Alternative Architectures

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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

$$y = activation(Mx + b)$$

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



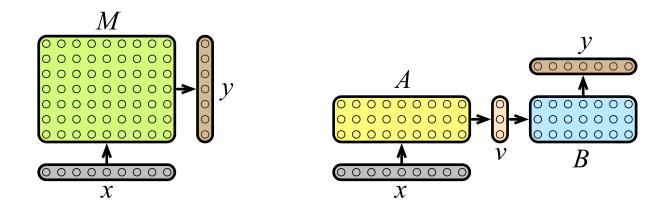
- One challenge: very large input and output vectors
- Number of parameters in matrix $M = |x| \times |y|$
- ⇒ Need to reduce size of matrix

Factored Decomposition



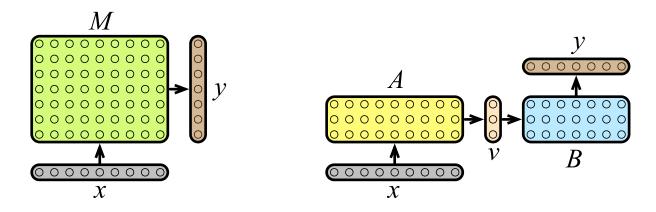
- One challenge: very large input and output vectors
- Number of parameters in matrix $M = |x| \times |y|$
- ⇒ Need to reduce size of matrix

• 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

$$y = \operatorname{activation}(M_1x_1 + M_2x_2 + b)$$

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• Another view

$$x = \operatorname{concat}(x_1, x_2)$$

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

• 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

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

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- Reduces varying length sentence representation into fixed sized vector
- Maybe weight the words, e.g., by attention



- Another elementary mathematical operation
- Three ways to multiply vectors



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

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



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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



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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

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- 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

$$W_1x + b_1$$

$$W_2x + b_2$$

Max Out



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- element-wise maximum

$$\max(x) = \max(W_1x + b_1, W_2x + b_2)$$

Max Out



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 - first branch out into multiple feed-forward layers

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- element-wise maximum

$$\max(x) = \max(W_1x + b_1, W_2x + b_2)$$

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

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



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)

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- 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

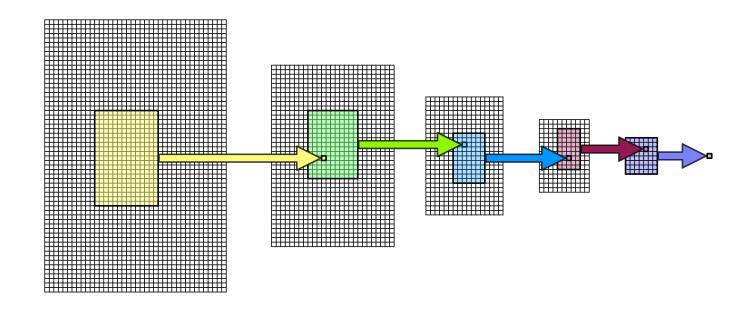
Attention



convolutional neural networks

Convolutional Neural Networks (CNN)

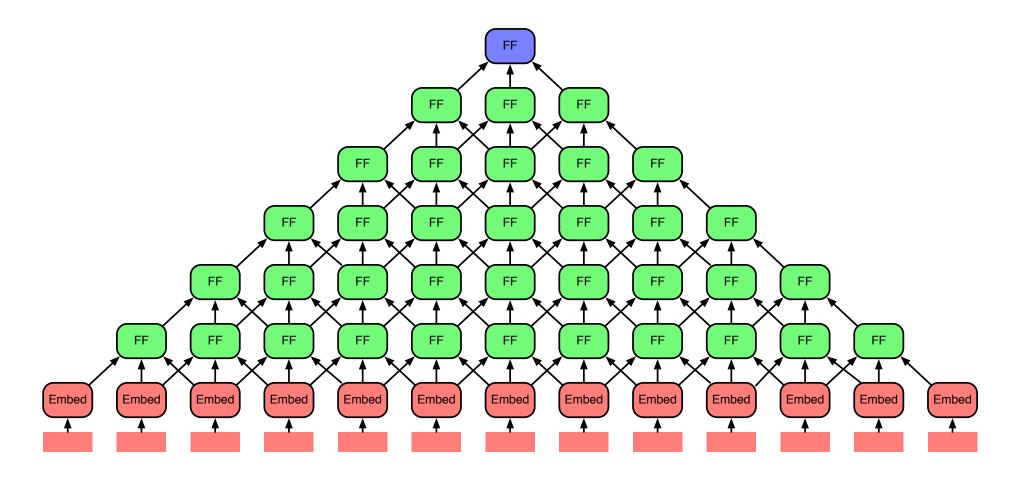




- Popular in image processing
- Regions of an image are reduced into increasingly smaller representation
 - matrix spanning part of image reduced to single value
 - overlapping regions

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 Neural Networks



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 - take a high dimensional input representation
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- 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



attention

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
- ⇒ Attention mechanism

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
 - 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: $a(s_{i-1}) = W_a s_{i-1}$

Attention of Luong et al. (2015)



• Luong et al. (2015) demonstrate good results with the dot product

$$a(s_{i-1}, h_j) = s_{i-1}^T h_j$$

- No trainable parameters
- Additional changes
- Currently more popular

General View of Dot-Product Attention



Three element

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

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

Scaled Dot-Product Attention



- Refinement of query, key, and value
- Scale it down to lower-dimensional vectors (e.g., 512 from 4096)
- Using a weight matrix for each: QW^Q , KW^K , VW^V

Multi-Head Attention



- Add redundancy
 - say, 16 attention weights
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 - say, 16 attention weights
 - each based on its own parameters
- 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



- Finally, a very different take at attention
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- Now: refine representation of input words in the encoder
 - representation of an input word mostly depends on itself
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 - previously: recurrent neural networks (considers left or right context)
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- Self attention:

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



• Formal definition (based on sequence of vectors h_j , packed into matrix H

$$self-attention(H) = softmax \left(\frac{HH^T}{\sqrt{|h|}}\right)H$$

- Association between every word representation h_j any other context word h_k
 - computed by dot product
 - results in a vector of raw association values

$$HH^T$$

• Scaled by the size of the word representation vectors |h|, and softmax

$$\operatorname{softmax}\left(\frac{HH^T}{\sqrt{|h|}}\right)$$

• Resulting vector of normalized association values used to weigh context words

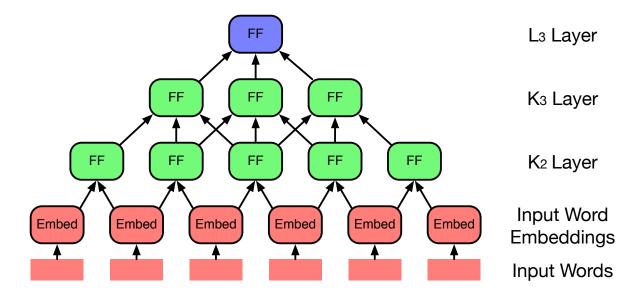


convolutional machine translation

Convolutional Machine Translation



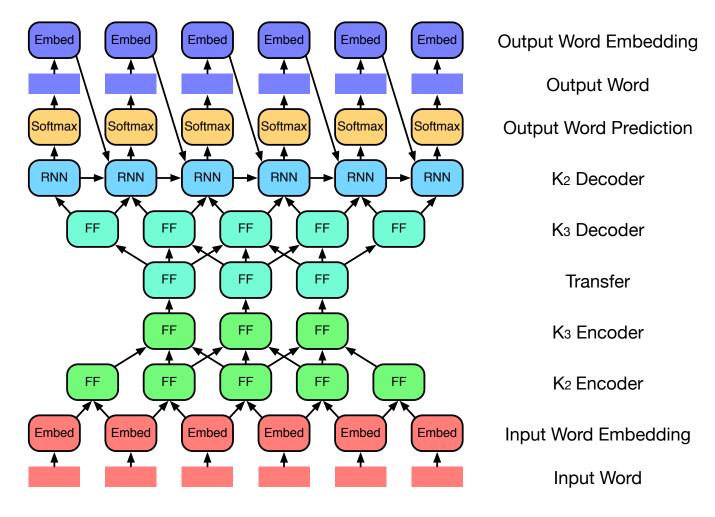
- First end-to-end neural machine translation model of the modern era [Kalchbrenner and Blunsom, 2013]
- Encoder



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

Refinement





- Convolutions do not result in a single sentence embedding but a sequence
- Decoder is also informed by a recurrent neural network

CNNs With Attention

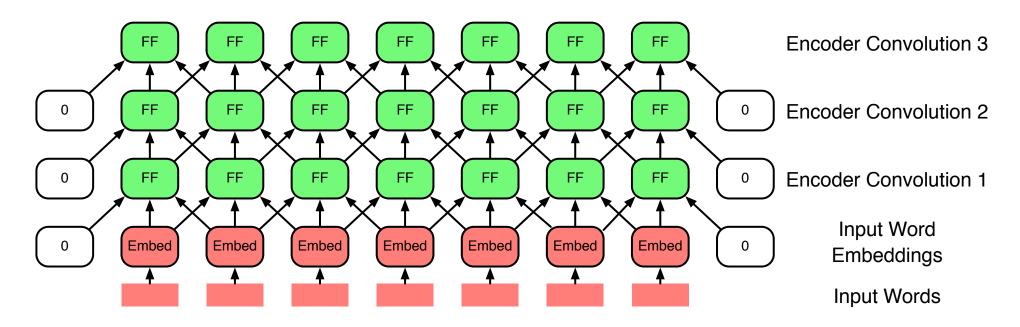


[Gehring et al. 2017]

- Combination of
 - convolutional neural networks
 - attention
- Sequence-to-sequence attention, mainly as before
- Recurrent neural networks replaced by convolutional layers

Encoder

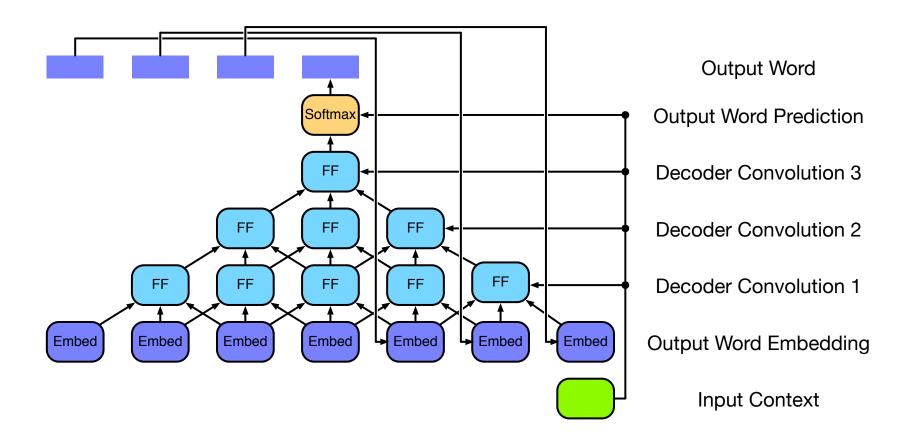




- Stacked encoder convolutions
- Not shortening representations
- But: faster processing due to more parallelism

Decoder





- Decoder state computed by convolutional layers over previous output words
- Each convolutional state also informed by the input context (using attention)



transformer

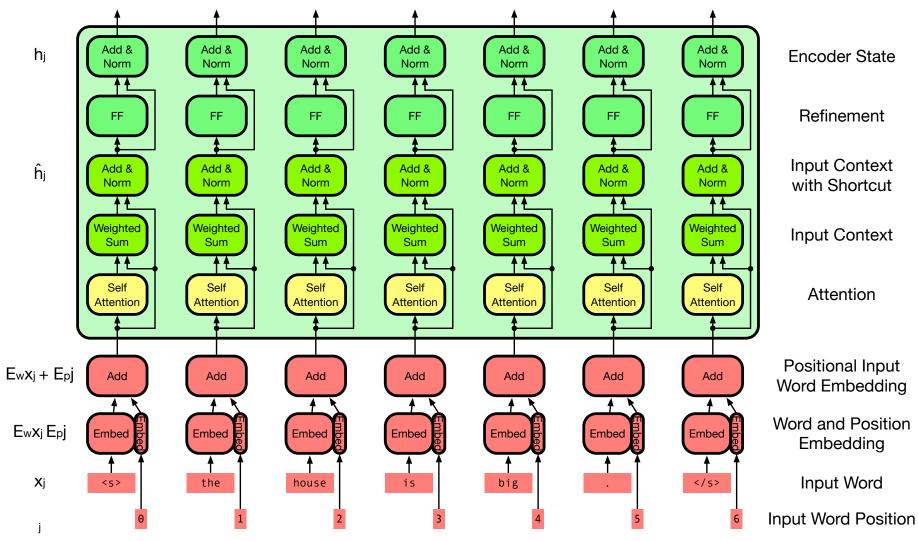
Self Attention: Transformer



- 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)

Encoder





Sequence of self-attention layers



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

$$self-attention(H) = softmax(\frac{HH^T}{\sqrt{|h|}})H$$



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- Shortcut connection

$$self$$
-attention $(h_j) + h_j$



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self-attention
$$(h_j) + h_j$$

• Layer normalization

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



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• Feed-forward step with ReLU activation function

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



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Feed-forward step with ReLU activation function

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

• Again, shortcut connection and layer normalization

layer-normalization(relu(
$$W\hat{h}_j + b$$
) + \hat{h}_j)

Stacked Self Attention Layers



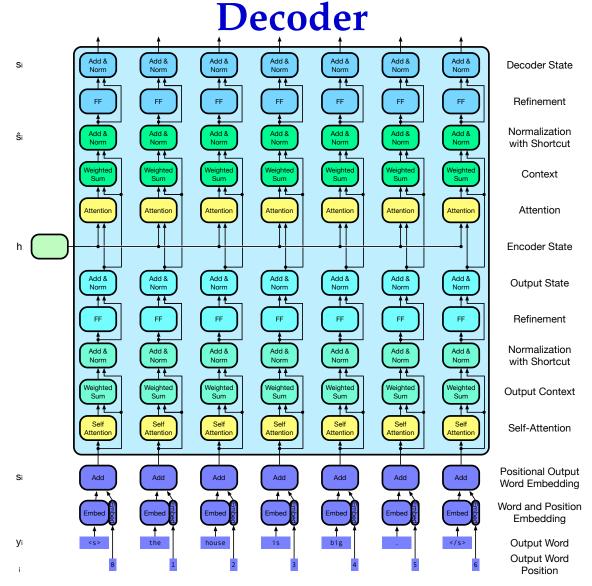
- Stack several such layers (say, D = 6)
- Start with input word embedding

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

• Stacked layers

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





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

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 ($k \le i$)
 - resulting representation $\tilde{s_i}$

$$\operatorname{self-attention}(\tilde{S}) = \operatorname{softmax}\Big(\frac{SS^T}{\sqrt{|h|}}\Big)S$$

Attention in the Decoder



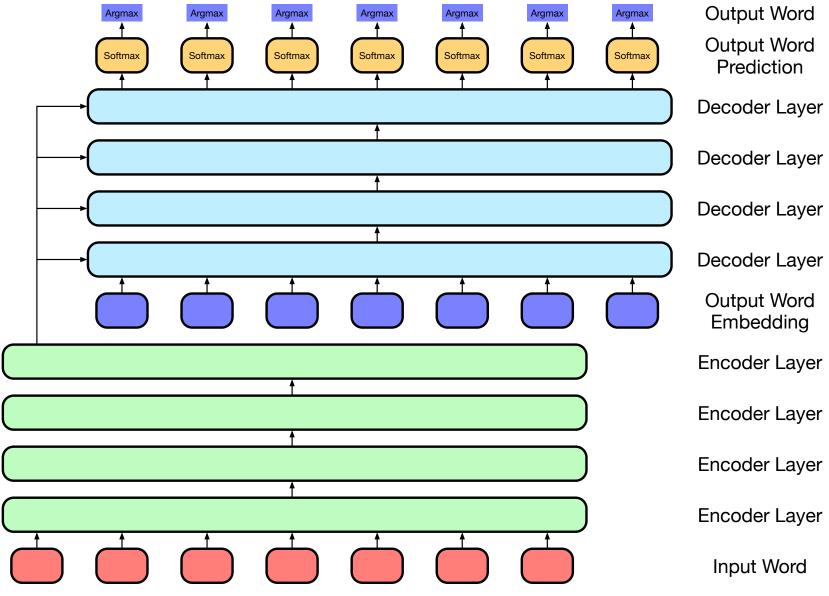
- Original intuition of attention mechanism: focus on relevant input words
- $\bullet\,$ Computed with dot product $\tilde{S}H^T$
- ullet Compute attention between the decoder states \tilde{S} and the final encoder states H

$$\operatorname{attention}(\tilde{S}, H) = \operatorname{softmax}\Big(\frac{SH^T}{\sqrt{|h|}}\Big)H$$

• Note: attention mechanism formally mirrors self-attention

Full Decoder





Full Decoder



• Self-attention

$$self-attention(\tilde{S}) = softmax \left(\frac{SS^T}{\sqrt{|h|}}\right)S$$

- shortcut connections
- layer normalization
- feed-forward layer
- Attention

$$\operatorname{attention}(\tilde{S}, H) = \operatorname{softmax}\Big(\frac{SH^T}{\sqrt{|h|}}\Big)H$$

- shortcut connections
- layer normalization
- feed-forward layer
- Multiple stacked layers

Mix and Match



- Encoder may be multiple layers of either
 - recurrent neural networks
 - self-attention layers
- Decoder may be multiple layers of either
 - recurrent neural networks
 - self-attention layers
- Also possible: self-attention encoder, recurrent neural network deocder
- Even better: both self-attention and recurrent neural network, merged at the end