

I want to know what attention is
I want you to show me

*Introduction to attention in NLP
(a practitioner's perspective)*

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Intuition

Given a collection of input representations,
the attention mechanism:

1. finds relevance scores for input representations based on our current point of interest
2. uses the relevance scores to weigh the input representations
3. aggregates those into a single representation

Basic terminology

Given a collection of input representations (**keys**),
the attention mechanism:

1. finds relevance scores for input representations based on our current point of interest (**query**)
2. uses the relevance scores to weigh the input representations (**values**)
3. aggregates those into a single representation (**context vector**)

Two main reasons for using attention:

- to improve model's performance,
- for interpretability (visual highlights of attention weights to analyse a model's prediction).

Different foci in literature:

- establishing relevance & compatibility
- memory addressing
- feature selection
- discovering alignment
- interpretability tool

A generalised view of attention

$$e = f(q, K)$$

f is a compatibility function

q is a query vector, $q \in \mathbb{R}^{n(q)}$

K are key vectors, $K \in \mathbb{R}^{n(k) \times d(k)}$

“Energy” scores e contain information about the relevance of a key to the query

$$a = g(e)$$

g is a distribution function (commonly softmax)

Attention weights a are the primary outcome of the attention mechanism.

They are applied to the input representation $V \in \mathbb{R}^{n(v) \times d(k)*}$, yielding a context vector c :

$$c = \sum_{i=1}^{d(k)} a_i v_i$$

* K and V can be obtained via the same weight matrix.

Diagram of the attention mechanism (1/2)

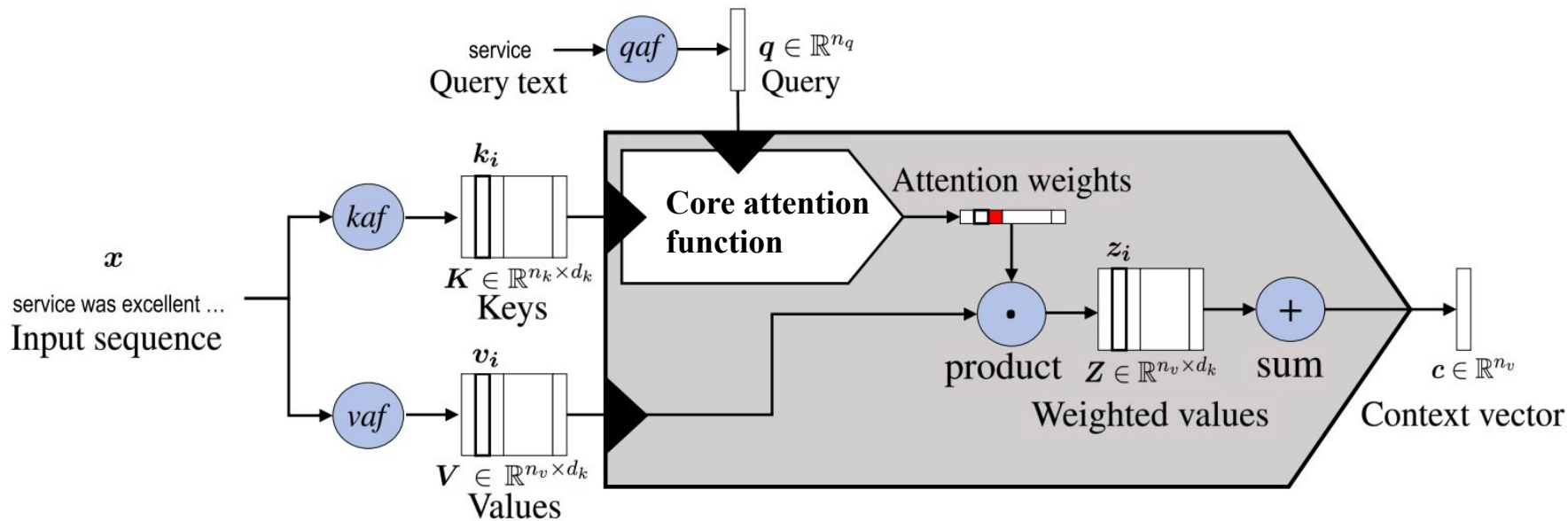
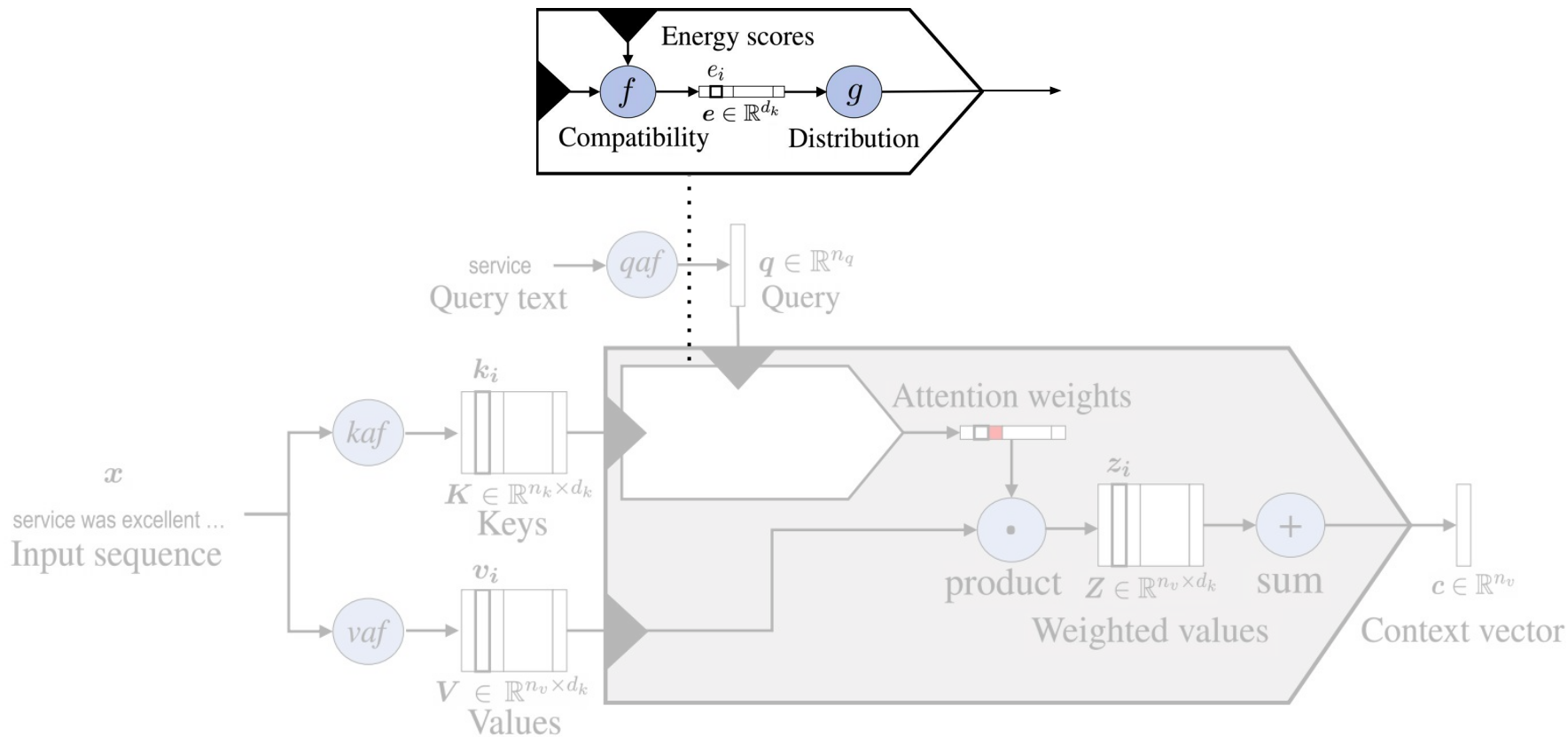


Diagram of the attention mechanism (2/2)



More on compatibility function $f(q, K)$

Some common approaches:

- $q^T K$ (dot product)
- $\text{cosine}(q, K)$
- $(q^T K) / \sqrt{n}$: scaled dot product, e.g. in Transformer; n =key vector dimension, for stability of gradient computation

Parameterised:

- $q^T W K$ (bilinear or general)
- $\text{act}(q^T W K + b)$ (MLP)
- $w_{\text{imp}}^T \text{act}(W_1 q + W_2 K + b)$ (additive)
- deep attention, convolution-based attention...

Attention in machine translation

Place of attention in neural machine translation (MT)

Recurrent neural network (RNN) for MT, without attention (Sutskever et al., 2014):

$$\text{encoder: } h_t^e = f(x_t, h_{t-1}^e)$$

$$\text{decoder: } h_t^d = f(y_{t-1}, h_{t-1}^d, c); P(y_t | y_{<t}, c) = g(h_t, y_{t-1}, c)$$

$c = h_T^e$ (context vector, here set to be encoder's final state)

h_t^d is decoder's newly generated hidden state,

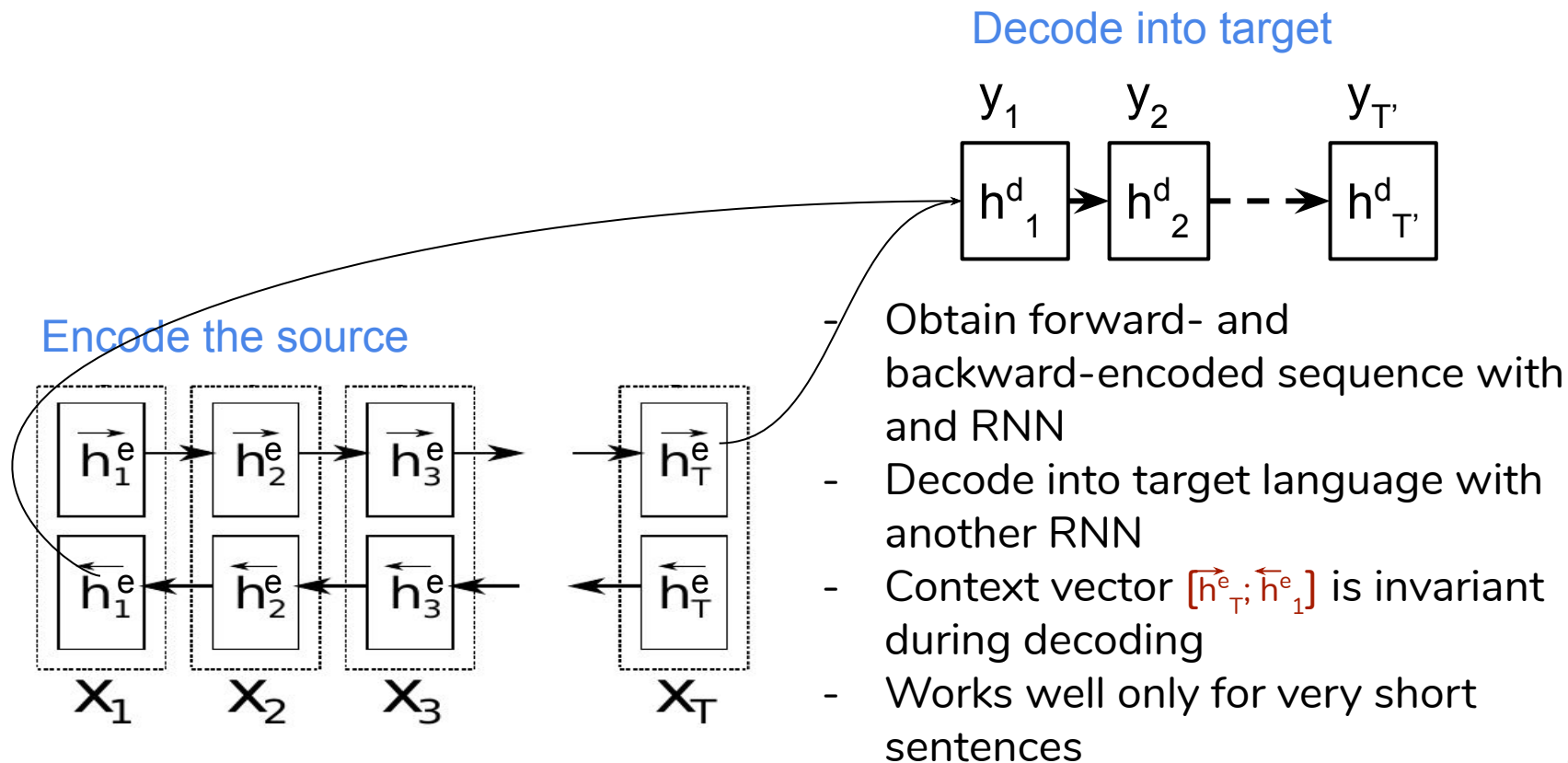
f is a non-linear activation function

g is a non-linear activation function producing valid probabilities

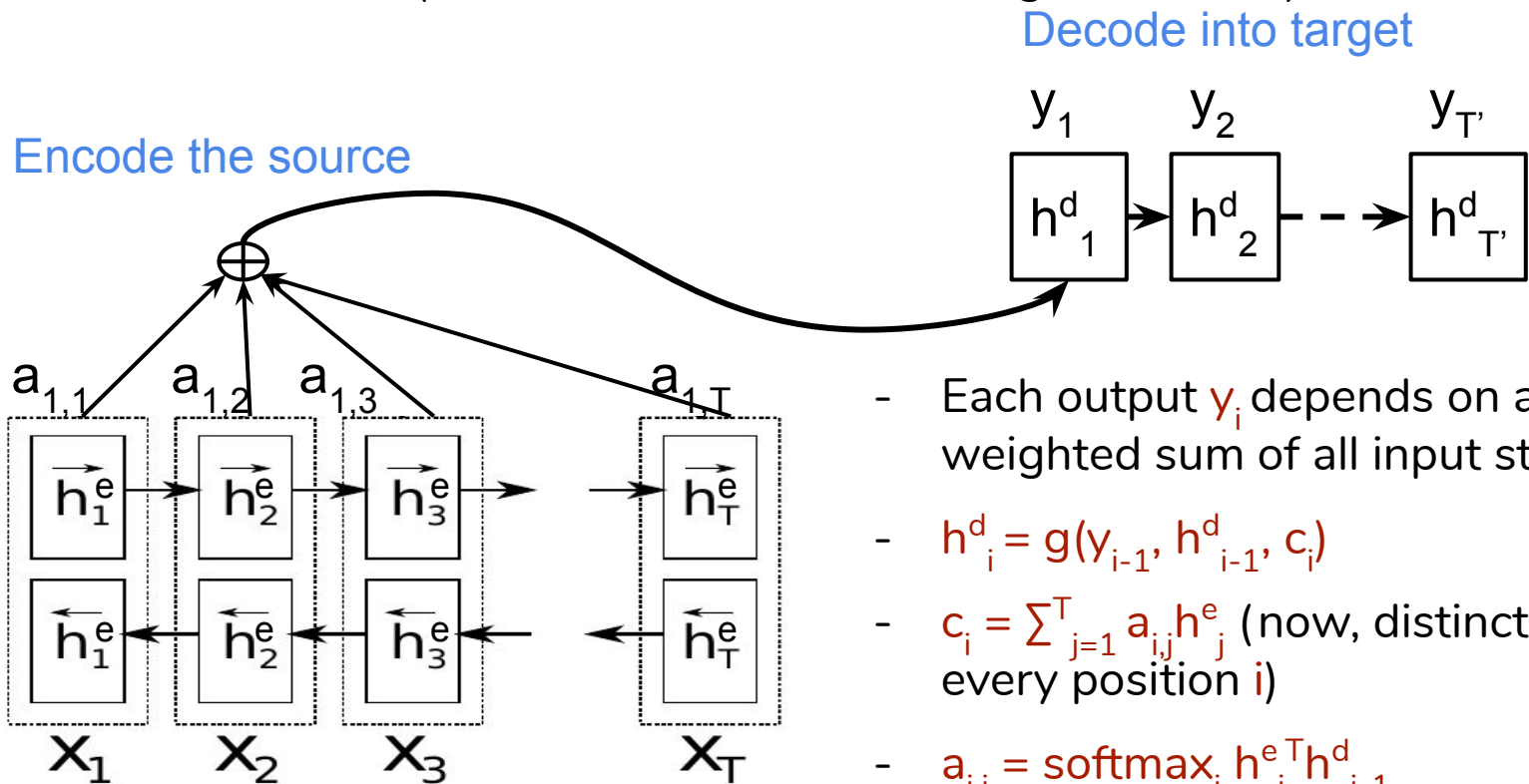
Input sentence is encoded into a single vector c^*

"You can't cram the meaning of a whole sentence into a single vector!" (R. Mooney)

A neural MT model without attention

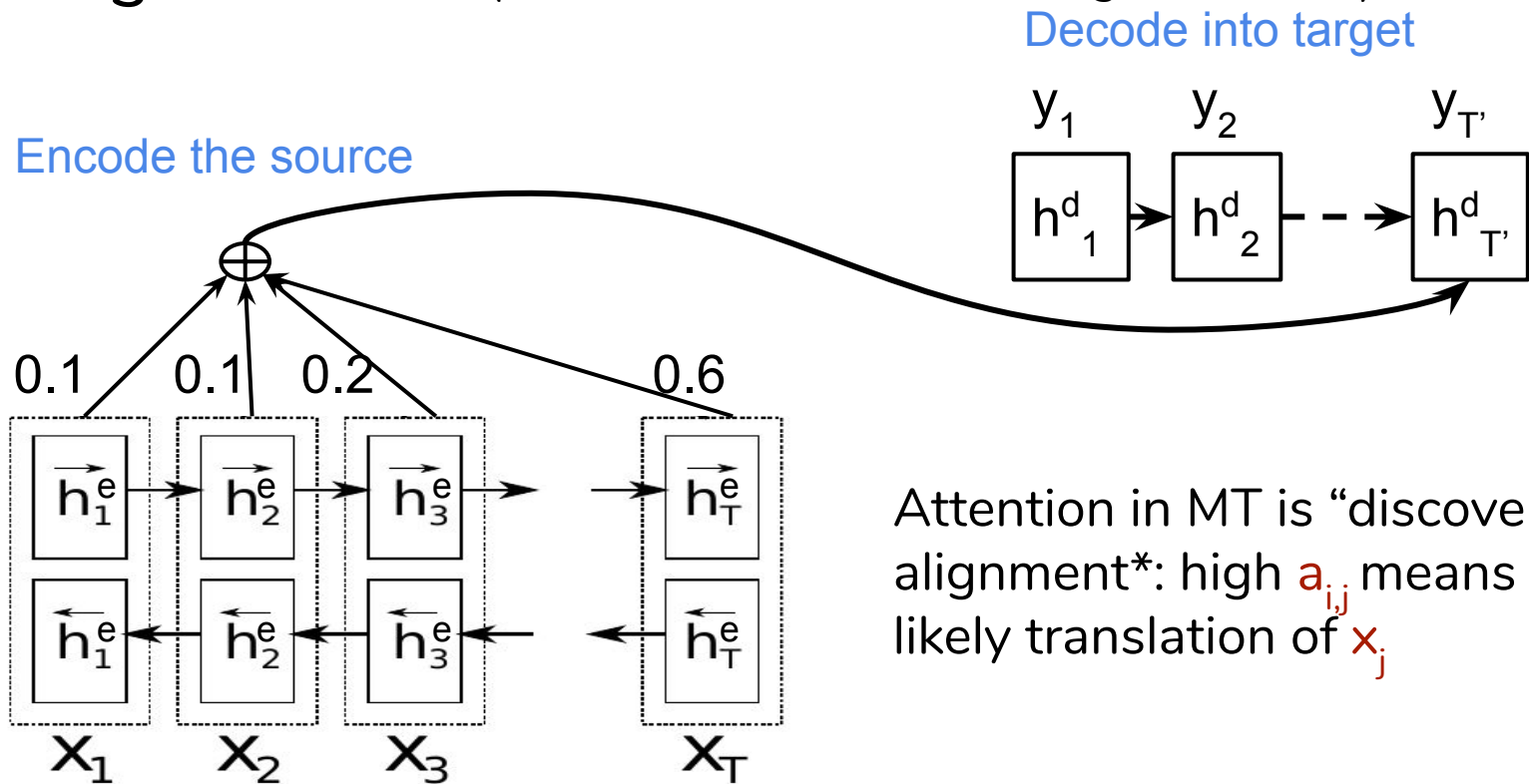


With attention (Bahdanau et al. 2014, Luong et al. 2015)



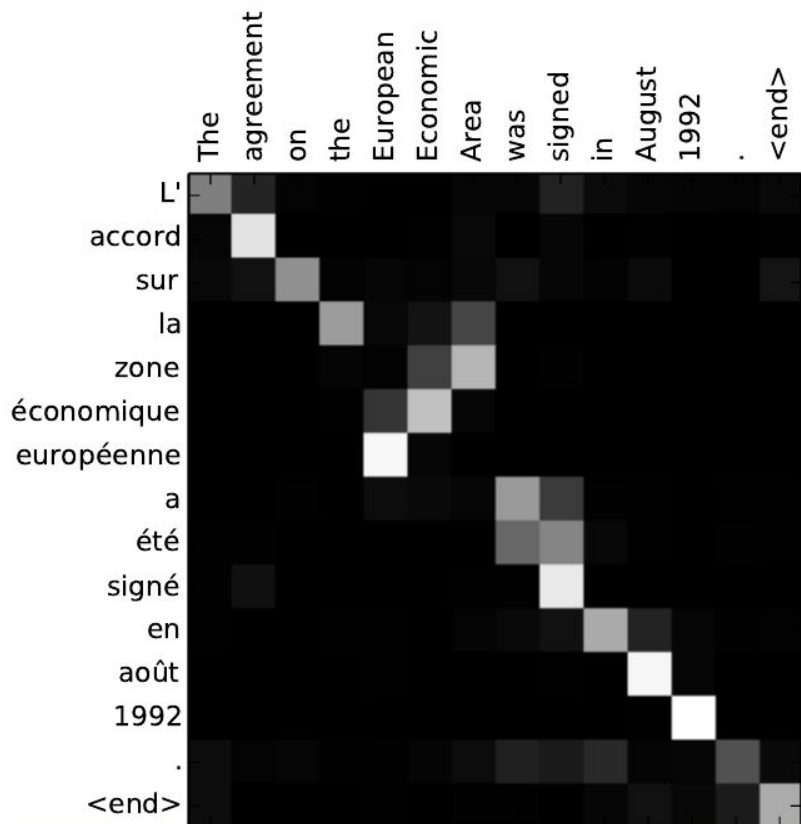
- Each output y_i depends on a weighted sum of all input states
- $h_i^d = g(y_{i-1}, h_{i-1}^d, c_i)$
- $c_i = \sum_{j=1}^T a_{i,j} h_j^e$ (now, distinct c at every position i)
- $a_{i,j} = \text{softmax}_j h_j^{eT} h_{i-1}^d$
- $(h_j^e = [\vec{h}_j^e; \overleftarrow{h}_j^e])$

Adding attention (Bahdanau et al. 2014, Luong et al. 2015)



Alignment matrix from attention weights

(Bahdanau et al. 2014)



- See word to word translation
- Although attention is a soft alignment, the result is peaky, low-entropy
- Local reordering

A few attention variants

Special case of one input sequence

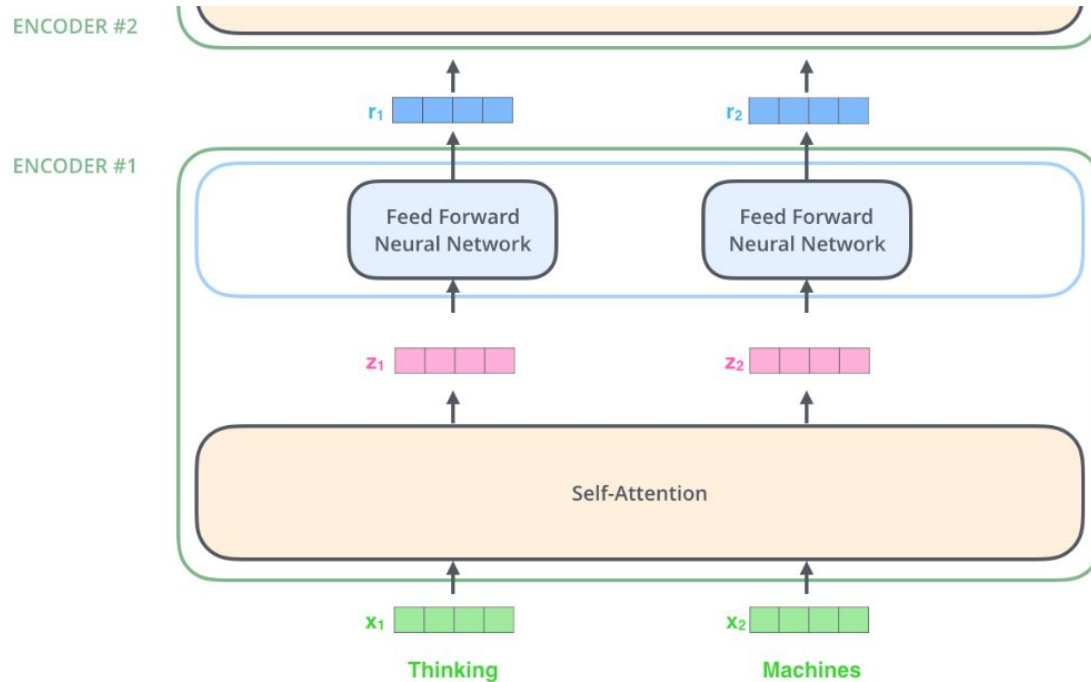
Self-attention:

- $e = f(q, K)$ stays the same, but $x_q \in X_K$
- Relating different positions of the same input to compute its representation
- Intuition: ability to discover lexical relations between tokens

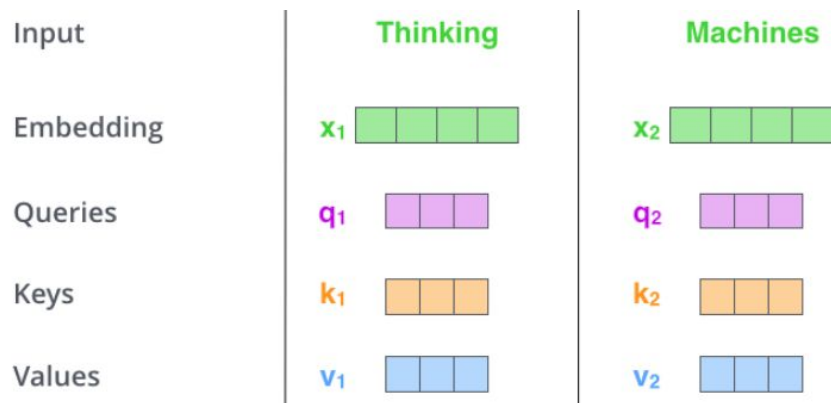
Transformer (Vaswani et al., 2017):

- overcomes sequential computation with an architecture in which “recurrency” is achieved through attention (and positional encoding)
 - self-attention for encoder inputs
 - self-attention for decoder inputs (up to current token)
 - encoder-decoder attention

Attention in Transformer connects different parts of the input



Each word is represented as a key, a query and a value, all with distinct weights



Each of q/k/v's use multiple weight matrices (“heads”), not only one

Hard attention and biasing the attention distribution

Make a zero-one decision about where to attend (i.e. uses a single sample instead of a distribution)

- harder to train (reinforcement learning)

Other approaches to encouraging sparsity: gumbel softmax, Gaussian noise

While most often we don't have access to attention's target distribution, sometimes knowledge about the desired weight distribution may be available, e.g.

- relevant sentences in a document are somehow marked,
- pre-trained attention weights exist from another task.

Two-way attention and co-attention

Represent the query as a matrix: $Q \in \mathbb{R}^{n(q) \times d(q)}$

Energy (“affinity”) scores: $E = f(Q, K)$, $E \in \mathbb{R}^{d(q) \times d(k)}$

Then the normalisation direction (row- vs. column-wise) on E determines whether we get attention weights for keys or values:

$$A^Q = g(E) \in \mathbb{R}^{d(q) \times d(k)}$$

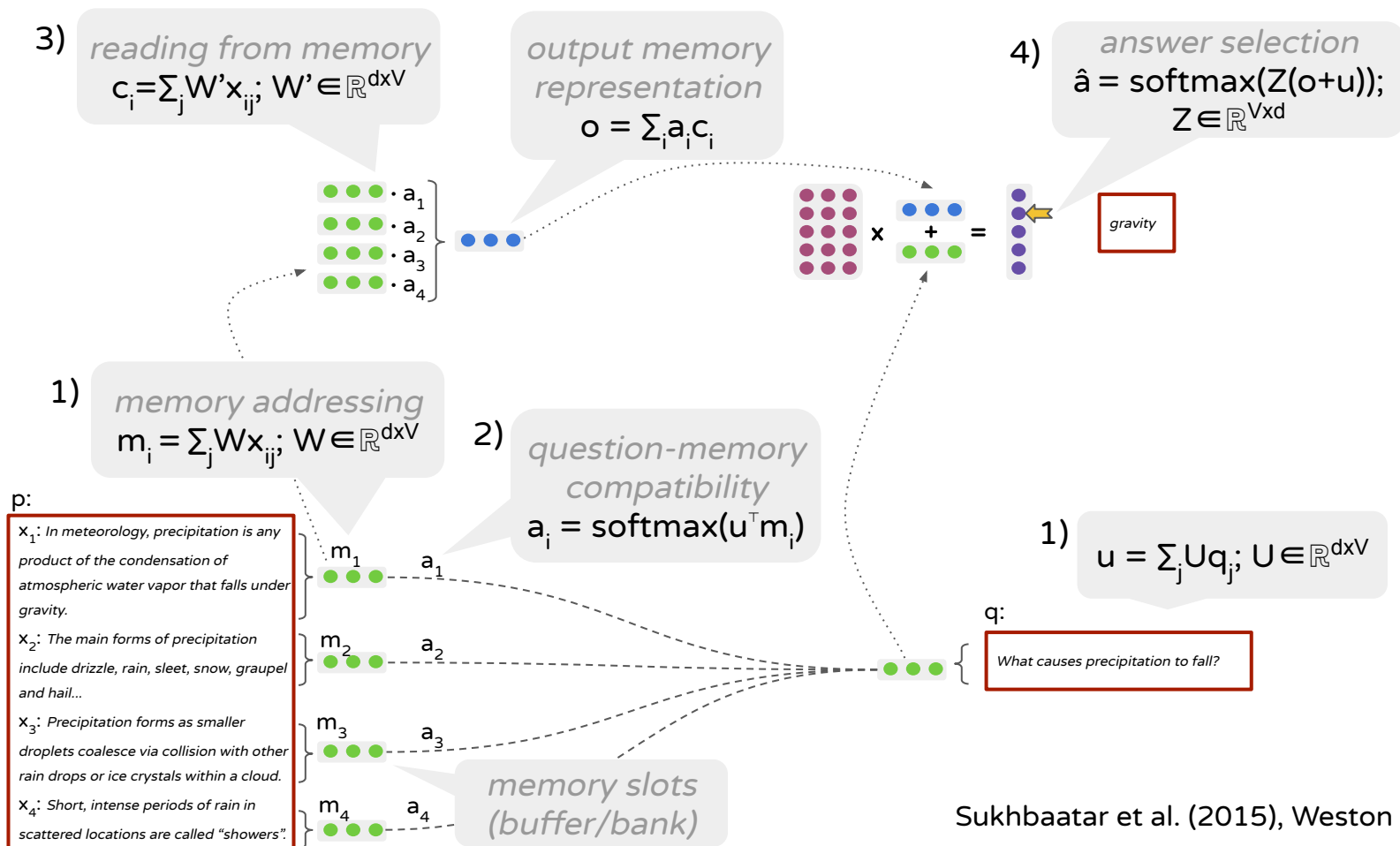
$$A^K = g(E^\top) \in \mathbb{R}^{d(k) \times d(q)}$$

E.g. instead of representing a sentence with a single vector (say, final LSTM state), have one vector per word

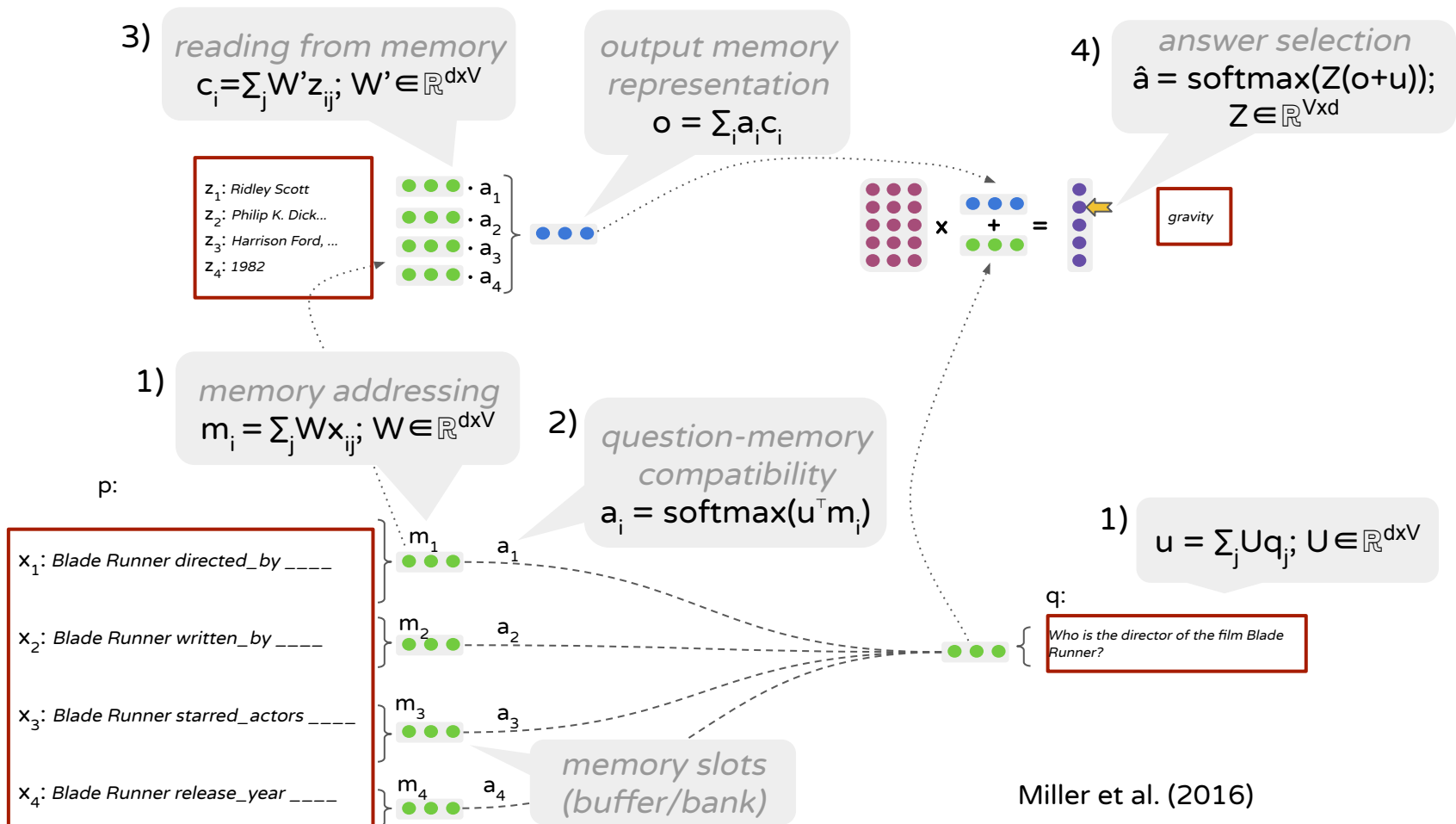
- word-by-word attention in textual entailment (Rocktäschel et al., 2015)
- document word-question word attention in QA (Xiong et al., 2016)

Attention for reading from memory

Attention in a simple memory network

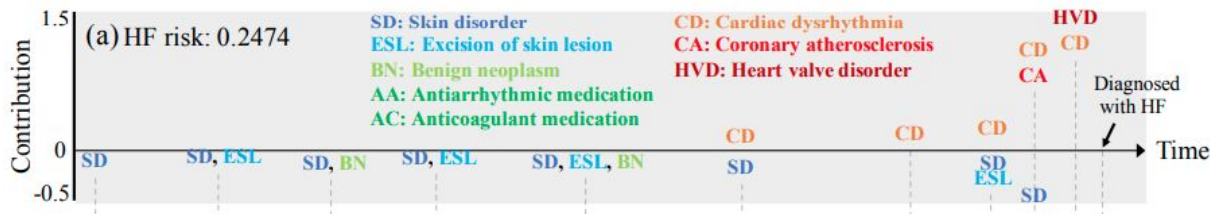
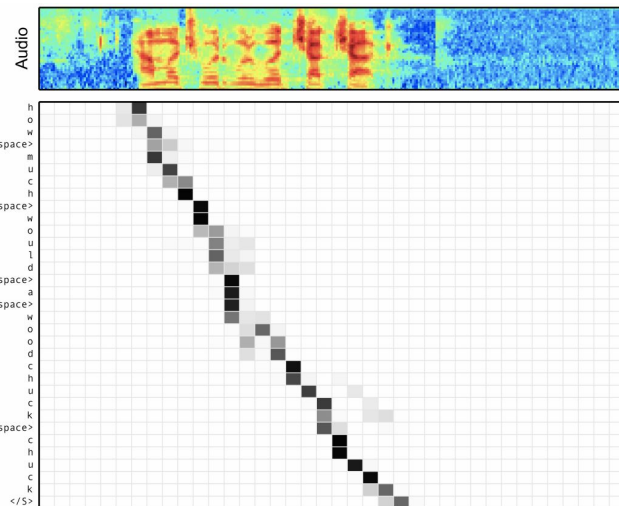


Attention keys and values can be obtained from different inputs



Attention in other fields

- Vision
 - image captioning, e.g. Xu et al. (2015)
 - object classification, e.g. Mnih et al. (2014)
- Speech recognition
 - encoding feature vectors from audio frames and decoding into sequence of phonemes (Chorowski et al., 2015)
- Clinical sequential modeling
 - salient medical codes for prediction of heart failure (Choi et al., 2016)



Useful references

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