Alternative Architectures

Philipp Koehn

10 October 2024

Alternative Architectures

- We introduced one translation model
  - attentional seq2seq model
  - core organizing feature: recurrent neural networks
- Other core neural architectures
  - convolutional neural networks
  - attention
- But first: look at various components of neural architectures

components

Components of Neural Networks

- Neural networks originally inspired by the brain
  - a neuron receives signals from other neurons
  - if sufficiently activated, it sends signals
  - feed-forward layers are roughly based on this

- Computation graph
  - any function possible, as long as it is partially differentiable
  - not limited by appeals to biological validity

- *Deep learning* maybe a better name

Feed-Forward Layer

- Classic neural network component

- Given an input vector x, matrix multiplication M with adding a bias vector b

$$Mx + b$$

- Adding a non-linear activation function

$$y = \text{activation}(Mx + b)$$

- Notation

$$y = FF_{\text{activation}}(x) = a(Mx + b)$$

Feed-Forward Layer

- Historic neural network designs: several feed-forward layers
  - input layer
  - hidden layers
  - output layer

- Powerful tools for a wide range of machine learning problems

- Matrix multiplication also called **affine transforms**
  - appeals to its geometrical properties
  - straight lines in input still straight lines in output

Factored Decomposition

- One challenge: very large input and output vectors

- Number of parameters in matrix $M = |x| \times |y|$

$\Rightarrow$ Need to reduce size of matrix

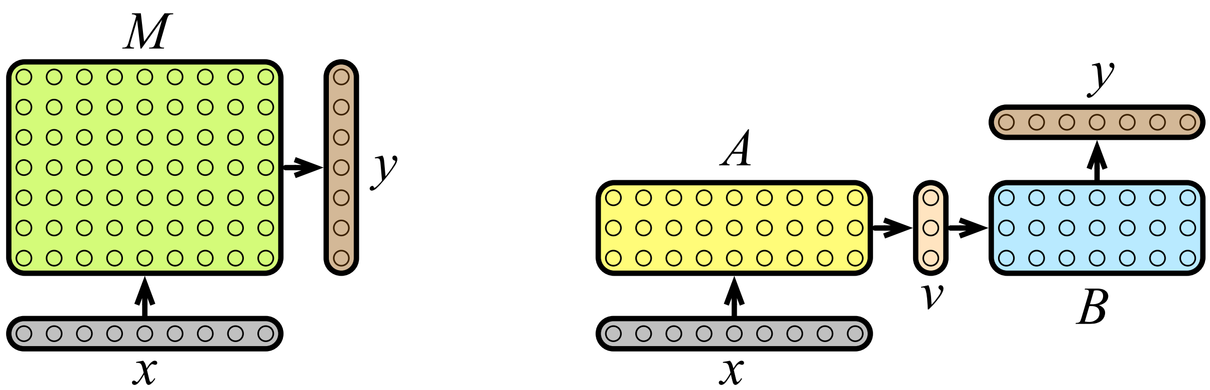
Factored Decomposition

- One challenge: very large input and output vectors

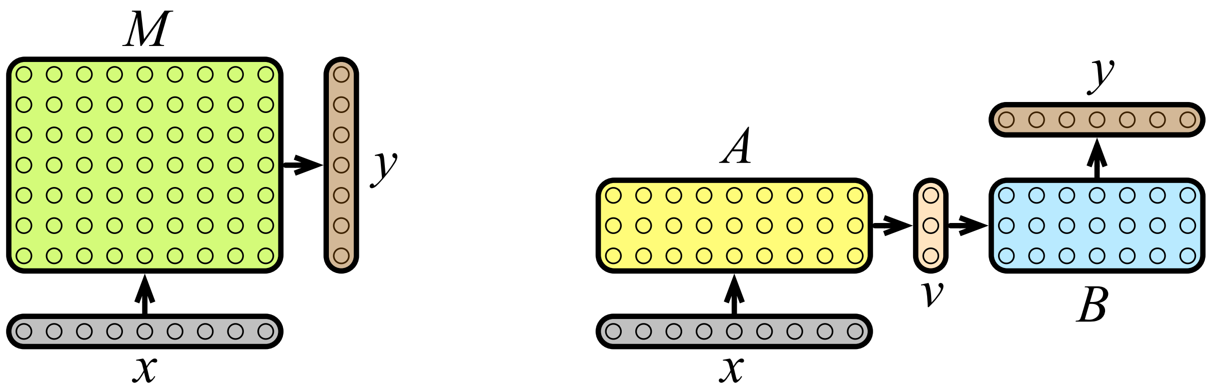
- Number of parameters in matrix $M = |x| \times |y|$

$\Rightarrow$ Need to reduce size of matrix

- Solution: first reduce to smaller representation



Factored Decomposition: Math



- Intuition
  - given highly dimension vector x
  - first map to into lower dimensional vector v (matrix A)
  - then map to output vector y (matrix B)

$$v = Ax$$
$$y = Bv = BAx$$

- Example
  - $|x|$ = 20,000, $|y|$ = 50,000 $\rightarrow$ M = 1,000,000,000
  - $|v|$ = 100 $\rightarrow$ A = 20,000 $\times$ 100 = 2,000,000, B = 100 $\times$ 50,000 = 5,000,000
  - reduction from 1,000,000,000 to 7,000,000

Factored Decomposition: Interpretation

- Vector v is a bottleneck feature
- Forced to captures salient features
- One example: word embeddings

basic mathematical operations

Concatenation

- Often multiple input vectors to processing step

- For instance recurrent neural network
  - input word
  - previous state

- Combined in feed-forward layer

$$y = \text{activation}(M_1 x_1 + M_2 x_2 + b)$$

Concatenation

- Often multiple input vectors to processing step
- For instance recurrent neural network
  - input word
  - previous state
- Combined in feed-forward layer

$$y = \text{activation}(M_1 x_1 + M_2 x_2 + b)$$

- Another view

$$x = \text{concat}(x_1, x_2)$$
$$y = \text{activation}(Mx + b)$$

- Splitting hairs here, but concatenation useful generally

Addition

- Adding vectors: very simplistic, but often done

- Example: compute sentence embeddings s from word embeddings $w_1, ..., w_n$

$$s = \sum_{i}^{n} w_i$$

- Reduces varying length sentence representation into fixed sized vector

Addition

- Adding vectors: very simplistic, but often done

- Example: compute sentence embeddings s from word embeddings $w_1, ..., w_n$

$$s = \sum_i^n w_i$$

- Reduces varying length sentence representation into fixed sized vector

- Maybe weight the words, e.g., by attention

Multiplication

- Another elementary mathematical operation
- Three ways to multiply vectors

Multiplication

- Another elementary mathematical operation
- Three ways to multiply vectors
  - element-wise multiplication

$$v \odot u = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \odot \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \begin{pmatrix} v_1 \times u_1 \\ v_2 \times u_2 \end{pmatrix}$$

Multiplication

- Another elementary mathematical operation

- Three ways to multiply vectors
  - element-wise multiplication

$$v \odot u = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \odot \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \begin{pmatrix} v_1 \times u_1 \\ v_2 \times u_2 \end{pmatrix}$$

  - dot product

$$v \cdot u = v^T u = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}^T \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = v_1 \times u_1 + v_2 \times u_2$$

    used for simple version of attention mechanism

Multiplication

- Another elementary mathematical operation

- Three ways to multiply vectors
  - element-wise multiplication

$$v \odot u = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \odot \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \begin{pmatrix} v_1 \times u_1 \\ v_2 \times u_2 \end{pmatrix}$$

  - dot product

$$v \cdot u = v^T u = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}^T \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = v_1 \times u_1 + v_2 \times u_2$$

    used for simple version of attention mechanism

  - third possibility: vu^T, not commonly done

Maximum

- Goal: reduce the dimensionality of representation

- Example: detect if a face is in image
  - any region of image may have positive match
  - represent different regions with element in a vector
  - maximum value: any region has a face

Maximum

- Goal: reduce the dimensionality of representation

- Example: detect if a face is in image
  - any region of image may have positive match
  - represent different regions with element in a vector
  - maximum value: any region has a face

- Max pooling
  - given: n dimensional vector
  - goal: reduce to $\frac{n}{k}$ dimensional vector
  - method: break up vector into blocks of k elements, map each into single value

Max Out

- Max out
  - first branch out into multiple feed-forward layers

$$W_1 x + b_1$$
$$W_2 x + b_2$$

Max Out

- Max out
  - first branch out into multiple feed-forward layers

$$W_1 x + b_1$$
$$W_2 x + b_2$$

  - element-wise maximum

$$\text{maxout}(x) = \max(W_1 x + b_1, W_2 x + b_2)$$

Max Out

- Max out
  - first branch out into multiple feed-forward layers

$$W_1 x + b_1$$
$$W_2 x + b_2$$

  - element-wise maximum

$$\text{maxout}(x) = \max(W_1 x + b_1, W_2 x + b_2)$$

- ReLu activation is a maxout layer: maximum of feed-forward layer and 0

$$\text{ReLu}(x) = \max(Wx + b, 0)$$

processing sequences

Recurrent Neural Networks

- Already described recurrent neural networks at length
  - propagate state s
  - over time steps t
  - receiving an input x_t at each turn

$$s_t = f(s_{t-1}, x_t)$$

(state may computed may as a feed-forward layer)

Recurrent Neural Networks

- Already described recurrent neural networks at length
  - propagate state s
  - over time steps t
  - receiving an input x_t at each turn

$$s_t = f(s_{t-1}, x_t)$$

(state may computed may as a feed-forward layer)

- More successful
  - gated recurrent units (GRU)
  - long short-term memory cells (LSTM)

Recurrent Neural Networks

- Already described recurrent neural networks at length
  - propagate state s
  - over time steps t
  - receiving an input x_t at each turn

$$s_t = f(s_{t-1}, x_t)$$

(state may computed may as a feed-forward layer)

- More successful
  - gated recurrent units (GRU)
  - long short-term memory cells (LSTM)
- Good fit for sequences, like words in a sentence
  - humans also receive word by word
  - most recent words most relevant

  $\rightarrow$ closer to current state
- But computational problematic: very long computation chains

Alternative Sequence Processing

- Convolutional neural networks

- Attention

convolutional neural networks

Convolutional Neural Networks

- Key step
  - take a high dimensional input representation
  - map to lower dimensional representation

- Several repetitions of this step

Convolutional Neural Networks

- Key step
  - take a high dimensional input representation
  - map to lower dimensional representation

- Several repetitions of this step

- Examples
  - map 50×50 pixel area into scalar value
  - combine 3 or more neighboring words into a single vector

Convolutional Neural Networks

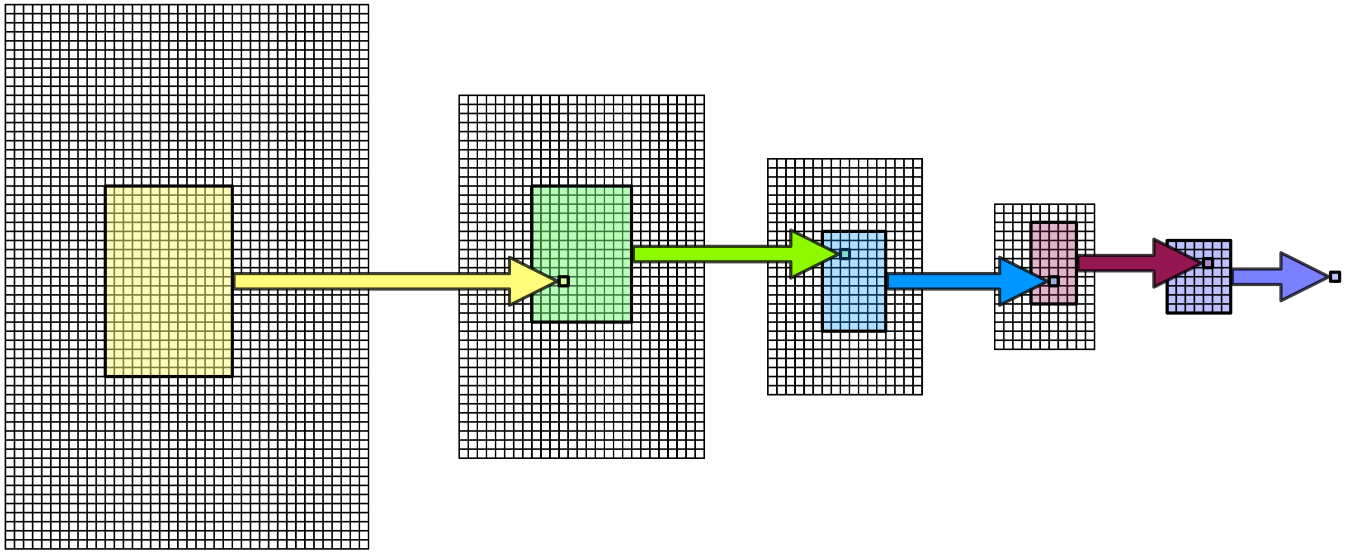
- Key step
  - take a high dimensional input representation
  - map to lower dimensional representation

- Several repetitions of this step

- Examples
  - map 50×50 pixel area into scalar value
  - combine 3 or more neighboring words into a single vector

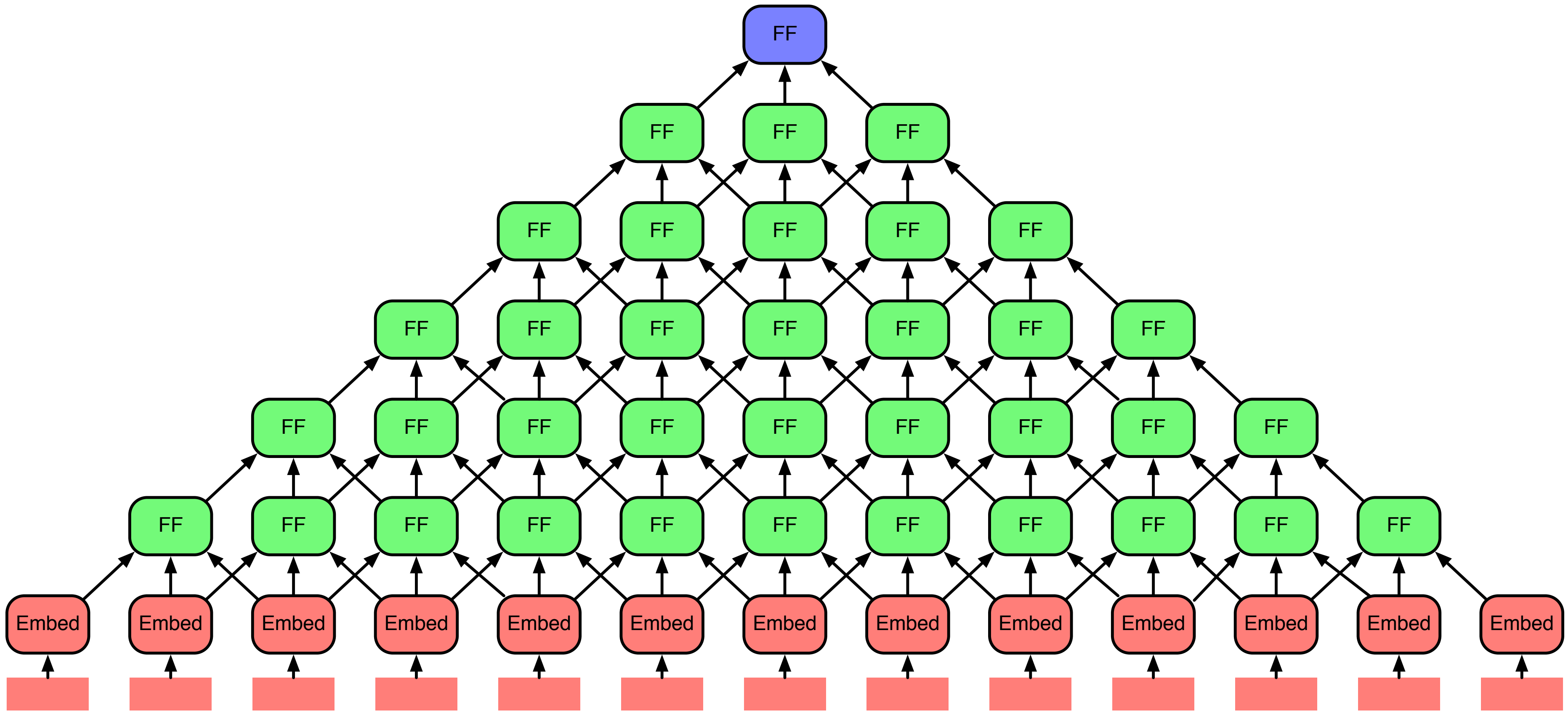
- Machine translation
  - encode input sentence into single vector
  - decode this vector into a sentence in the output language

CNNs for Vision



- Popular in image processing
- Regions of an image are reduced into increasingly smaller representation
  - matrix spanning part of image reduced to single value
  - overlapping regions

CNNs for Language



- Map words into fixed-sized sentence representation

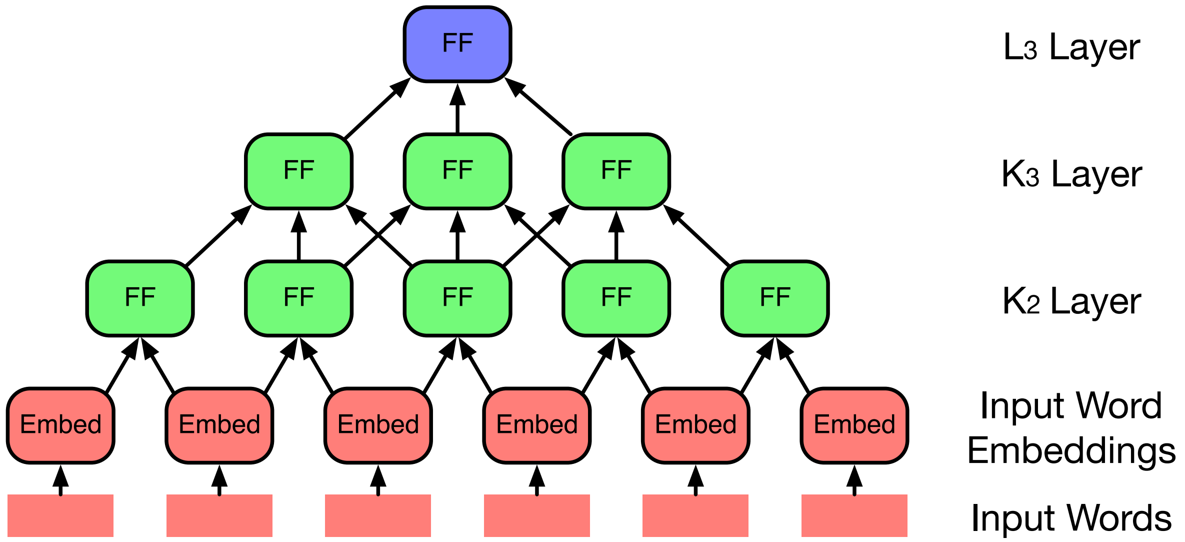
Hierarchical Structure and Language

- Syntactic and semantic theories of language
  - language is recursive
  - central: verb
  - dependents: subject, objects, adjuncts
  - their dependents: adjectives, determiners
  - also nested: relative clauses
- How to compute sentence embeddings active research topic

Convolutional Machine Translation

- First end-to-end neural machine translation model of the modern era [Kalchbrenner and Blunsom, 2013]

- Encoder



  - always two convolutional layers, with different size
  - here: K_2 and K_3

- Decoder similar

attention

Attention

- Machine translation is a structured prediction task
  - output is not a single label
  - output structure needs to be built, word by word

Attention

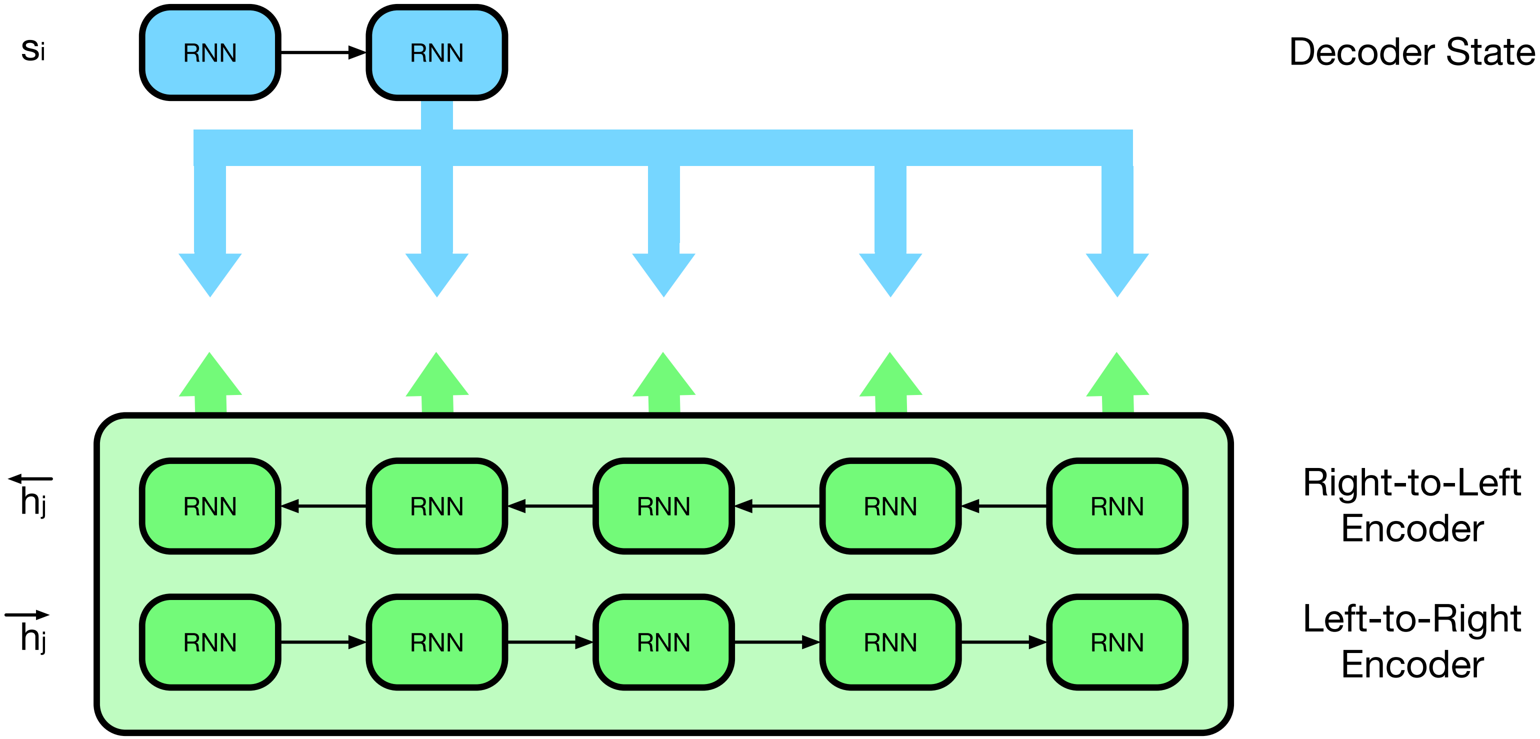
- Machine translation is a structured prediction task
  - output is not a single label
  - output structure needs to be built, word by word
- Relevant information for each word prediction varies

Attention

- Machine translation is a structured prediction task
  - output is not a single label
  - output structure needs to be built, word by word
- Relevant information for each word prediction varies
- Human translators pay attention to different parts of the input sentence when translating

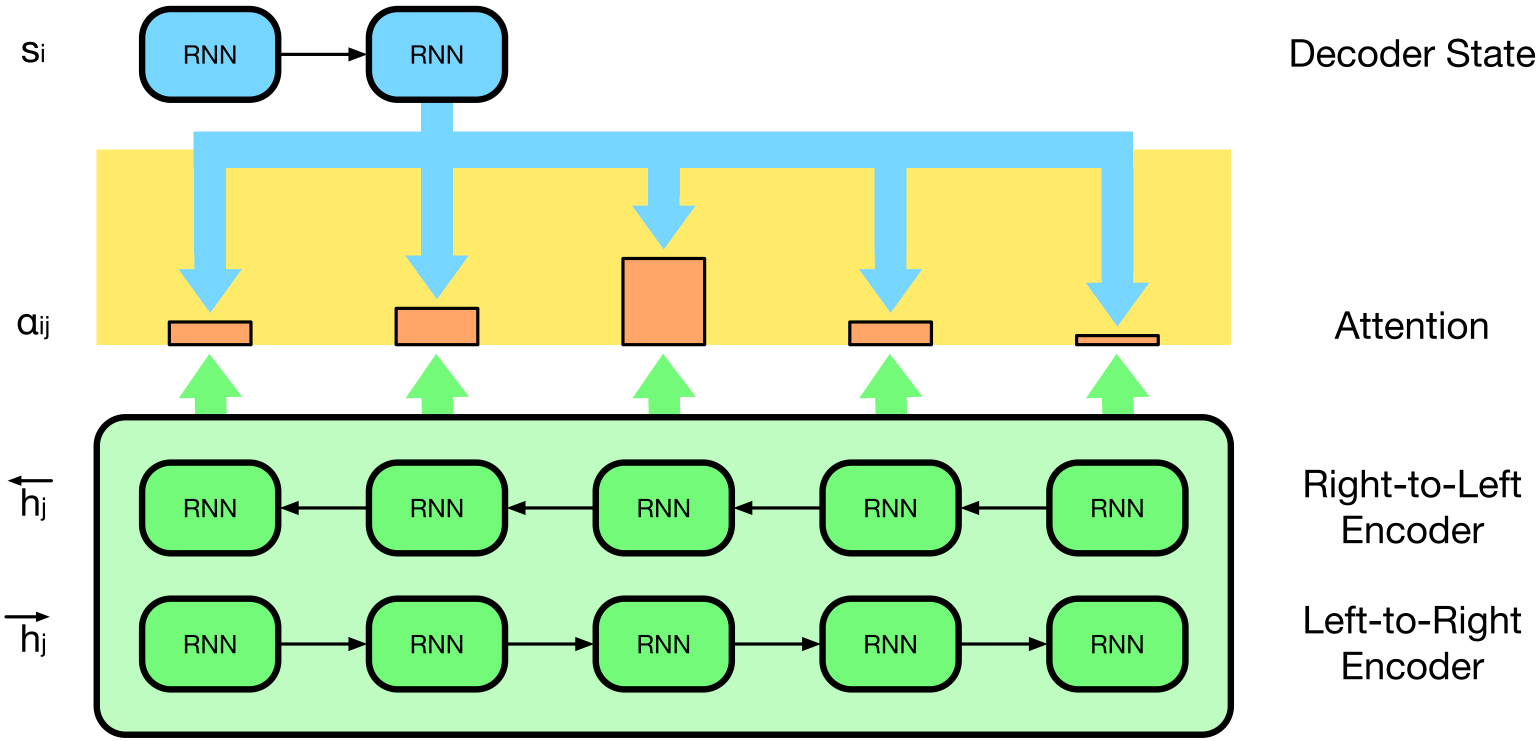
$\Rightarrow$ Attention mechanism

Attention



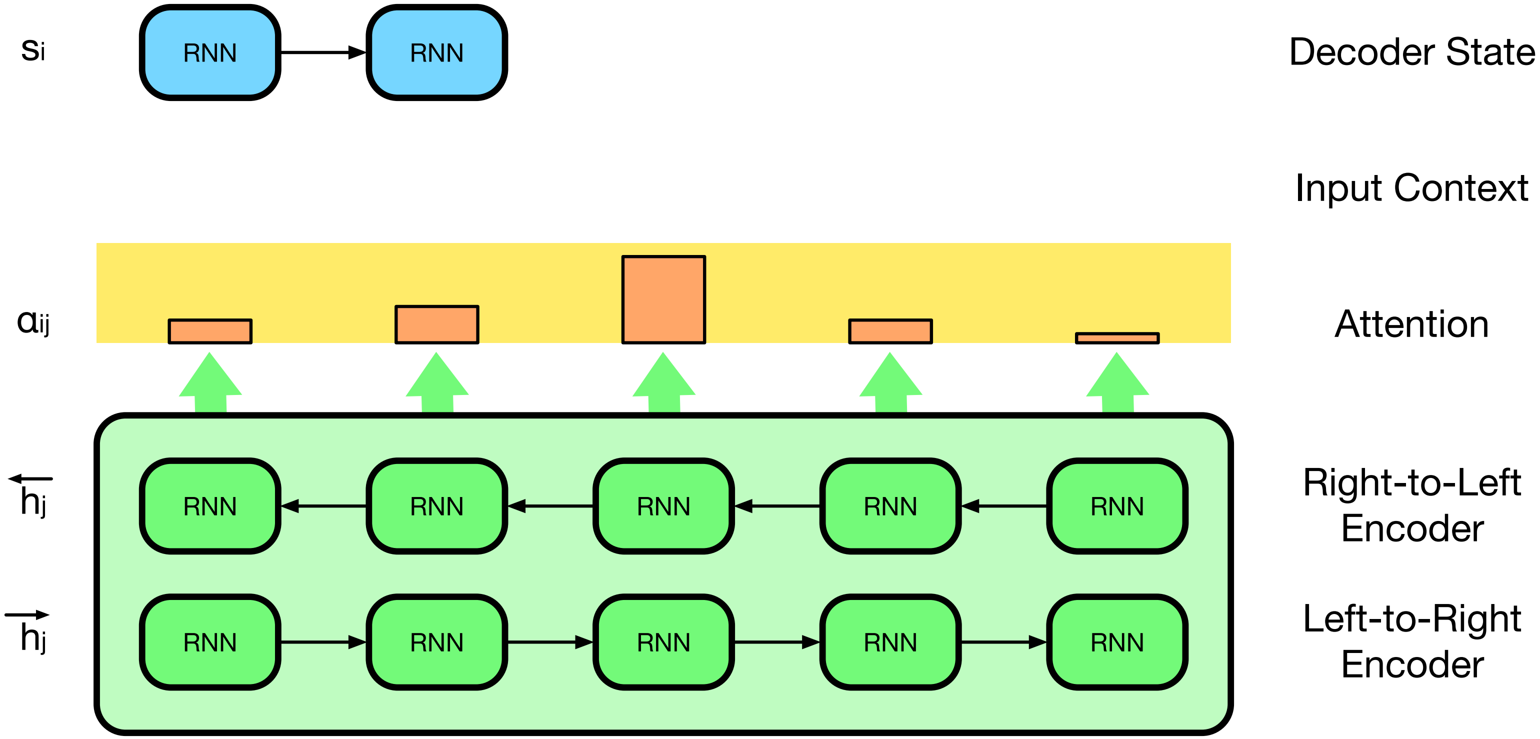
- Given what we have generated so far (decoder hidden state)
- ... which words in the input should we pay attention to (encoder states)?

Attention



- Given: – the previous hidden state of the decoder s_{i-1}
  – the representation of input words $h_j = (\overleftarrow{h_j}, \overrightarrow{h_j})$
- Predict an alignment probability $a(s_{i-1}, h_j)$ to each input word j (modeled with with a feed-forward neural network layer)

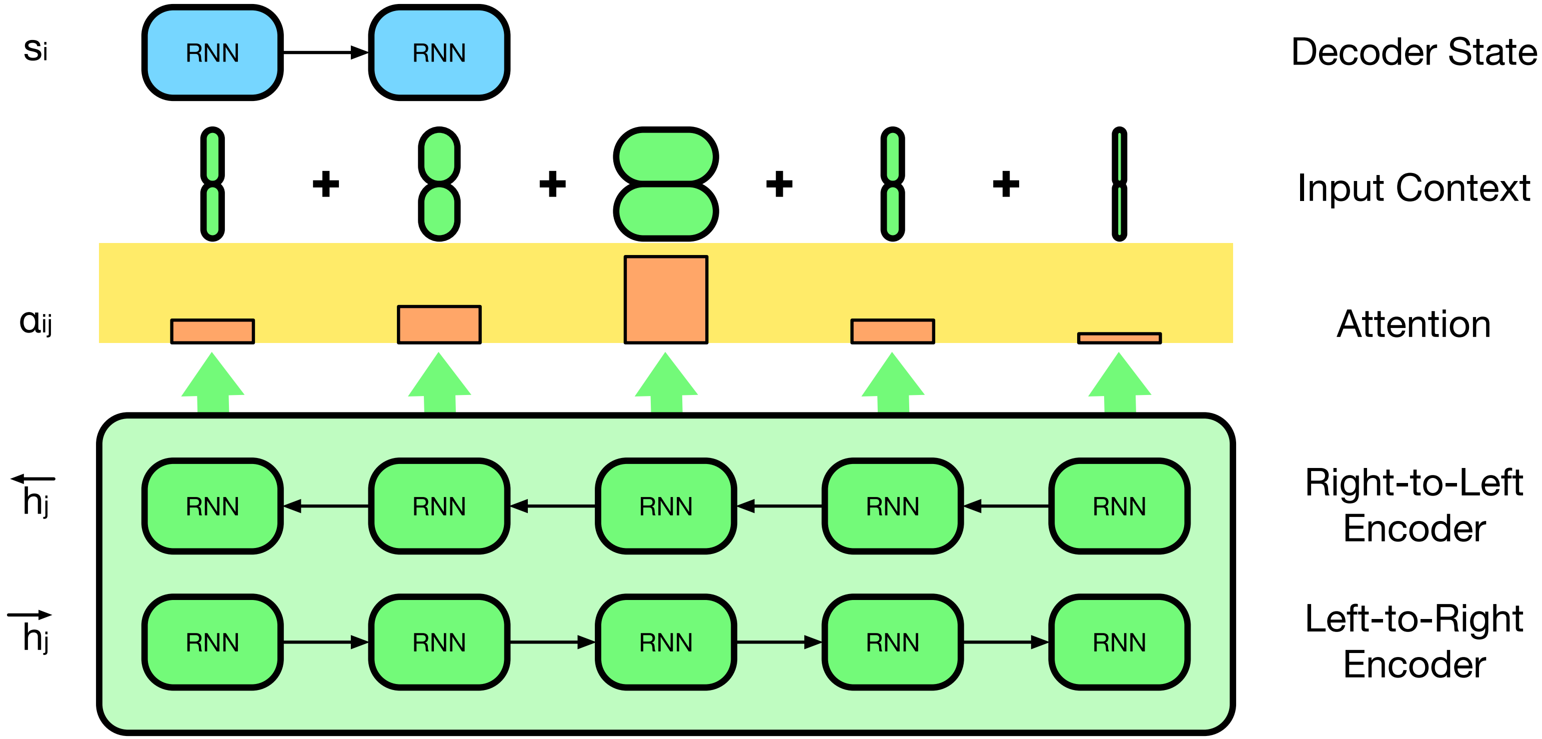
Attention



- Normalize attention (softmax)

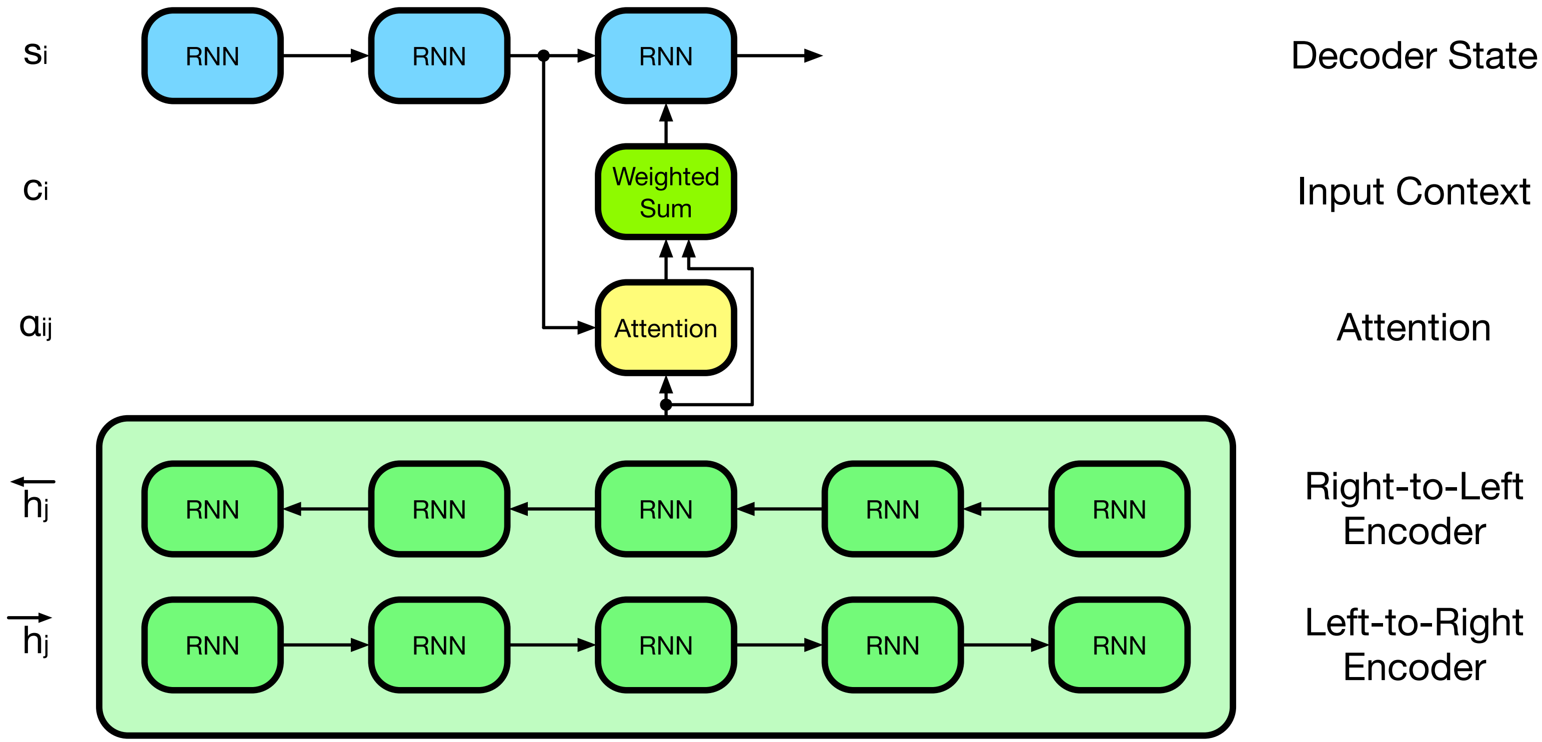
$$\alpha_{ij} = \frac{\exp(a(s_{i-1}, h_j))}{\sum_k \exp(a(s_{i-1}, h_k))}$$

Attention



- Relevant input context: weigh input words according to attention: $c_i = \sum_j \alpha_{ij} h_j$

Attention



- Use context to predict next hidden state and output word

Computing Attention

- Attention mechanism in neural translation model (Bahdanau et al., 2015)
  - previous hidden state s_{i-1}
  - input word embedding h_j
  - trainable parameters b, W_a, U_a, v_a

$$a(s_{i-1}, h_j) = v_a^T \tanh(W_a s_{i-1} + U_a h_j + b)$$

Computing Attention

- Attention mechanism in neural translation model (Bahdanau et al., 2015)
  - previous hidden state s_{i-1}
  - input word embedding h_j
  - trainable parameters b, W_a, U_a, v_a

$$a(s_{i-1}, h_j) = v_a^T \tanh(W_a s_{i-1} + U_a h_j + b)$$

- Other ways to compute attention (Luong et al., 2015)
  - Dot product: $a(s_{i-1}, h_j) = s_{i-1}^T h_j$
  - Scaled dot product: $a(s_{i-1}, h_j) = \frac{1}{\sqrt{|h_j|}} s_{i-1}^T h_j$
  - General: $a(s_{i-1}, h_j) = s_{i-1}^T W_a h_j$
  - Local: $a(s_{i-1}) = W_a s_{i-1}$

General View of Dot-Product Attention

- Three elements

  Query : decoder state
  Key : encoder state
  Value : encoder state

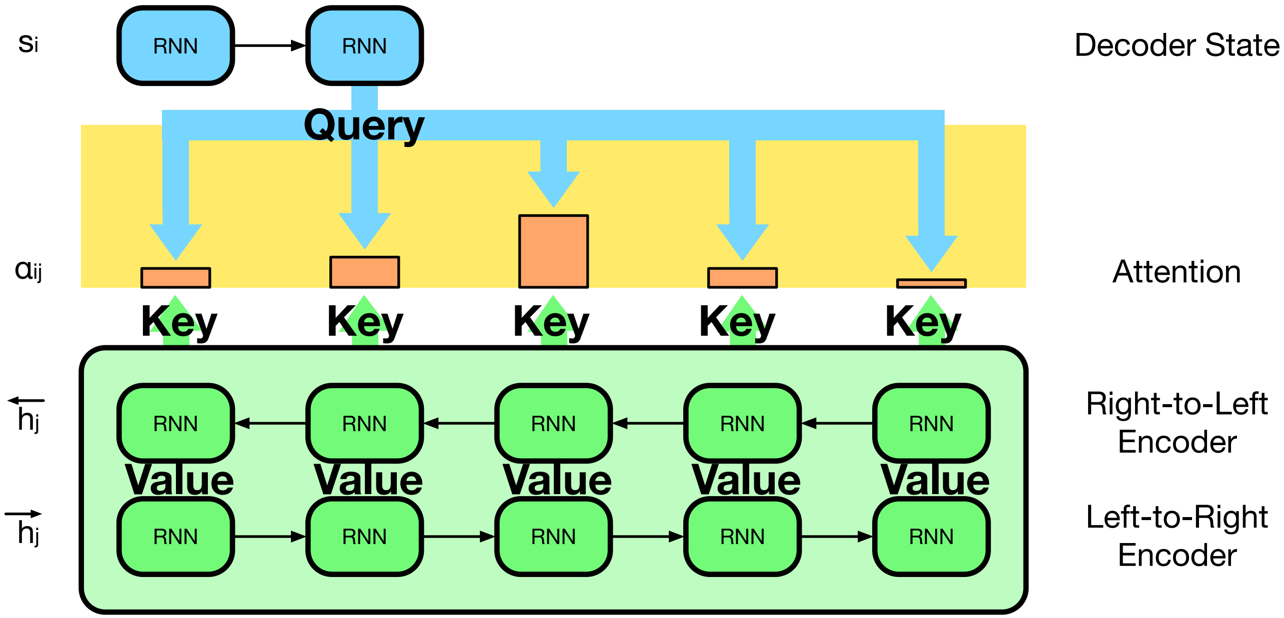
- Intuition
  - given a query (the decoder state)
  - we check how well it matches keys in the database (the encoder states)
  - and then use the matching score to scale the retrieved value (also the encoder state)

- Computation

$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$

General View of Dot-Product Attention

$$\text{Attention}(Q, K, V)$$



- Query: encoder state, Key and Value: decoder state

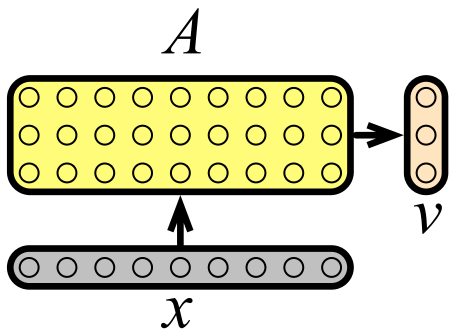
$$\text{Attention}(S, H, H)$$

Dimensionality Reduction

- Instead of simple dot product of query and key vectors QK^T...
- Multiply with weight matrices W^Q and W^K

Dimensionality Reduction

- Instead of simple dot product of query and key vectors QK^T...
- Multiply with weight matrices W^Q and W^K
- Also reduce the size of the vectors



- New computation: $\text{Attention}(QW^Q, KW^K, V)$

Self Attention

- Finally, a very different take at attention
- Motivation so far: need for alignment between input words and output words

Self Attention

- Finally, a very different take at attention
- Motivation so far: need for alignment between input words and output words
- Now: refine representation of input words in the encoder
  - representation of an input word mostly depends on itself
  - but also informed by the surrounding context
  - previously: recurrent neural networks (considers left or right context)
  - now: attention mechanism

Self Attention

- Finally, a very different take at attention

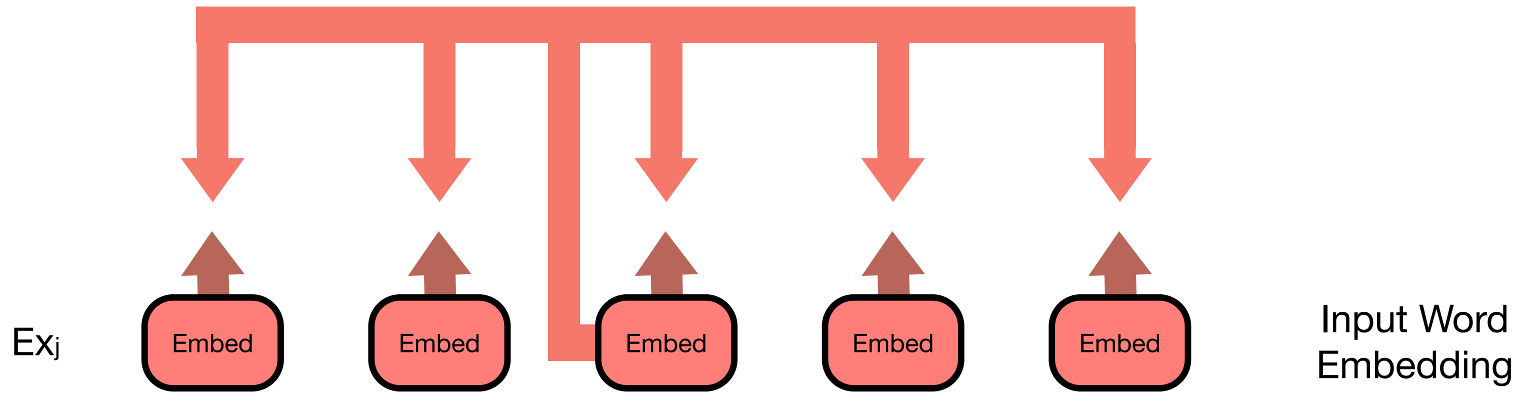
- Motivation so far: need for alignment between input words and output words

- Now: refine representation of input words in the encoder
  - representation of an input word mostly depends on itself
  - but also informed by the surrounding context
  - previously: recurrent neural networks (considers left or right context)
  - now: attention mechanism

- Self attention:

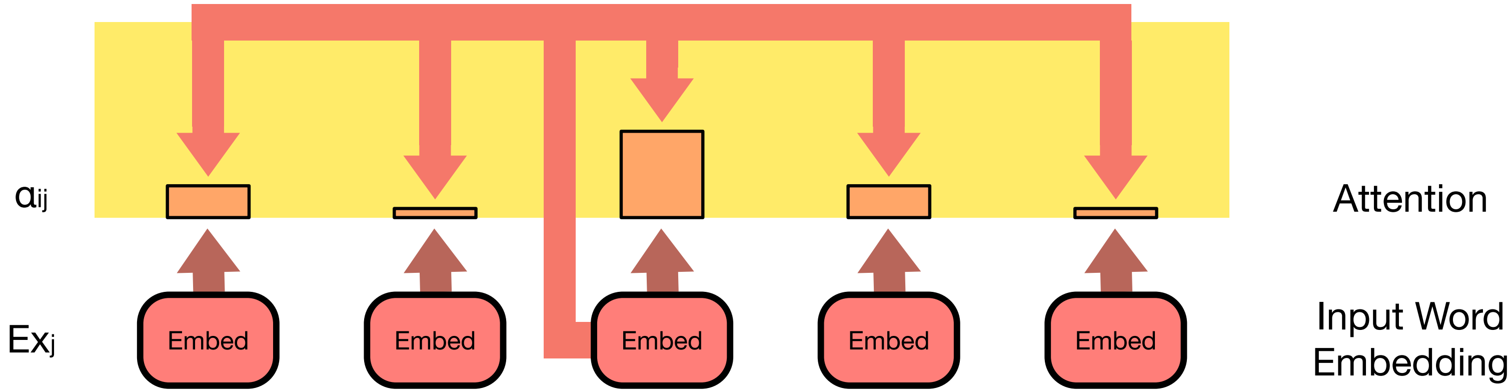
  Which of the surrounding words is most relevant to refine representation?

Self Attention



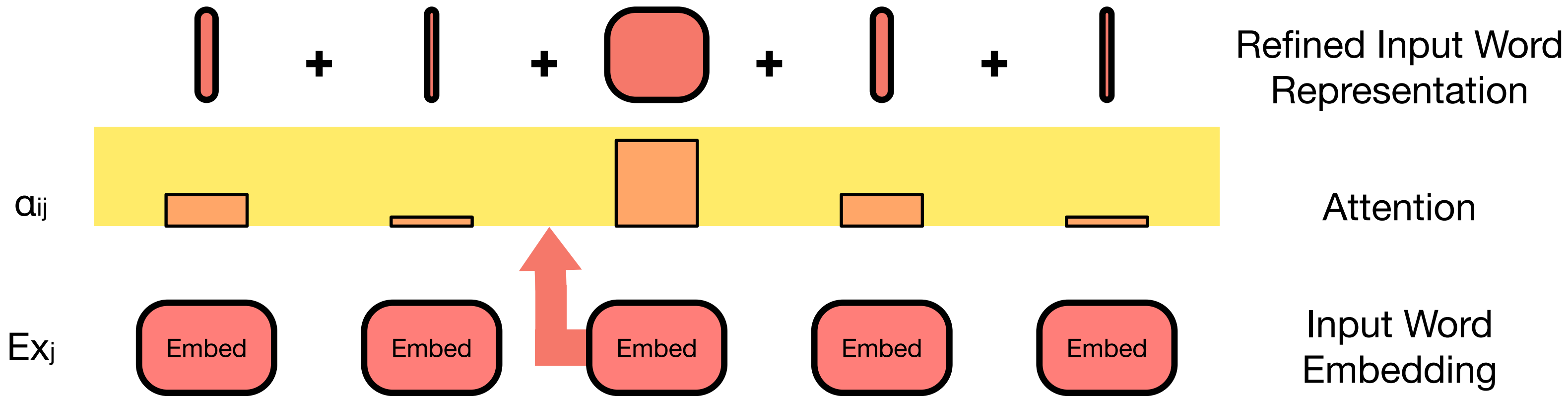
- Given: input word embeddings
- Task: consider how each should be refined in view of others
- Needed: how much attention to pay to others

Self Attention



- Computation of attention weights as before
  - Key: word embedding (or generally: encoder state for word H)
  - Query: word embedding (or generally: encoder state for word H)
- Again, multiple with weight matrices: Q=HW^Q and K=HW^K
- Attention weights: QK^T

Self Attention



- Full self attention

$$\text{self-attention}(H) = \text{Attention}(HW^Q, HW^K, H)$$

- Resulting vector uses weighted context words

Multi-Head Attention

- Add redundancy
  - say, 16 attention weights
  - each based on its own parameters W_i^Q, W_i^K, W_i^V

Multi-Head Attention

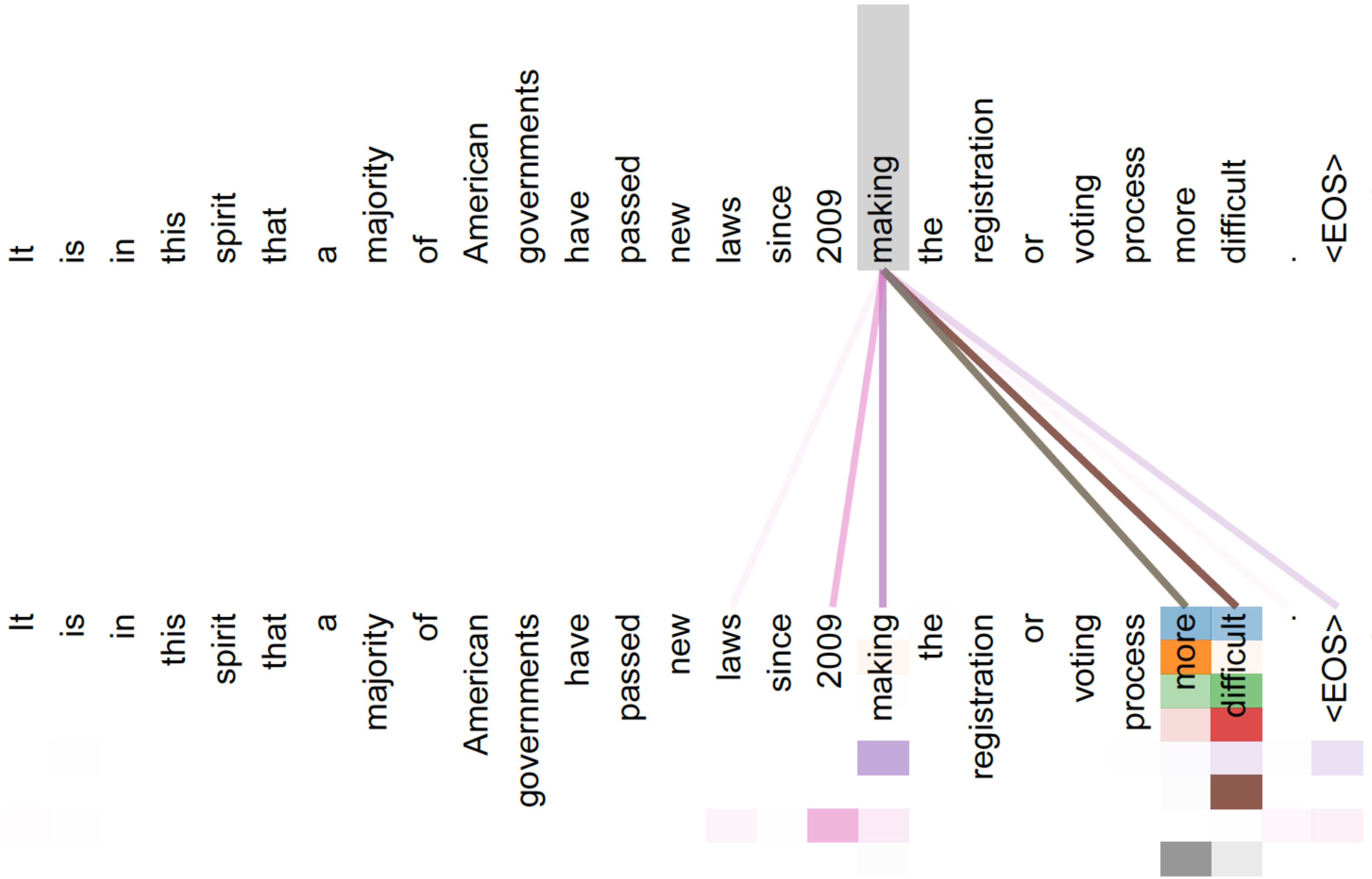
- Add redundancy
  - say, 16 attention weights
  - each based on its own parameters W_i^Q, W_i^K, W_i^V

- Formally:

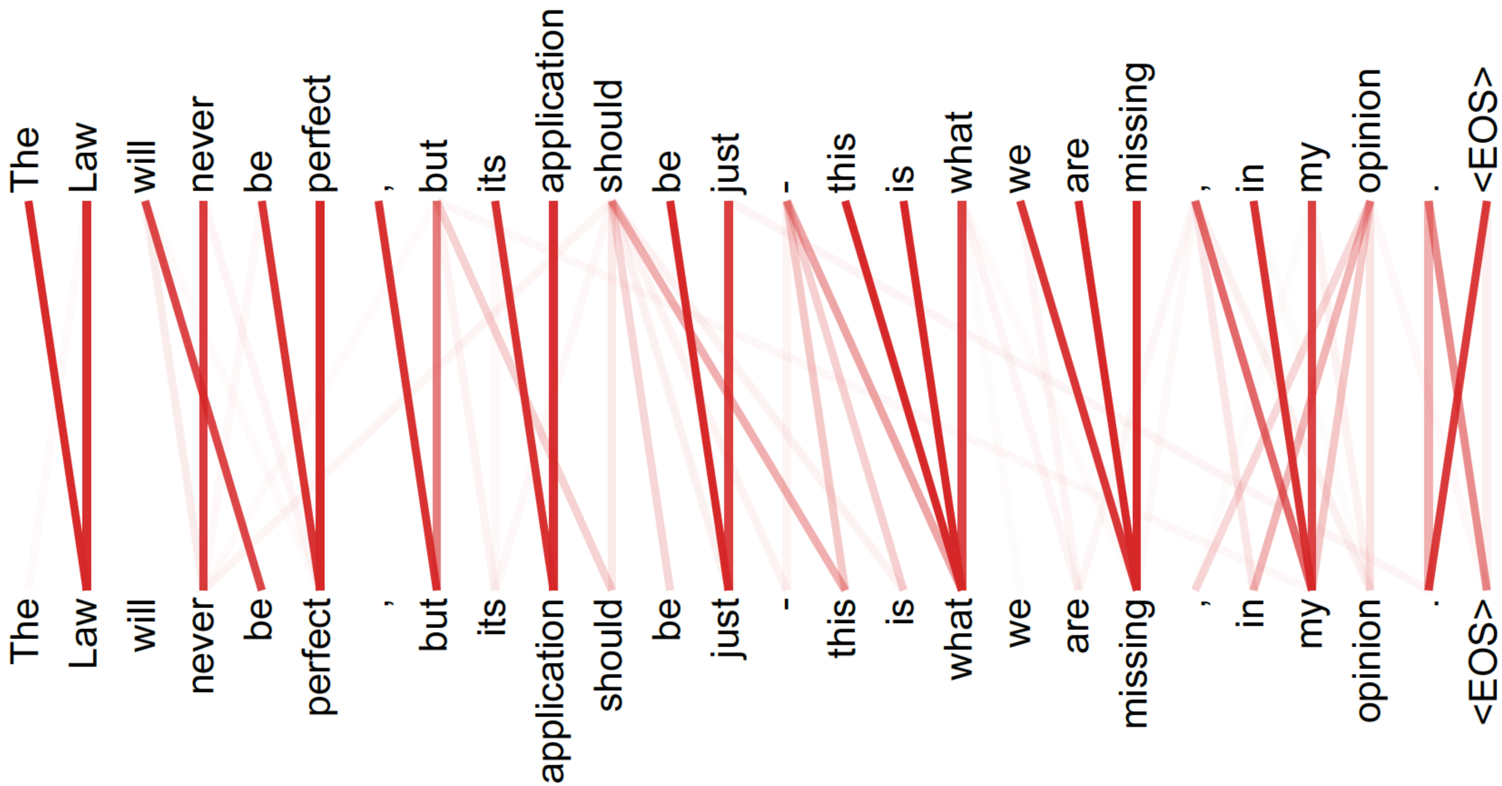
$$\begin{aligned} \text{head}_i &= \text{Attention}(QW_i^Q, KW_i^K, VW_i^V) \\ \text{MultiHead}(Q, K, V) &= \text{Concat}(\text{head}_1, ..., \text{head}_h)W^O \end{aligned}$$

- Multi-head attention is a form of ensembling

Multi-Head Attention



Multi-Head Attention



"Many of the attention heads exhibit behaviour that seems related to the structure of the sentence."

transformer

Self Attention: Transformer

- Self-attention in encoder
  - refine word representation based on relevant context words
  - relevance determined by self attention

Self Attention: Transformer

- Self-attention in encoder
  - refine word representation based on relevant context words
  - relevance determined by self attention
- Self-attention in decoder
  - refine output word predictions based on relevant previous output words
  - relevance determined by self attention

Self Attention: Transformer

- Self-attention in encoder
  - refine word representation based on relevant context words
  - relevance determined by self attention
- Self-attention in decoder
  - refine output word predictions based on relevant previous output words
  - relevance determined by self attention
- Also regular attention to encoder states in decoder

Self Attention: Transformer

- Self-attention in encoder
  - refine word representation based on relevant context words
  - relevance determined by self attention
- Self-attention in decoder
  - refine output word predictions based on relevant previous output words
  - relevance determined by self attention
- Also regular attention to encoder states in decoder
- Currently most successful model

  (maybe only with self attention in decoder, but regular recurrent decoder)

Self Attention Layer

- Given: input word representations h_j, packed into a matrix $H = (h_1, ..., h_j)$
- Self attention

$$\text{self-attention}(H) = \text{MultiHead}(H, H, H)$$

Self Attention Layer

- Given: input word representations h_j, packed into a matrix $H = (h_1, ..., h_j)$
- Self attention
$$\text{self-attention}(H) = \text{MultiHead}(H, H, H)$$
- Shortcut connection
$$\text{self-attention}(h_j) + h_j$$

Self Attention Layer

- Given: input word representations h_j, packed into a matrix $H = (h_1, ..., h_j)$
- Self attention

$$\text{self-attention}(H) = \text{MultiHead}(H, H, H)$$

- Shortcut connection

$$\text{self-attention}(h_j) + h_j$$

- Layer normalization

$$\hat{h}_j = \text{layer-normalization}(\text{self-attention}(h_j) + h_j)$$

Self Attention Layer

- Given: input word representations h_j, packed into a matrix $H = (h_1, ..., h_j)$

- Self attention

$$\text{self-attention}(H) = \text{MultiHead}(H, H, H)$$

- Shortcut connection

$$\text{self-attention}(h_j) + h_j$$

- Layer normalization

$$\hat{h}_j = \text{layer-normalization}(\text{self-attention}(h_j) + h_j)$$

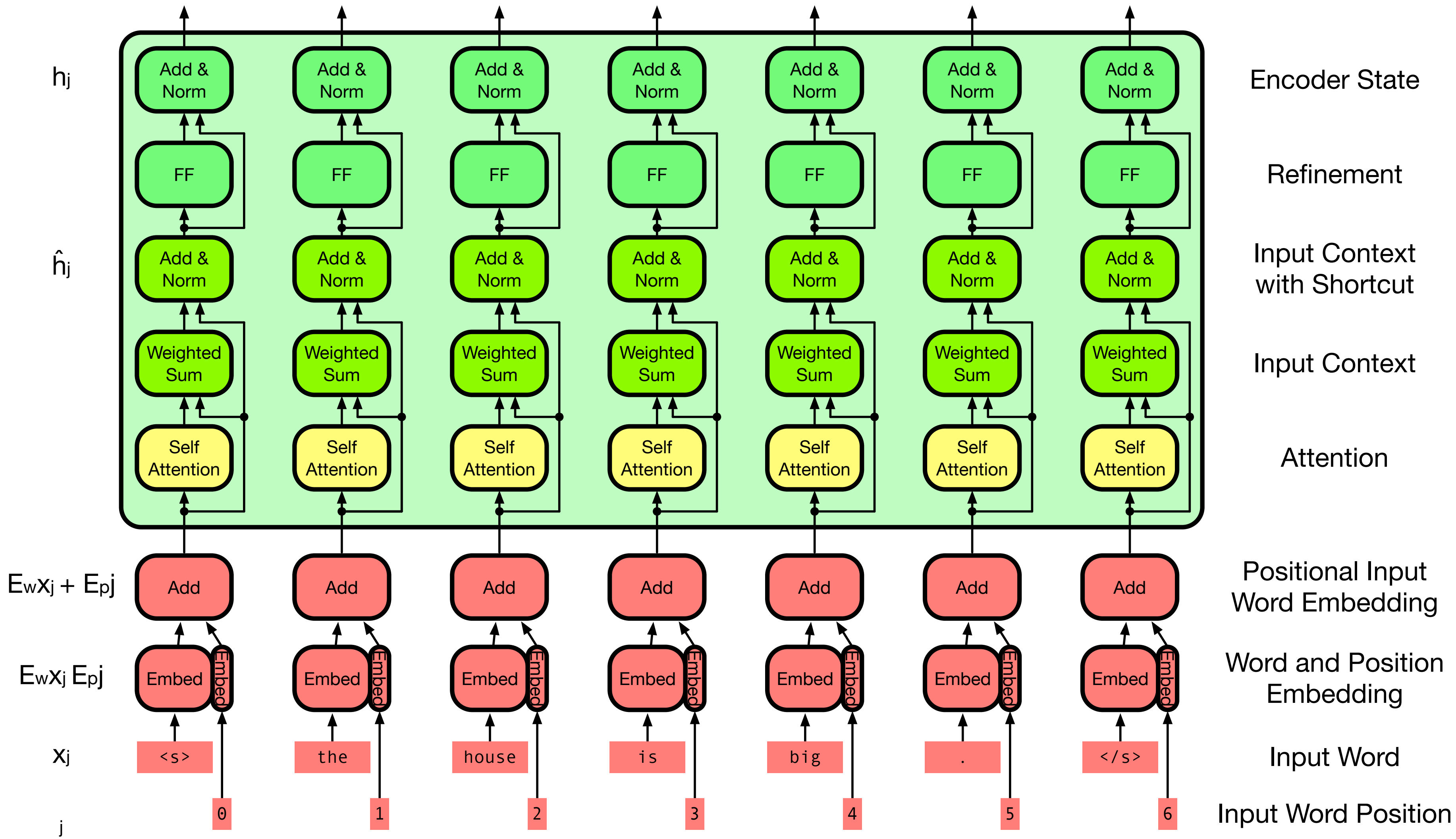
- Feed-forward step with ReLU activation function

$$\text{relu}(W\hat{h}_j + b)$$

Self Attention Layer

- Given: input word representations h_j, packed into a matrix $H = (h_1, ..., h_j)$
- Self attention
$$\text{self-attention}(H) = \text{MultiHead}(H, H, H)$$
- Shortcut connection
$$\text{self-attention}(h_j) + h_j$$
- Layer normalization
$$\hat{h}_j = \text{layer-normalization}(\text{self-attention}(h_j) + h_j)$$
- Feed-forward step with ReLU activation function
$$\text{relu}(W\hat{h}_j + b)$$
- Again, shortcut connection and layer normalization
$$\text{layer-normalization}(\text{relu}(W\hat{h}_j + b) + \hat{h}_j)$$

Encoder



Sequence of self-attention layers

Self-Attention in the Decoder

- Same idea as in the encoder
- Output words are initially encoded by word embeddings $s_i = Ey_i$.
- Self attention is computed over previous output words
  - association of a word s_i is limited to words s_k $(k \leq i)$
  - resulting representation $\tilde{s}_i$

$$\text{self-attention}(\tilde{S}) = \text{MultiHead}(\tilde{S}, \tilde{S}, \tilde{S})$$

Attention in the Decoder

- Original intuition of attention mechanism: focus on relevant input words

- Computed with dot product $\tilde{S}H^T$

- Compute attention between the decoder states $\tilde{S}$ and the final encoder states H

$$\text{attention}(\tilde{S}, H) = \text{MultiHead}(\tilde{S}, H, H)$$

- Note: attention mechanism formally mirrors self-attention

Full Decoder

- Self-attention

$$\text{self-attention}(\tilde{S}) = \text{MultiHead}(\tilde{S}, \tilde{S}, \tilde{S})$$

  - shortcut connections
  - layer normalization

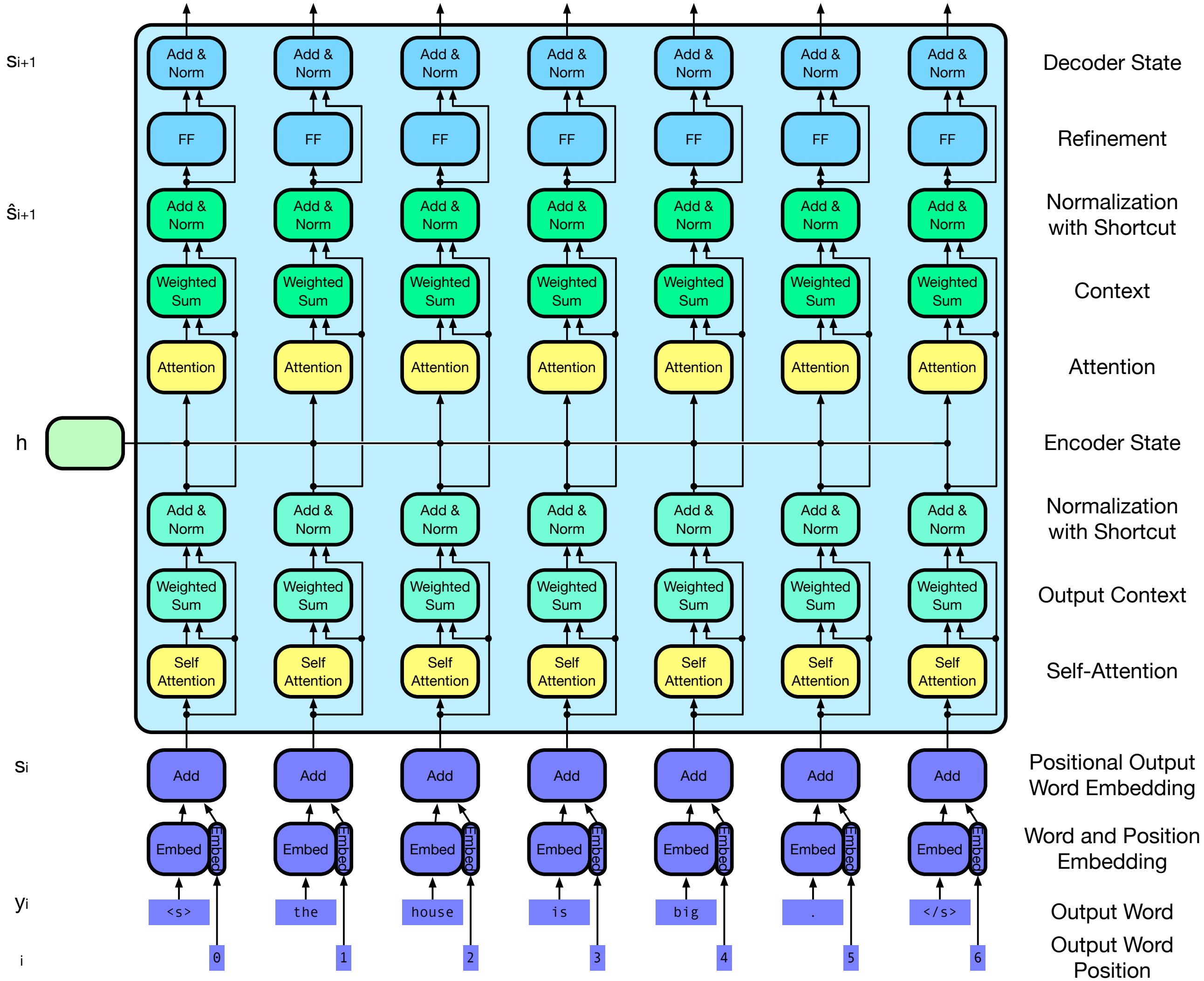
- Attention

$$\text{attention}(\tilde{S}, H) = \text{softmaxMultiHead}(\tilde{S}, H, H)$$

  - shortcut connections
  - layer normalization
  - feed-forward layer

- Multiple stacked layers

Decoder



Decoder computes attention-based representations of the output in several layers, initialized with the embeddings of the previous output words

Multiple Layers

- Stack several transformer layers (say, $D = 6$)

- Encoder
  - Start with input word embedding

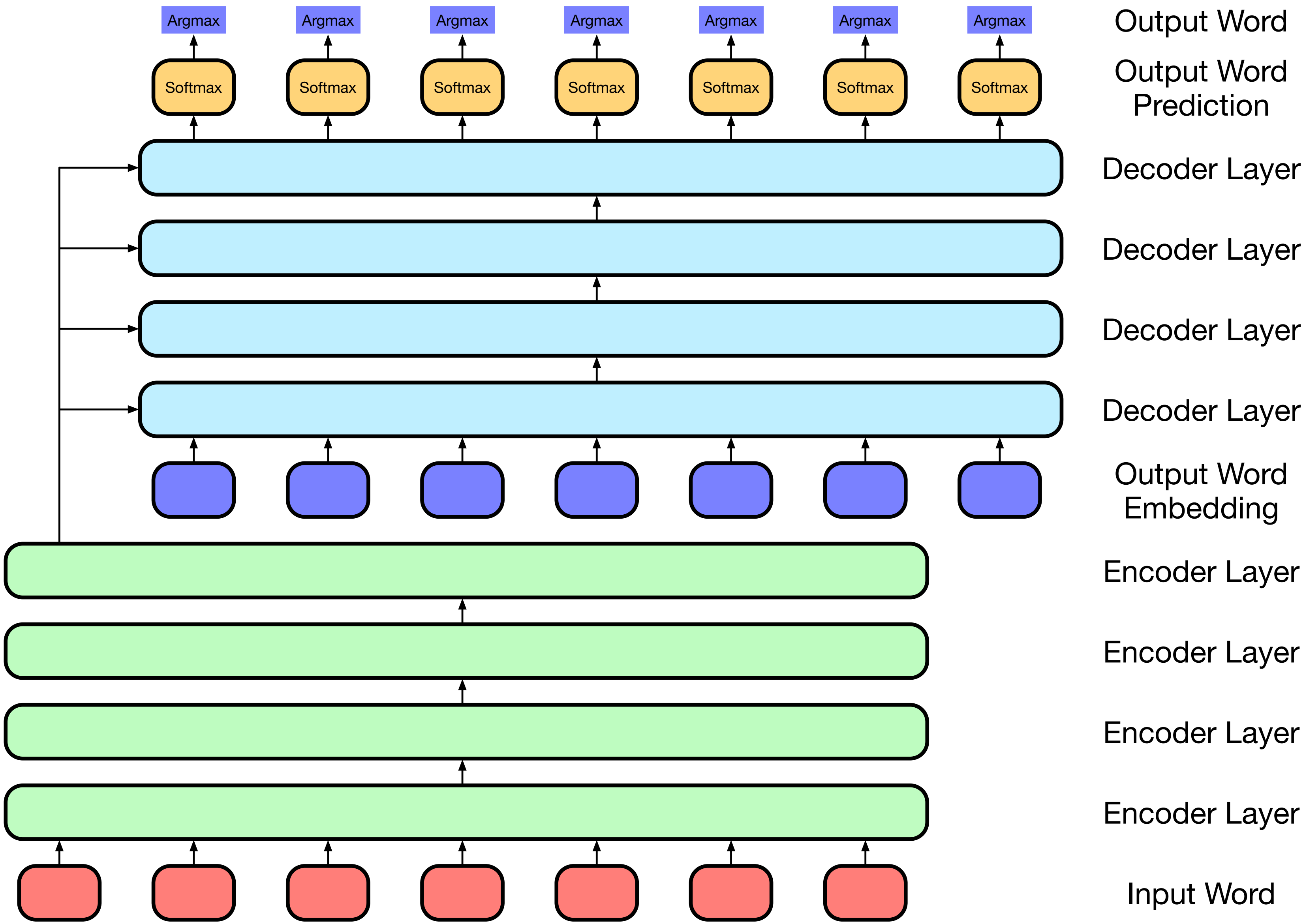
$$h_{0,j} = Ex_j$$

  - Stacked layers

$$h_{d,j} = \text{self-attention-layer}(h_{d-1,j})$$

- Same for decoder

Multiple Layers in Encoder and Decoder



questions?