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# 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

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

- Notation

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

# Feed-Forward Layer



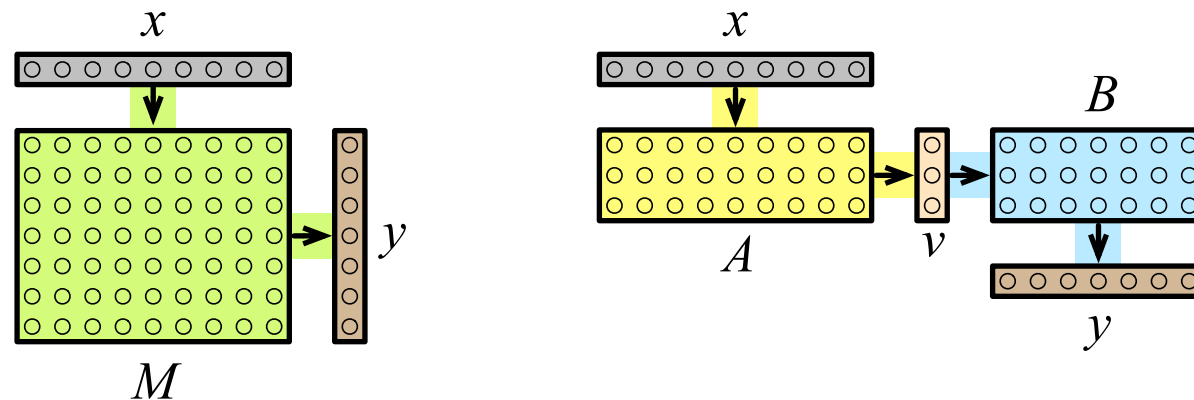
- Historic neural network designs: several feed-forward layers
  - input layer
  - hidden layers
  - output layer
- Powerful tools for a wide range of machine learning problems
- Matrix multiplication also called **affine transforms**
  - appeals to its geometrical properties
  - straight lines in input still straight lines in output

# Factored Decomposition

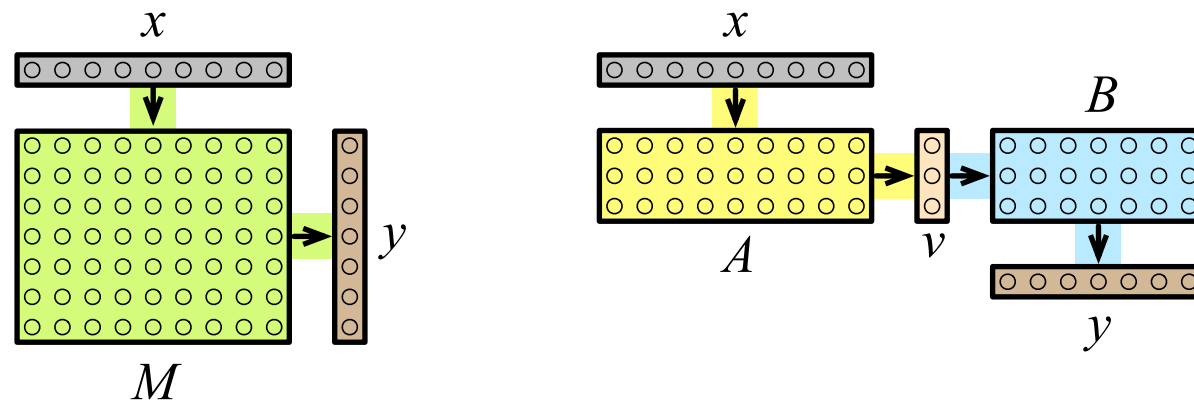
- One challenge: very large input and output vectors
- Number of parameters in matrix  $M = |x| \times |y|$

⇒ 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 capture 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

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

- Another view

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

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

- Splitting hairs here, but concatenation useful generally

- Adding vectors: very simplistic, but often done
- Example: compute sentence embeddings  $s$  from word embeddings  $w_1, \dots, w_n$

$$s = \sum_i^n w_i$$

- 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■
  - element-wise multiplication

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

- 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

- 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
  - first branch out into multiple feed-forward layers

$$W_1x + b_1$$

$$W_2x + b_2$$

- element-wise maximum

$$\text{maxout}(x) = \max(W_1x + b_1, W_2x + b_2)$$

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

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

# processing sequences



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

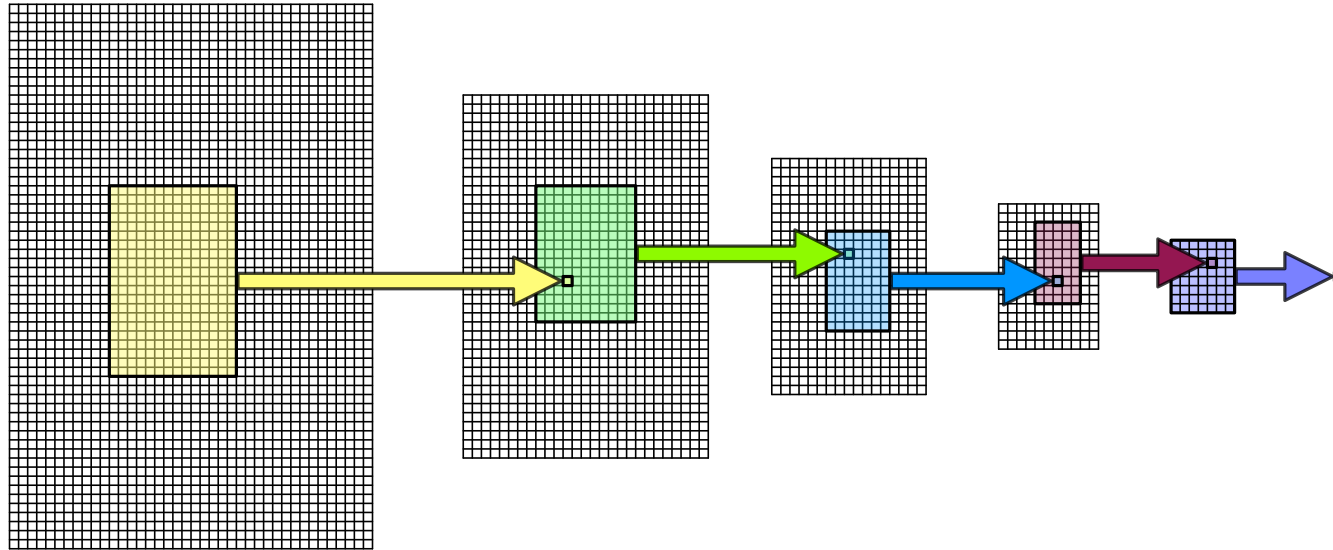
# Alternative Sequence Processing



- Convolutional neural networks
- Attention

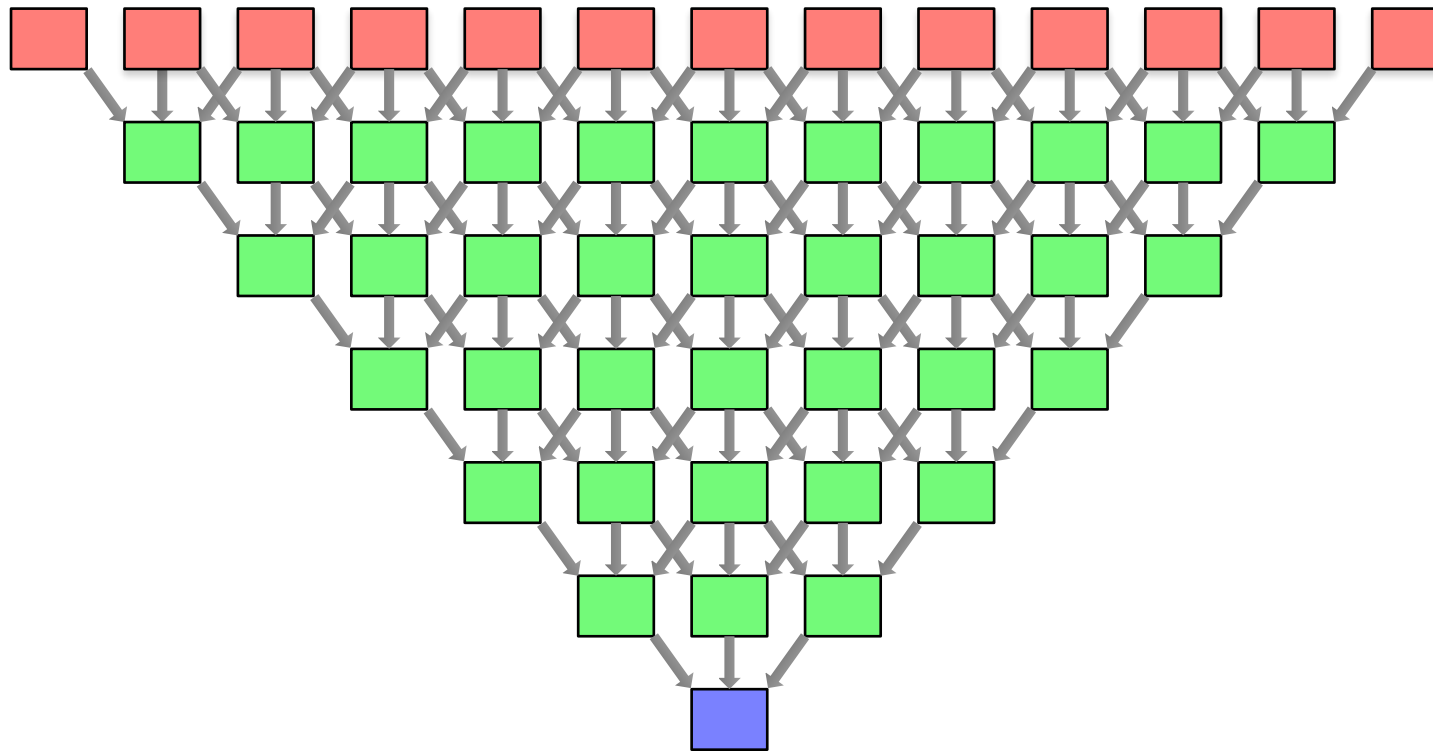
# convolutional neural networks

# 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

- Key step
  - take a high dimensional input representation
  - map to lower dimensional representation
- Several repetitions of this step
- Examples
  - map  $50 \times 50$  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



- 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

- 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)

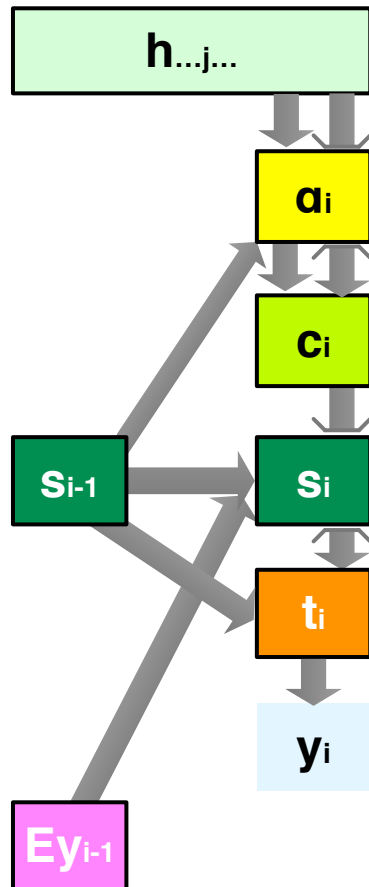
- Luong et al. (2015) demonstrate good results with the dot product

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

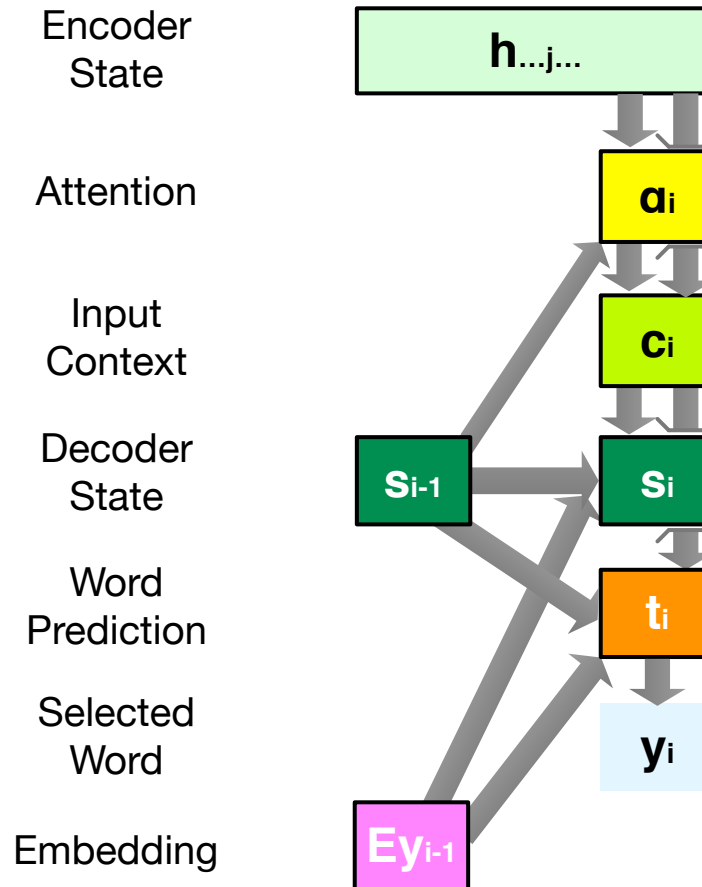
- No trainable parameters
- Additional changes
- Currently more popular

# Attention of Luong et al. (2015)

Luong et al. (2015)



Bahdanau et al. (2015)



# Attention of Luong et al. (2015)

Luong et al. (2015)

Attention

$$\alpha_{ij} = \text{softmax FF}(s_{i-1}, h_j)$$

Input context  $c_i = \sum_j \alpha_{ij} h_j$

Output word

$$p(y_t | y_{<t}, x) = \text{softmax}(W \text{ FF}_{\tanh}(s_{i-1}, c_i))$$

Decoder state

$$s_i = \text{FF}_{\tanh}(s_{i-1}, Ey_{i-1})$$

Bahdanau et al. (2015)

Attention

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Output word

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Decoder state

$$s_i = \text{FF}_{\tanh}(s_{i-1}, Ey_{i-1}, c_i)$$

# Multi-Head Attention

- Add redundancy
  - say, 16 attention weights
  - each based on its own parameters■
- Formally, for each head  $k$  compute an associated between
  - decoder state  $s_{i-1}$  at time step  $i$
  - encoder state  $h_j$  for the  $j$ th input word
  - using the softmax of some parameterized function  $a^k$

$$\alpha_{ij}^k = \text{softmax } a^k(s_{i-1}, h_j) \blacksquare$$

- Average the attention weights

$$\alpha_{ij} = \frac{1}{k} \sum_k \alpha_{ij}^k$$

- Multi-head attention is a form of ensembling

- Why just use a single scalar value to weight entire vectors?
  - learn weights for each element
  - computation of attention values returns vector instead of scalar■
- Architecturally, still a feed-forward neural network (or any of variants)

$$a(s_{i-1}, h_j) = \text{FF}^k(s_{i-1}, h_j) \blacksquare$$

- Softmax is now applied over each dimension  $d$

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

- Input context is now computed by a element-wise multiplication

$$c_i = \sum_j \alpha_{ij} \times h_j$$

- 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?



- Formal definition (based on sequence of vectors  $h_j$ , packed into matrix  $H$ )

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

- 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

$$H H^T$$

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

$$\text{softmax}\left(\frac{H H^T}{\sqrt{|h|}}\right)$$

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

- More familiar math, using word representation vectors  $h_j$

- Raw association  $\frac{HH^T}{\sqrt{|h|}}$

$$a_{jk} = \frac{1}{|h|} h_j h_k^T$$

- Normalized association (softmax)

$$\alpha_{jk} = \frac{\exp(a_{jk})}{\sum_{\kappa} \exp(a_{j\kappa})}$$

- Weighted sum

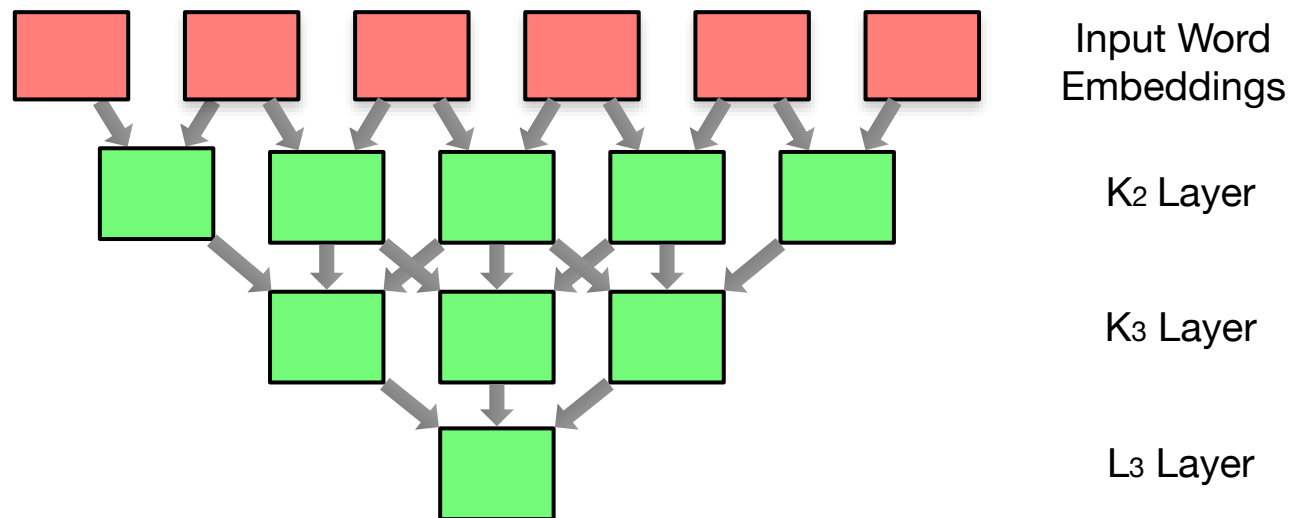
$$\text{self-attention}(h_j) = \sum_k \alpha_{jk} h_k$$

- More on this later (Transformer)

# convolutional machine translation

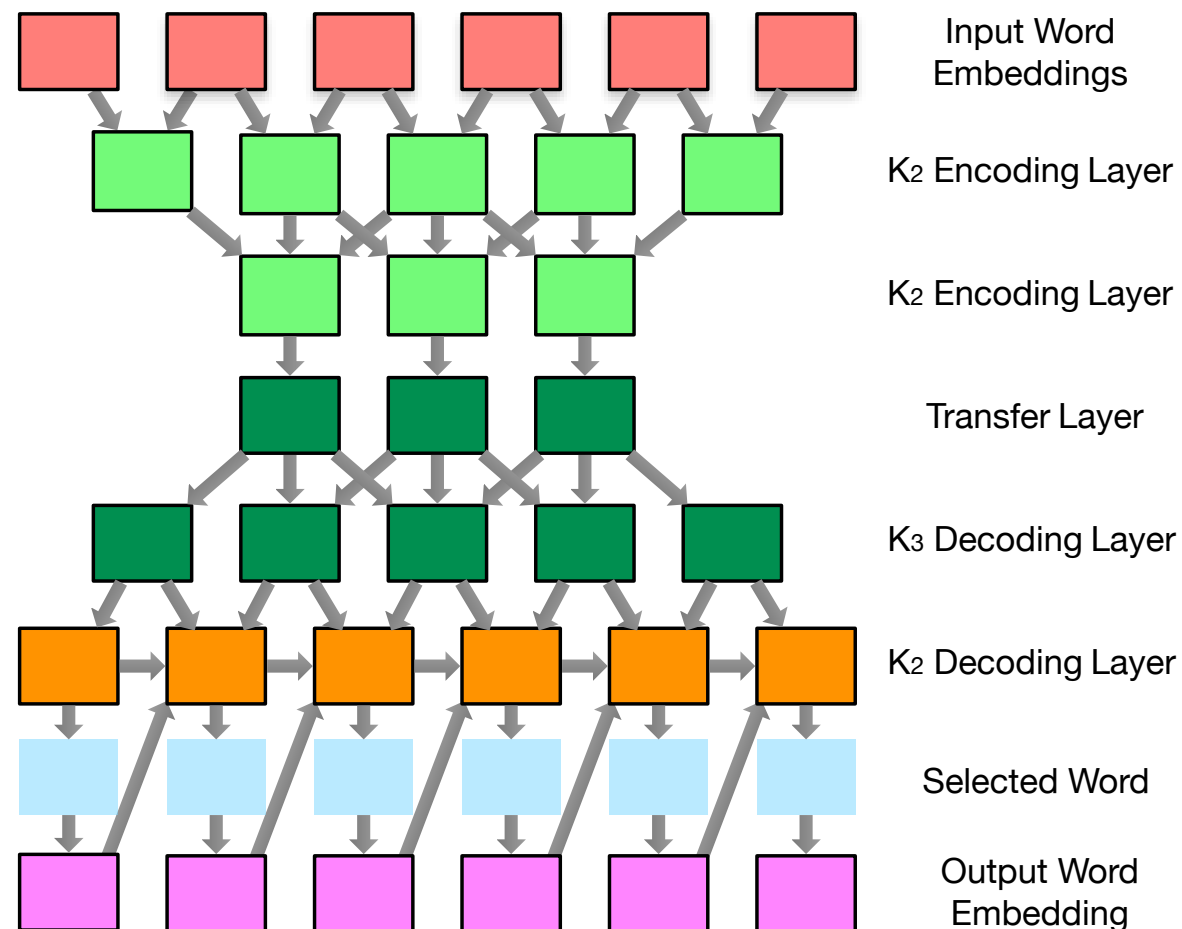
# Convolutional Machine Translation

- 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



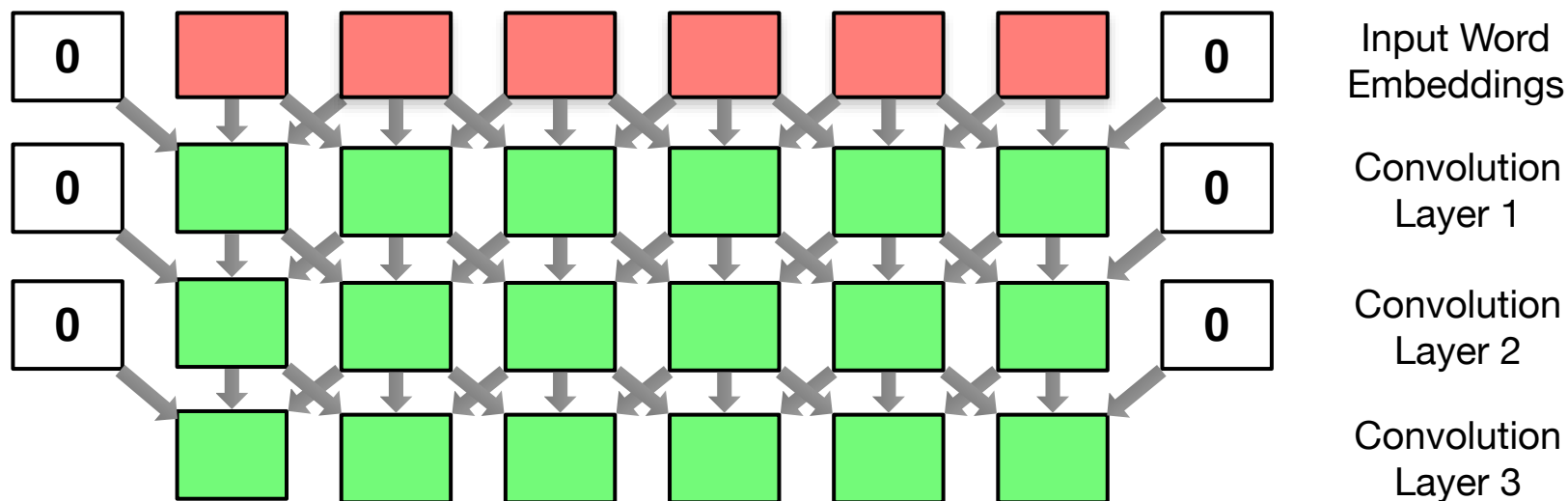
- Convolutions do not result in a single sentence embedding but a sequence
- Decoder is also informed by a recurrent neural network

# 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

- Start with input word embeddings  $Ex_j$

$$h_{0,j} = E x_j$$

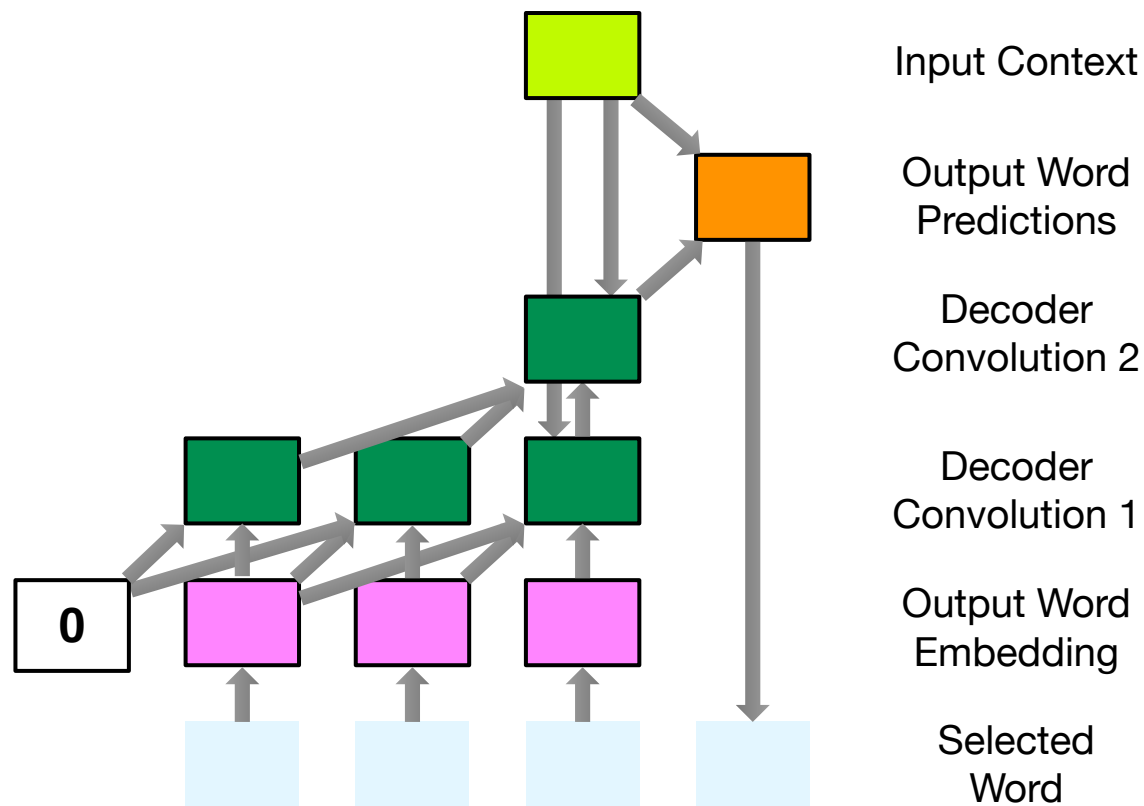
- Progress through
  - sequence of layer encodings  $h_{d,j}$
  - at different depth  $d$
  - until maximum depth  $D$

$$h_{d,j} = f(h_{d-1,j-k}, \dots, h_{d-1,j+k})$$

- Details
  - function  $f$  is feed-forward layer with shortcut connection
  - final representation  $h_{D,j}$  may only be informed by partial sentence context
  - all words at one depth can be processed in parallel  $\rightarrow$  fast



# Decoder



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

- Recall: decoder recurrent neural network decoder

$$s_i = f(s_{i-1}, Ey_{i-1}, c_i)$$

- encoder state  $s_i$
  - embedding of previous output word  $Ey_{i-1}$
  - input context  $c_i$
- Now
  - state computation not depending on previous state  $s_{i-1}$  (not recurrent)
  - conditioned on the sequence of the  $\kappa$  most recent previous words

$$s_i = f(Ey_{i-\kappa}, \dots, Ey_{i-1}, c_i)$$

- Stacked convolutions

$$s_{1,i} = f(Ey_{i-\kappa}, \dots, Ey_{i-1}, c_i)$$

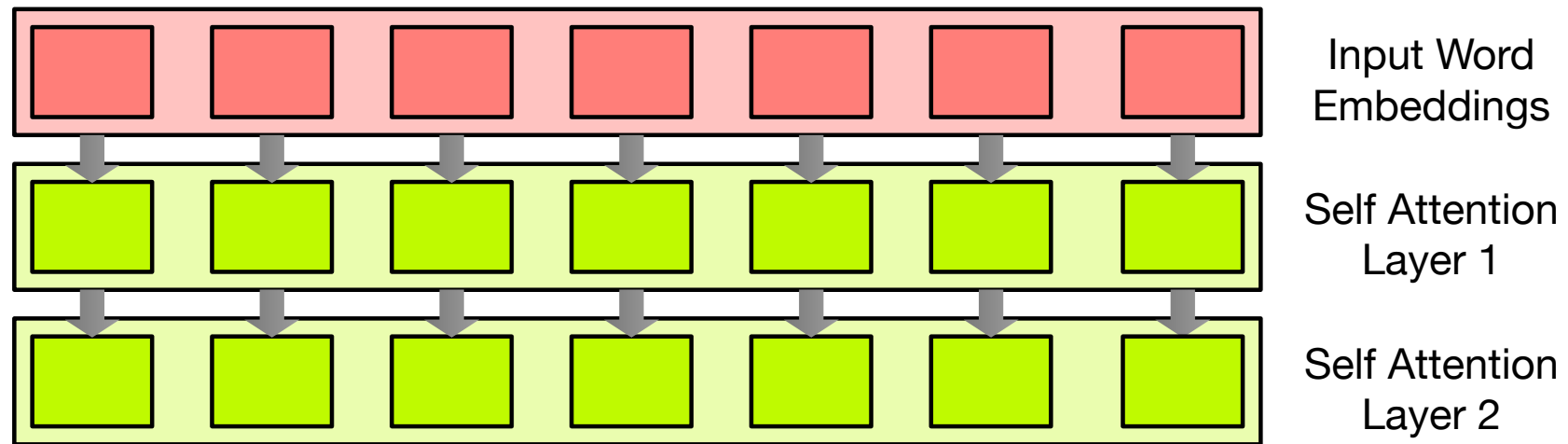
$$s_{d,i} = f(s_{d-1,i-\kappa-1}, \dots, s_{d-1,i}, c_i) \text{ for } d > 0, d \leq \hat{D}$$

- Attention mechanism fundamentally unchanged
- Input context  $c_i$  computed based on association  $a(s_{i-1}, h_j)$  between
  - encoder state  $h_j$
  - decoder state  $s_{i-1}$
- Now
  - encoder state  $h_{D,j}$
  - decoder state  $s_{\hat{D},i-1}$
- Refinement when computing the context vector  $c_i$ :  
shortcut connection between encoder state  $h_{D,j}$  and input word embedding  $x_j$

# 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

# Self Attention Layer

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

- Self attention

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

- 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

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

# Stacked Self Attention Layers

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

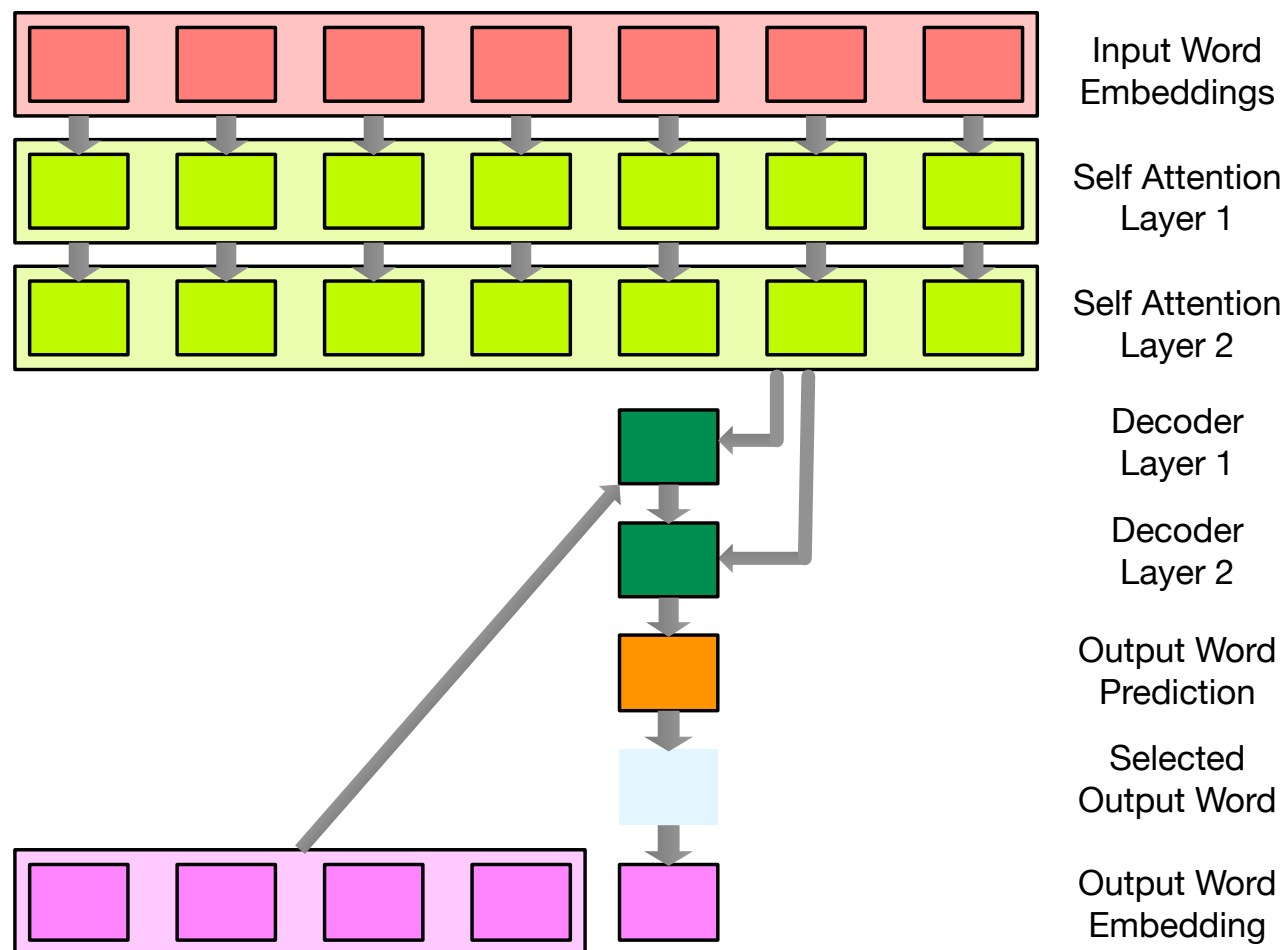
$$h_{0,j} = Ex_j$$

- Stacked layers

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



# Decoder



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  $s_k$  ( $k \leq i$ )
  - resulting representation  $\tilde{s}_i$

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

# 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  $H$

$$\text{attention}(\tilde{S}, H) = \text{softmax}\left(\frac{\tilde{S}H^T}{\sqrt{|h|}}\right)H$$

- Note: attention mechanism formally mirrors self-attention

- Self-attention

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

- shortcut connections
- layer normalization
- feed-forward layer

- Attention

$$\text{attention}(\tilde{S}, H) = \text{softmax}\left(\frac{\tilde{S} H^T}{\sqrt{|h|}}\right) H$$

- shortcut connections
- layer normalization
- feed-forward layer

- Multiple stacked layers

- 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