ensemble [39]		40.4		$8.0\cdot10^{20}$	
	GNMT + RL Ensemble [38]	26.30	41.16	$1.8\cdot 10^{20}$	$1.1\cdot 10^{21}$	
	ConvS2S Ensemble [9]	26.36	41.29	$7.7\cdot 10^{19}$	$1.2\cdot 10^{21}$	
65 Mpar	Transformer (base model)	27.3	38.1	3.3 •	10 ¹⁸ larges	t of the two
213 Mpar	Transformer (big)	28.4	41.8		10	DE/EN-FR

BLEU score: percentage of translated words that appear in the ground truth

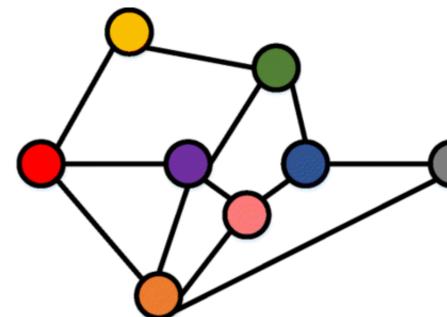


TRANSFORMERS AND GNN

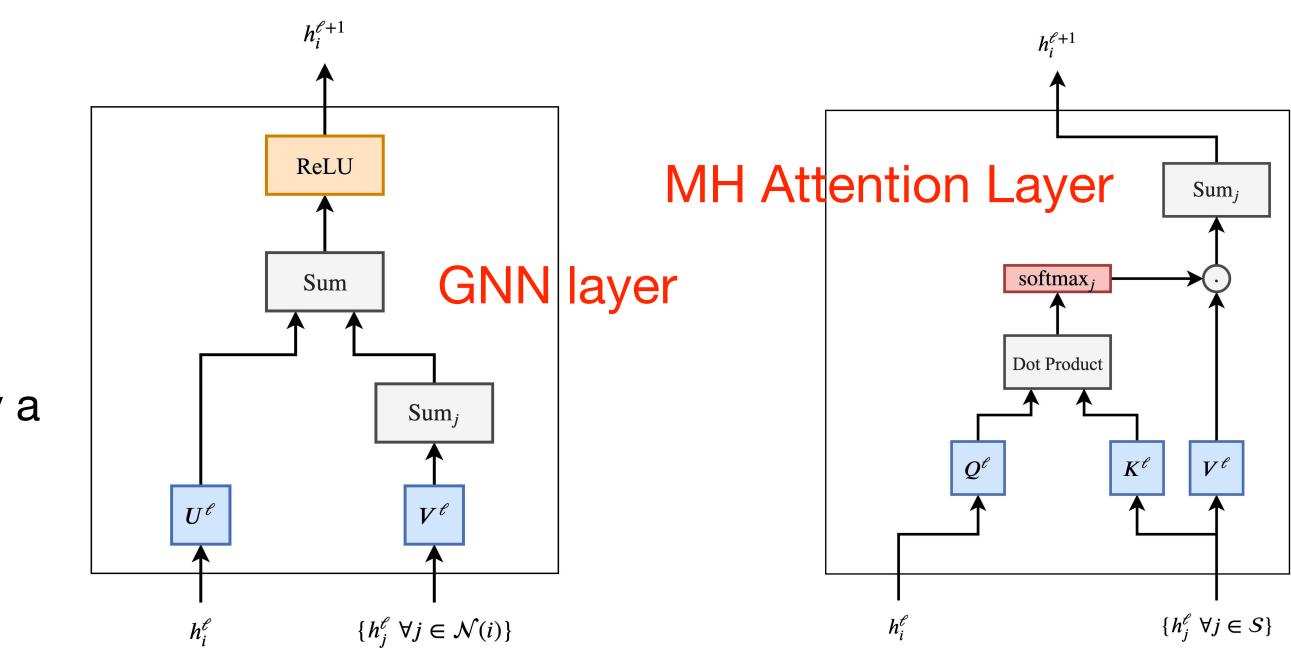
- there is a strong link between Graph Neural Networks and Transformers
- in the most simple form a GNN update the hidden feature of a given node, by message passing, i.e. by a non

$$j \in N(i)$$
 $h_i^{t+1} = \phi(U^t h_i^t + \sum_{j \in N(i)} (V^t h_j^t))$
non linear function
(i.e. ReLU, σ , ...) learnable weight matrices

- the sum over the neighbours node can be replaced by a permutation invariant aggregation function (ex. mean, max, ...), or with more powerful aggregators, like an attention mechanism
- Network (GAT), adding normalisation and an MLP we get something formally equivalent to a graph transformer
- a Transformer is a GNN with a multi-head attention as aggregation function
- local neighbourhood, aggregating features from each element of the sequence at each layer



linear transformation of the node feature added to an aggregation of the features of the neighbouring nodes:



• replacing the summation over the neighbours j with the attention mechanism, i.e., with a weighted sum, we'd get the Graph Attention

• while a GNN aggregate features from their local neighbourhood nodes $j \in N(i)$, transformers treat the whole input sequence as the









TRANSFORMERS EVOLUTIONS

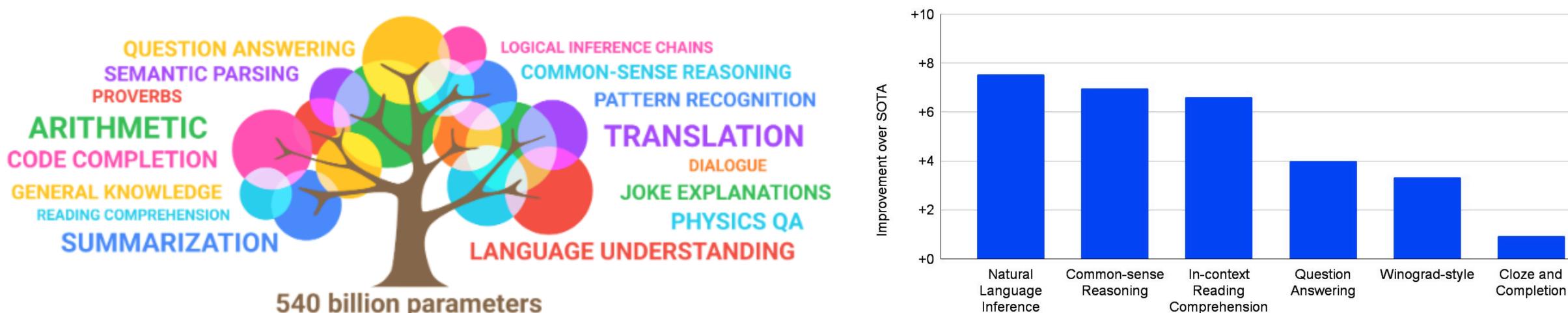
- the original transformer has spawn series of evolutions that today dominate NLP
- GPT (2018)/GPT2/GPT3 (GPT3: 175B paramaters): unsupervised multitask learned based on a decoder transformer (no encoder) that predicts next words based on previous words by computing $P(x_t|x_{1,...,x_{t-1}})$
- BERT (2019), 340M parameters: unsupervised bi-directional encoder transformer that predicts a missing word based on surrounding words by computing Softmax Classifier $P(x_t|x_{1,...,x_{t-1},x_{t+1,...,x_N})$ or the next sentence based on a previous sentence \mathbf{u}_1 \mathbf{u}_6 \mathbf{u}_3 Transformer's Encoder randomly mask one or multiple words in the sentence, the X_3 associated context is passed to a softmax classifier that produce Embedding Layer the probability of classifying the mat the [MASK] sat on the

correct missing word



Google - PalM (Pathways Language Model): <u>arXiv:2204.02311</u>

- 540B parameters
- single model that can generalize across different domains and tasks
- highly efficient training across multiple TPUs pods
- few-shot performance across most tasks, by significant margins in many cases



540 billion parameters

- tested on hundreds of language understanding and generation tasks: achieves state-of-the-art





Prompt

```
// Translate from C to Python
int add_one ( int x ){
 int m = 1;
 while (x&m) {
   x = x ^ m;
   m <<= 1;
 x = x^{m};
 return x; }
```

Prompt

def exercise5():

"""Marie ordered one chicken meal that costs \$12, 5 packs of milk that cost \$3 each, 4 apples that cost \$1.50 each, and some boxes of pizza. Marie paid a total of \$50. How many boxes of pizza did Marie order if box costs \$8.50?"""

```
def add_one(x: int):
  m = 1
  while (x & m):
    x = (x ^ m)
    m <<= 1
  x = (x ^ m)
  return x
```

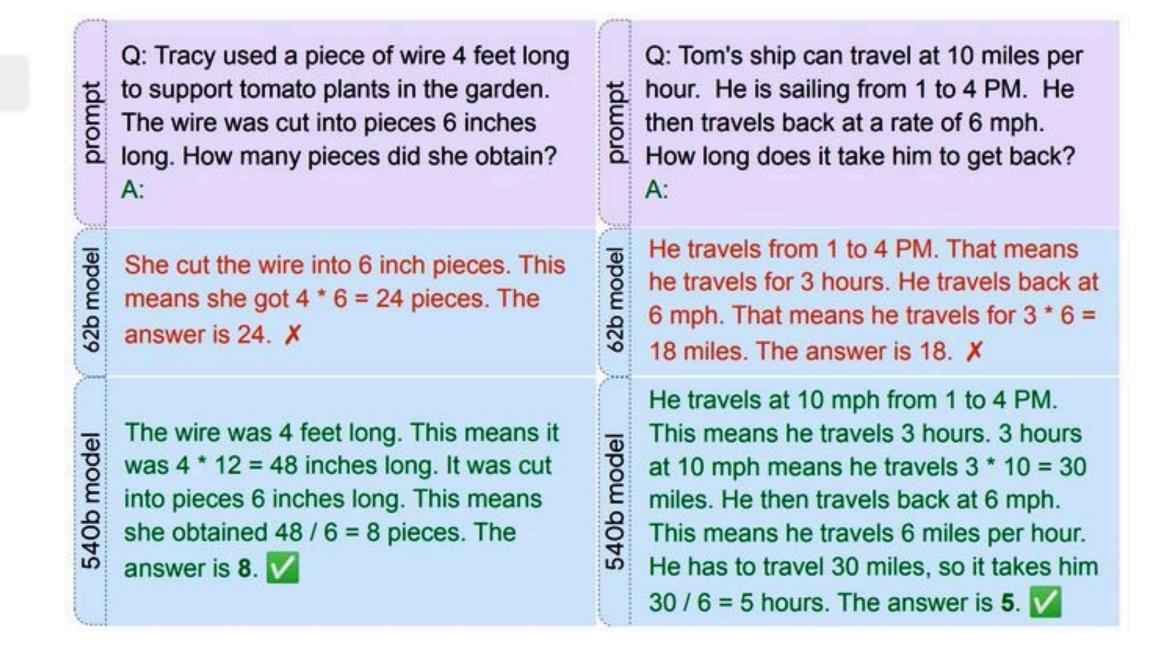
Model Response

Model Response

total_paid = 50 cost_of_pizza_per_box = 8.50 cost_of_meal = 12 cost_of_milk_per_pack = 3 cost_of_apples_per_apple = 1.50 packages_of_milk = 5

```
return float(total_paid - cost_of_meal-
cost_of_milk_per_pack * packages_of_milk -
cost_of_apples_per_apple * 4)/
cost_of_pizza_per_box
```

some PalM examples ...



Explaining a joke

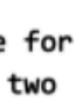
Prompt

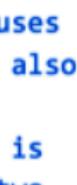
Explain this joke:

Joke: Did you see that Google just hired an eloquent whale for their TPU team? It showed them how to communicate between two different pods!

Model Response

Prediction: TPUs are a type of computer chip that Google uses for deep learning. A "pod" is a group of TPUs. A "pod" is also a group of whales. The joke is that the whale is able to communicate between two groups of whales, but the speaker is pretending that the whale is able to communicate between two groups of TPUs.







OpenAI - DALL·E 2: <u>https://openai.com/dall-e-2/</u>

- scaled down (3.5B parameters) evolution of the first version DALL-E (12B pars) released in 2021 which in turn is a scaled down evolution from GPT3 (175B pars)
- generative transformer (combines transformers with diffusion models) able to create new realistic images and art from based on a text description. It can combine concepts, attributes, and styles

TEXT DESCRIPTION

An astronaut Teddy bears A bowl of soup



TEXT DESCRIPTION

An astronaut Teddy bears A bowl of soup

riding a horse lounging in a tropical resort in space playing basketball with cats in space

"A rabbit detective sitting on a park bench and reading a newspaper in a victorian setting"





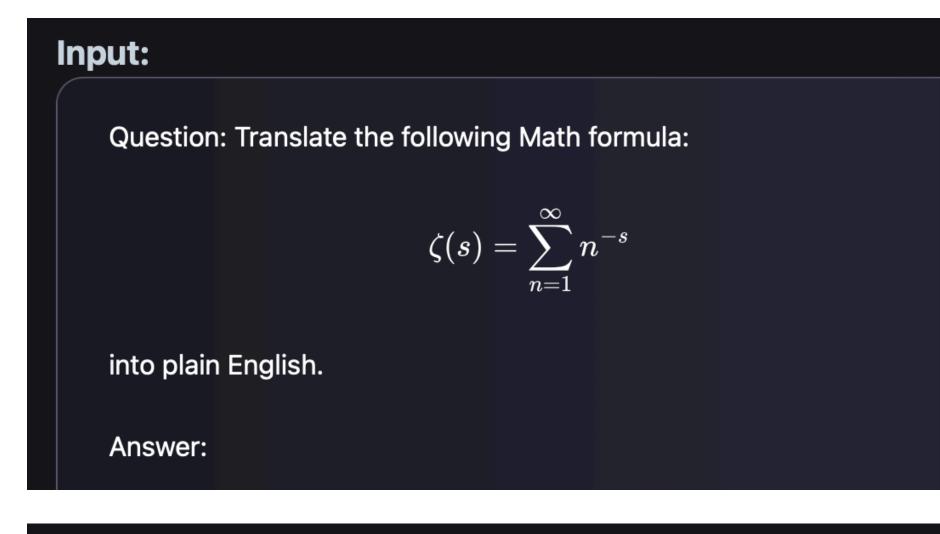
"macro 35mm film photography of a large family of mice wearing hats cozy by the fireplace"





Meta - Galactica: http://galactica.org/

- citations and help discover related papers



Input:

A paper that suggested to initialize model weights of linear layers with n inputs and m outputs using the following formula:

numpy.random.normal(0, numpy.sqrt(2 / n))

- transformer model (125B parameters) trained on a large corpus comprising more than 360 millions in-context citations and over 50 millions of unique references normalized across a diverse set of sources. Eenables to suggest

- on technical knowledge probes such as LaTeX equations, outperforms the latest GPT-3 and PaLM 540B on MATH.

GALACTICA Output:

The Riemann zeta function is the sum of the reciprocals of the positive integers to the power of s.

Answer: The Riemann zeta function is the sum of the reciprocals of the positive integers to the power of s.

GALACTICA Suggestions:

Delving Deep into Rectifiers: Surpassing Human-Level Performance on {ImageNet} Classification He et al., 2015



VISION TRANSFORMERS

- point-cloud analyst, etc. tasks
- - is based on the same original Transformer architecture of Vaswani et al.
 - needed to re-train the model is large enough (large enough means > 100M images)
- Simple idea:
 - split the images into patches
 - vectorise the patches into flat vectors lacksquare
 - add positional encodings vectors to preserve patch positions in the original image
 - feed the embedding to a transformer encoder tailored for a classification task



• the very same philosophy of the Transformer architecture can be applied to vision, signal analysis,

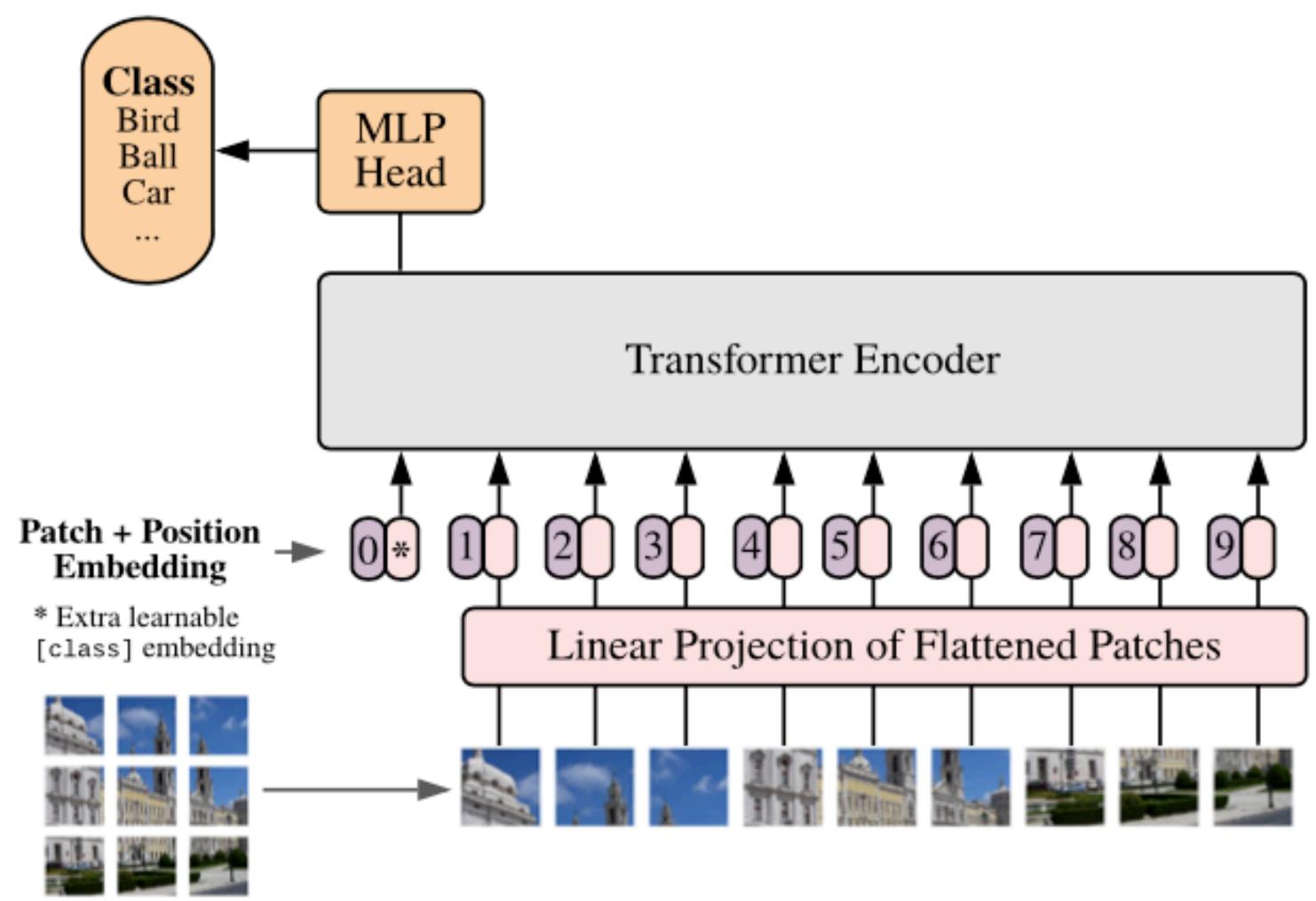
• Vision Transformer (ViT) has been proposed in 2021 by A. Dosovitsky et al. in <u>arXiv:2010.11929</u>

has shown to be able to surpass SOTA CNN architectures ResNet, but only if the dataset





Vision Transformer (ViT)



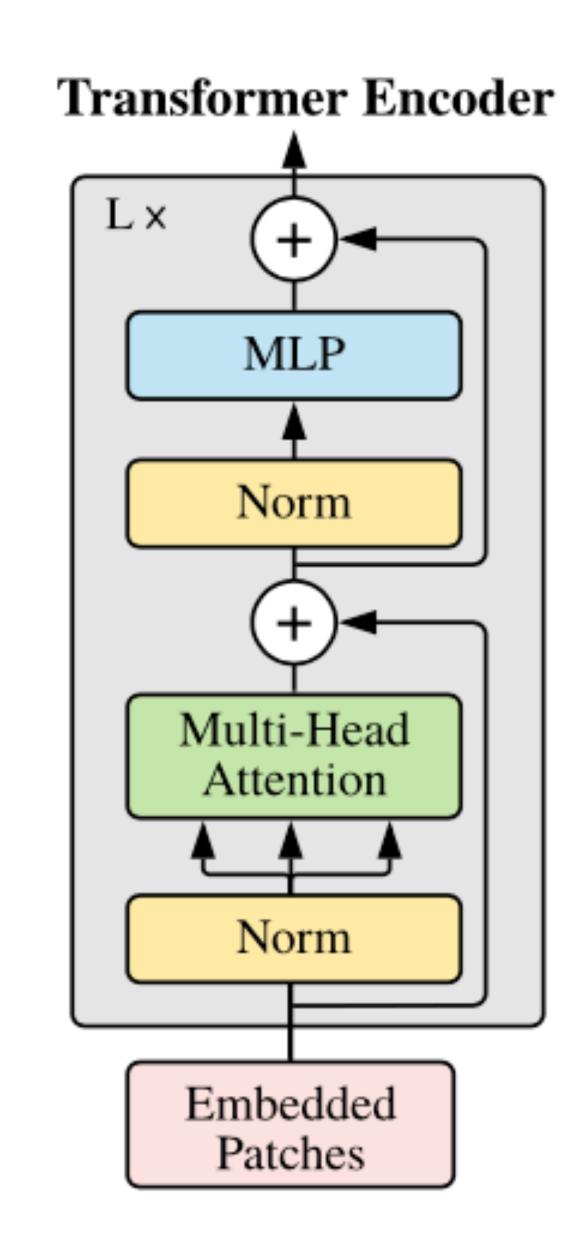
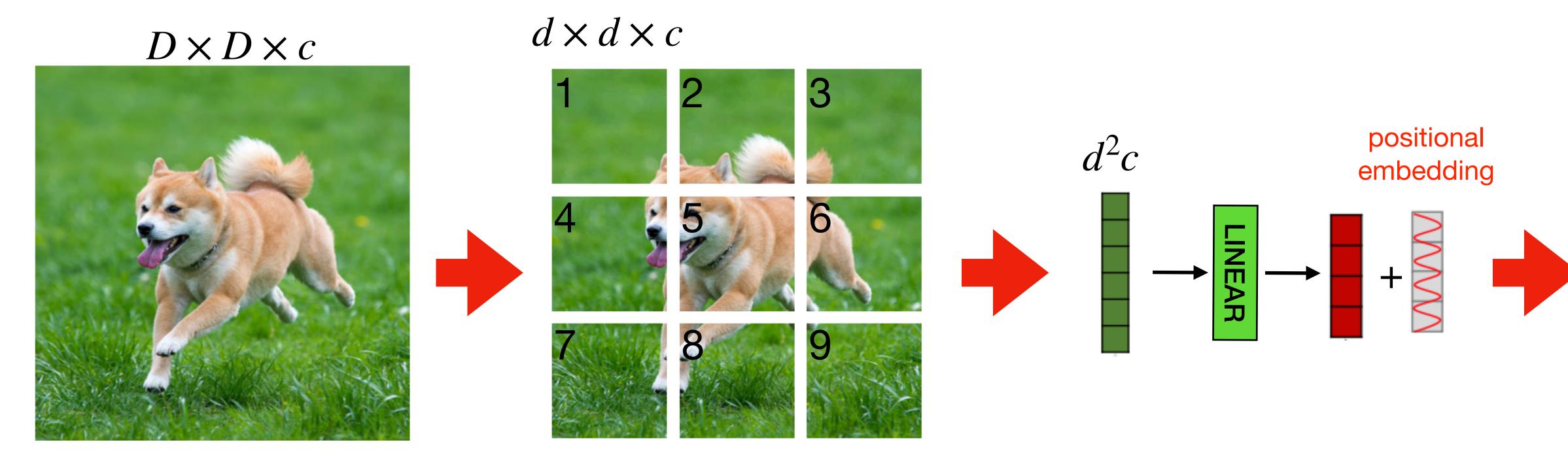


IMAGE PATCHING AND VECTORISATION

patches can overlap or not (the original paper uses not overlapping patches)



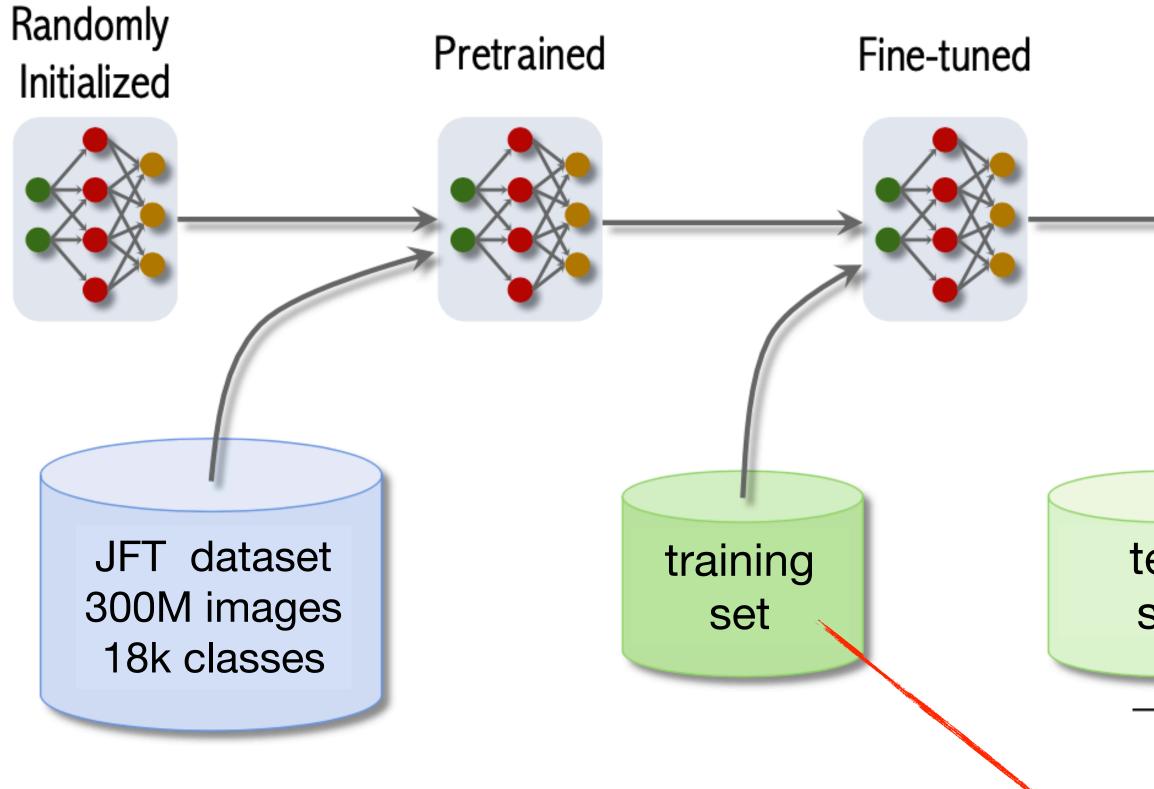
 \bullet

NOTE: VIT has much less image-specific inductive bias than CNNs. In CNNs, locality, two-dimensional neighbourhood structure, and translation equivariance, are baked into each layer throughout the whole model. In ViT, only MLP layers are local and translationally equivariant, while the self-attention layers are global. The two-dimensional neighborhood structure is only used when cutting the image into patches while the position embeddings is only 1D and the 2D spatial relations between the patches have to be learned





TRAINING AND PERFORMANCE



Test Accuracy				
est set	pertained on JFT		pertained or magenet-21 14M images 21k classes	k S
	Ours-JFT (ViT-H/14)	Ours-JFT (ViT-L/16)	Ours-I21k (ViT-L/16)	BiT-L (ResNet152x4)
ImageNet	88.55 ± 0.04	87.76 ± 0.03	85.30 ± 0.02	87.54 ± 0.02
ImageNet ReaL	90.72 ± 0.05	90.54 ± 0.03	88.62 ± 0.05	90.54
CIFAR-10	99.50 ± 0.06	99.42 ± 0.03	99.15 ± 0.03	99.37 ± 0.06
CIFAR-100	94.55 ± 0.04	93.90 ± 0.05	93.25 ± 0.05	93.51 ± 0.08
Oxford-IIIT Pets	97.56 ± 0.03	97.32 ± 0.11	94.67 ± 0.15	96.62 ± 0.23
Oxford Flowers-102	99.68 ± 0.02	99.74 ± 0.00	99.61 ± 0.02	99.63 ± 0.03
VTAB (19 tasks)	77.63 ± 0.23	76.28 ± 0.46	72.72 ± 0.21	76.29 ± 1.70
TPUv3-core-days	2.5k	0.68k	0.23k	9.9k





AN EXAMPLE OF PYTORCH IMPLEMENTATION OF VIT

<u>https://github.com/lucidrains/vit-pytorch</u>

```
class Attention(nn.Module):
     def __init__(self, dim, heads = 8, dim_head = 64, dropout = 0.):
         super().__init__()
        inner_dim = dim_head * heads
         project_out = not (heads == 1 and dim_head == dim)
         self.heads = heads
        self.scale = dim_head ** -0.5
         self.attend = nn.Softmax(dim = -1)
         self.dropout = nn.Dropout(dropout)
         self.to_qkv = nn.Linear(dim, inner_dim * 3, bias = False)
         self.to_out = nn.Sequential(
            nn.Linear(inner_dim, dim),
            nn.Dropout(dropout)
         ) if project_out else nn.Identity()
                                                                                 MatMul
    def forward(self, x):
        qkv = self.to_qkv(x).chunk(3, dim = -1)
                                                                          SoftMax
         q, k, v = map(lambda t: rearrange(t, 'b n (h d) -> b h r d',
                                                                         Mask (opt.)
         dots = torch.matmul(q, k.transpose(-1, -2)) * self.scale
                                                                             Scale
         attn = self.attend(dots)
         attn = self.dropout(attn)
                                                                            MatMul
         out = torch.matmul(attn, v)
         out = rearrange(out, 'b h n d -> b n (h d)')
                                                                                  Κ
         return self.to_out(out)
```

```
class Transformer(nn.Module):
   def __init__(self, dim, depth, heads, dim_head, mlp_dim, dropout = 0.):
       super().__init__()
       self.layers = nn.ModuleList([])
       for _ in range(depth):
          self.layers.append(nn.ModuleList([
              PreNorm(dim, Attention(dim, heads = heads, dim_head = dim_head, dropout = dropout)),
              PreNorm(dim, FeedForward(dim, mlp_dim, dropout = dropout))
          ]))
   def forward(self, x):
       for attn, ff in self.layers:
          x = attn(x) + x
          x = ff(x) + x
                               class ViT(nn.Module):
       return x
                                   def __init__(self, *, image_size, patch_size, num_clas
                                        super().__init__()
                                        image_height, image_width = pair(image_size)
                                        patch_height, patch_width = pair(patch_size)
     def forward(self, img):
         x = self.to_patch_embedding(img)
         b, n, _ = x.shape
         cls_tokens = repeat(self.cls_token, '1 n d -> b n d', b = b)
         x = torch.cat((cls_tokens, x), dim=1)
         x += self.pos_embedding[:, :(n + 1)]
         x = self.dropout(x)
         x = self.transformer(x)
         x = x.mean(dim = 1) if self.pool == 'mean' else x[:, 0]
         x = self.to_latent(x)
         return self.mlp_head(x)
```



