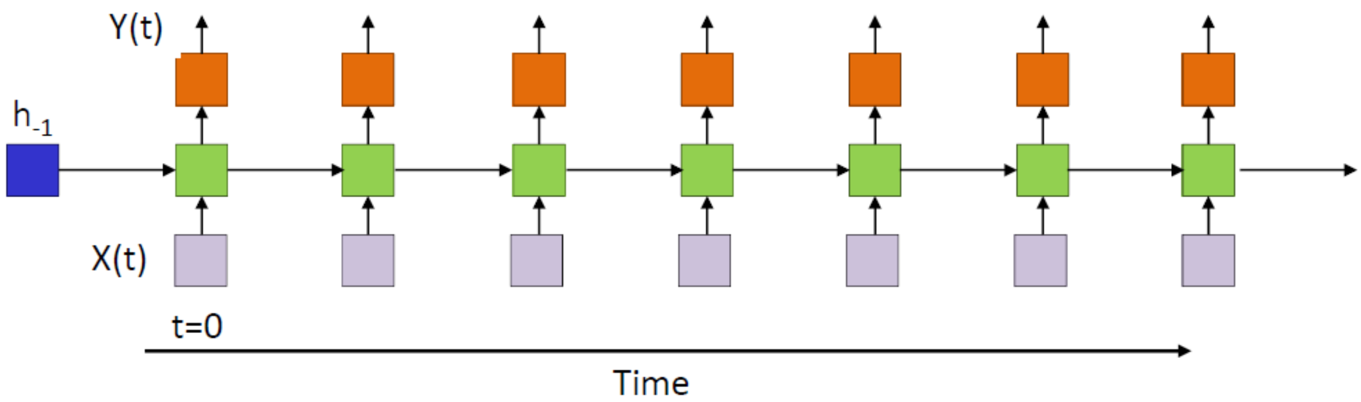
HW 2 Due 2/13

Recurrent Neural Networks

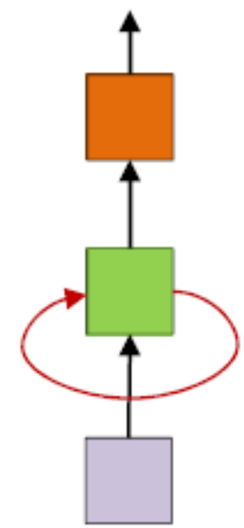
Recurrent Neural Network

- h_t: hidden state
- X_t: input
- Y_t: output
- $Y_t, h_t = f(h_{t-1}, X_t; \theta)$
- h_{-1}: initial state



Fully-connect NN vs. RNN

- RNN can be viewed as repeated applying fully-connected NNs
- $h_t = \sigma_1(W^{(1)}X_t + W^{(11)}h_{t-1} + b^{(1)})$
- $Y_t = \sigma_2(W^{(2)}h_t + b^{(2)})$
- σ_1, σ_2 are activation functions (sigmoid, ReLU, tanh, etc)



Practical issues of RNN

Linear RNN derivation

- $h_t = W^{(11)} h_{t-1} + W^{(1)} x_t$

$$\Rightarrow \quad h_k = \left(W^{(11)}\right)^{k+1} h_{-1} + \sum_{i=0}^{k} \left(W^{(11)}\right)^{k-i} W^{(1)} \cdot x_i$$

if $\lambda_{max}(W^{(11)}) < 1 \rightarrow$ exp small

$\Rightarrow$ forgetting x_i

for i small

Practical issues of RNN: training

Gradient explosion and gradient vanishing

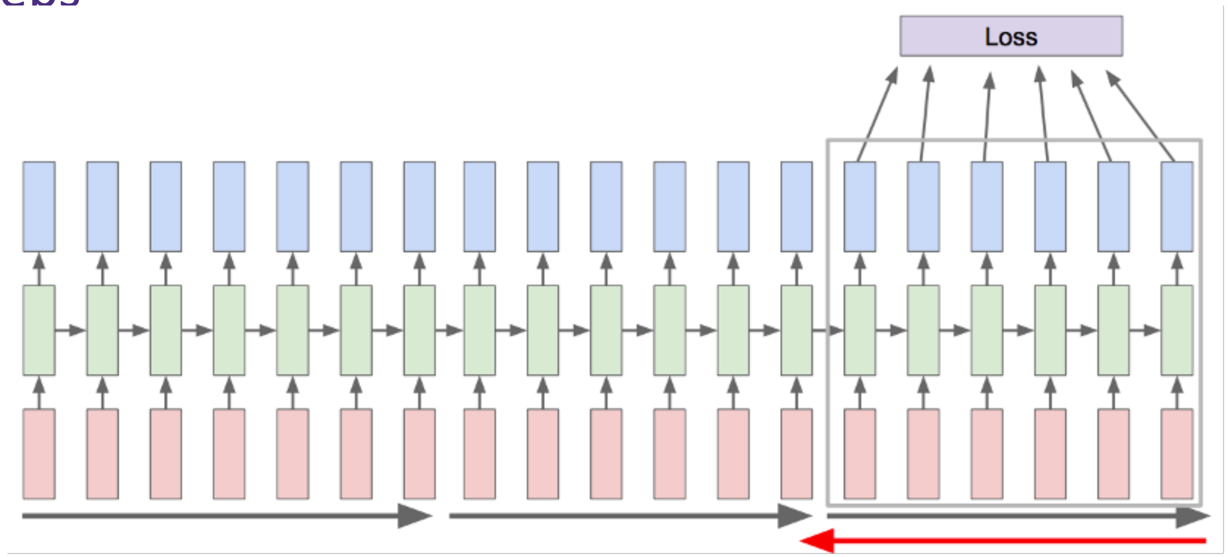
$$\frac{\partial L_k}{\partial h_0} \propto \underline{\left(W^{(hh)}\right)^k} \; \underbrace{\prod_{t=0}^{k} \sigma'(z_k)}_{\text{forgetting problem}}$$

Techniques for avoiding gradient explosion

- Gradient clipping

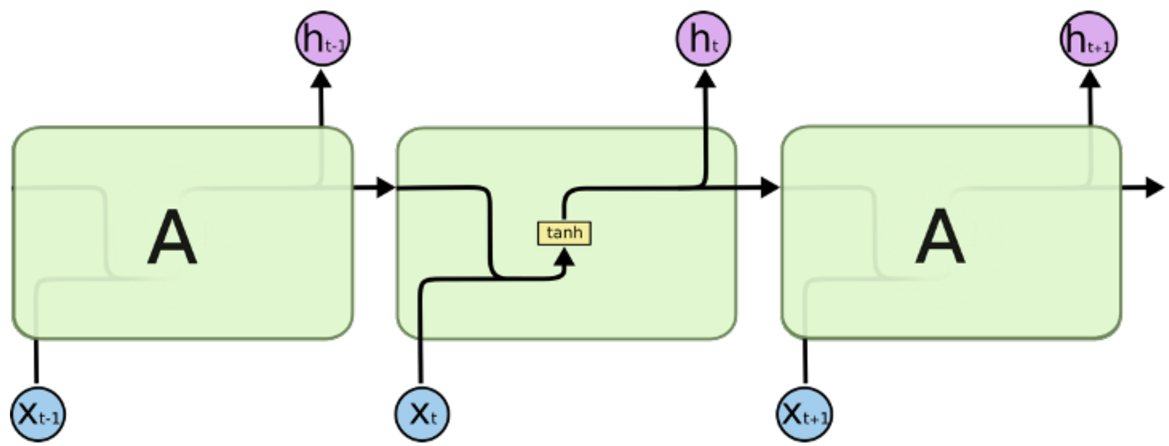
- Identity initialization

- Truncated backprop through time
  - Only backprop for a few steps

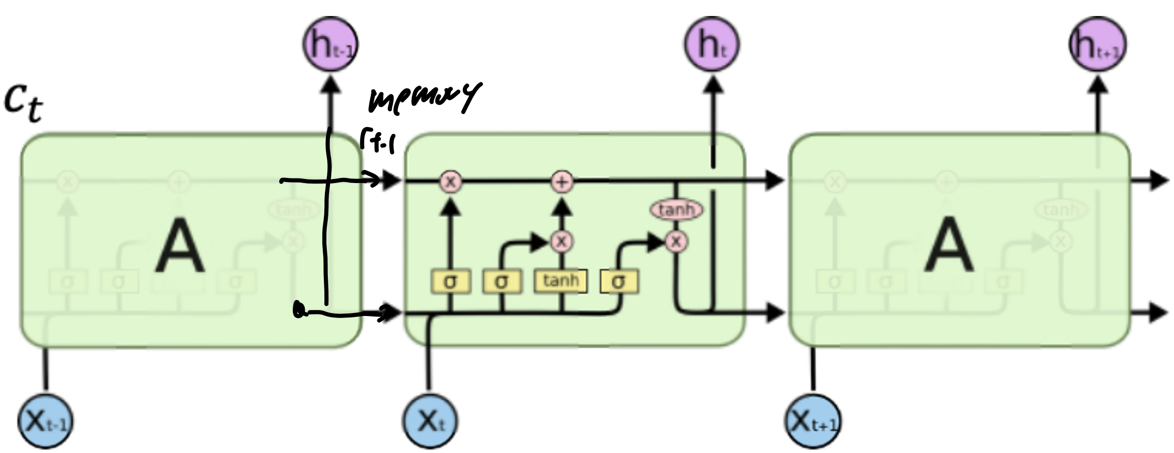


Preserve Long-Term Memory

- Difficult for RNN to preserve long-term memory
  - The hidden state h_t is constantly being written (short-term memory)
  - Use a separate cell to maintain long-term memory



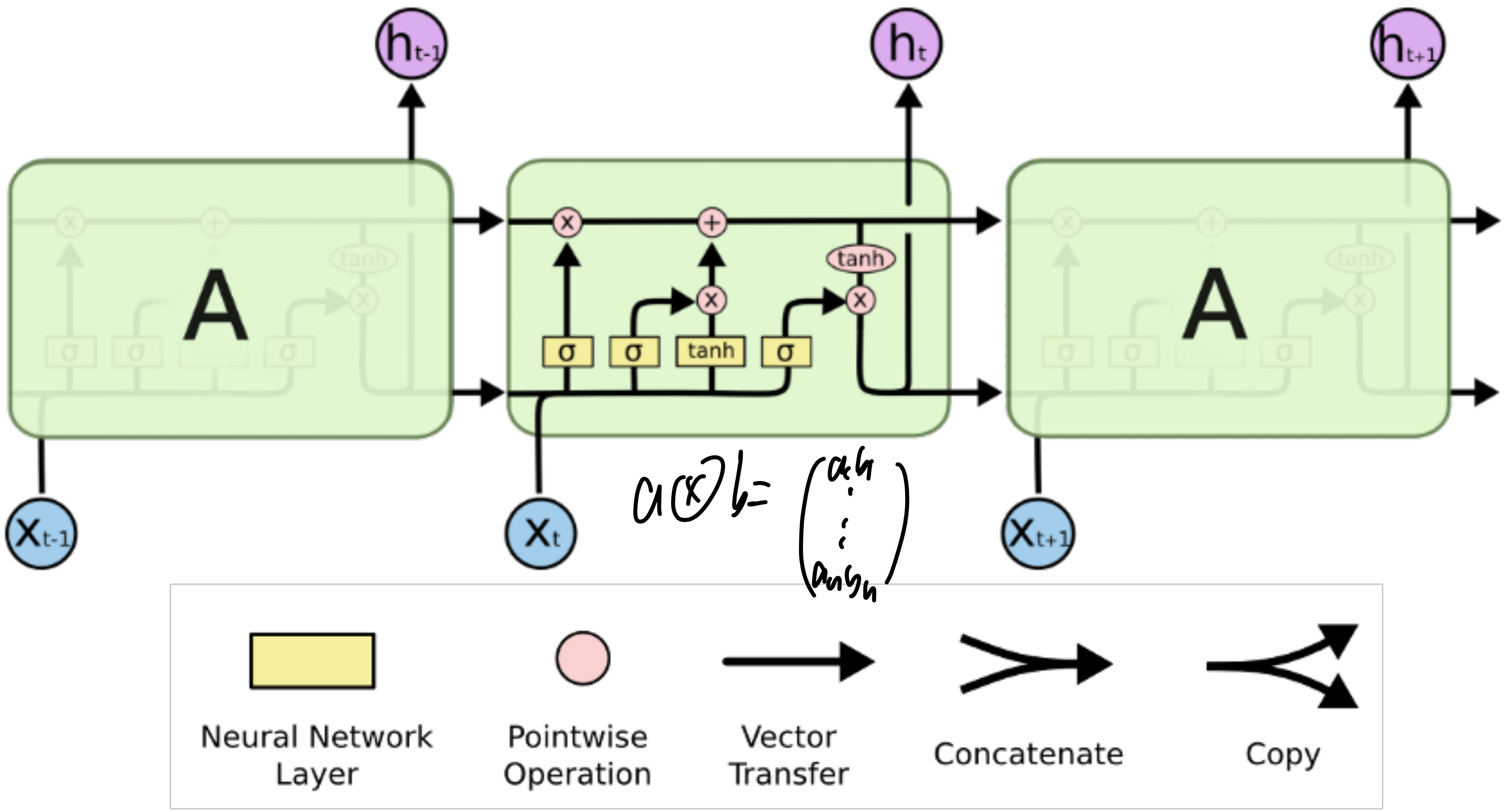
Memory c_t



Long Short-Term Memory Network

LSTM (Hochreitcher & Schmidhuber, ’97)

- RNN architecture for learning long-term dependencies
- σ: layer with sigmoid activation

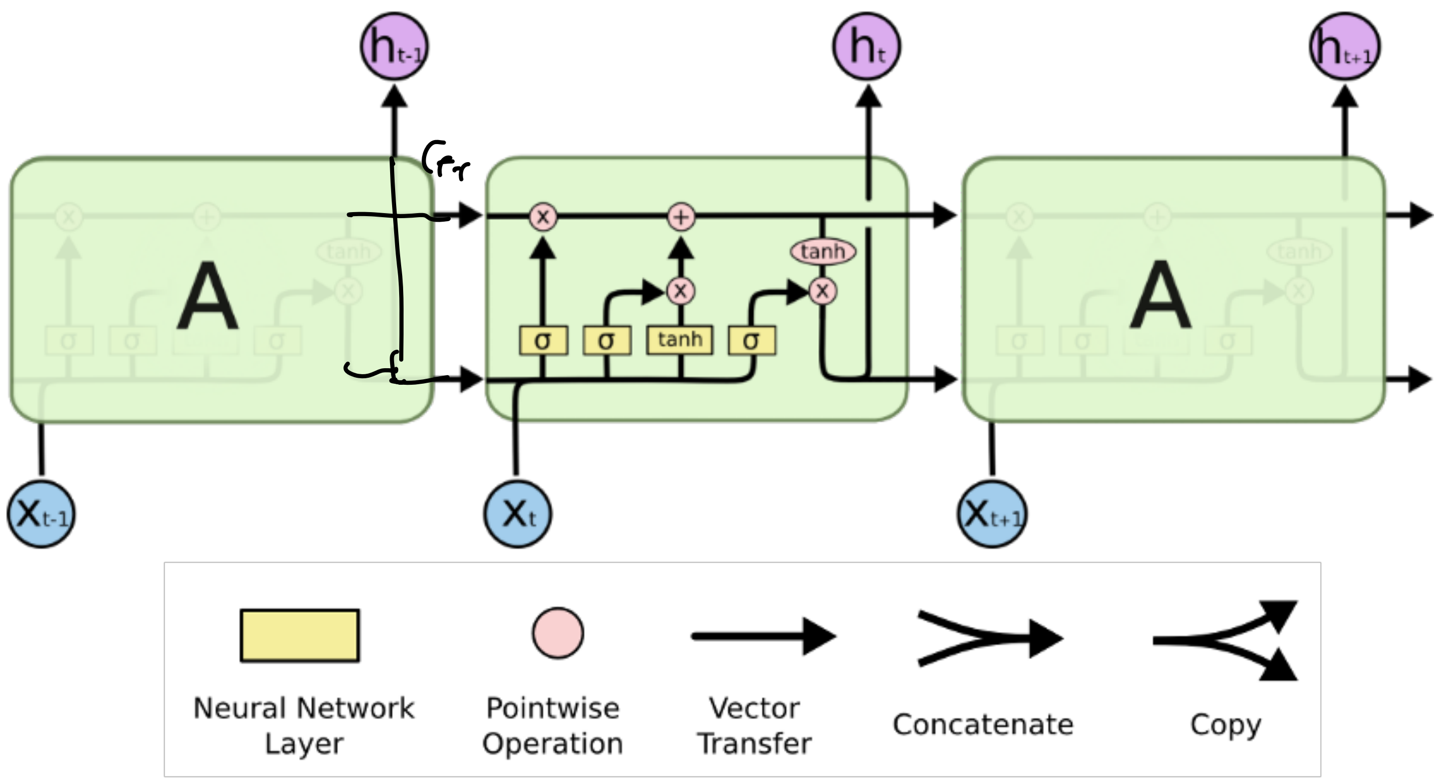


$a \otimes b = \begin{pmatrix} a_1 b_1 \\ \vdots \\ a_n b_n \end{pmatrix}$

Long Short-Term Memory Network

LSTM (Hochreitcher & Schmidhuber, ’97)

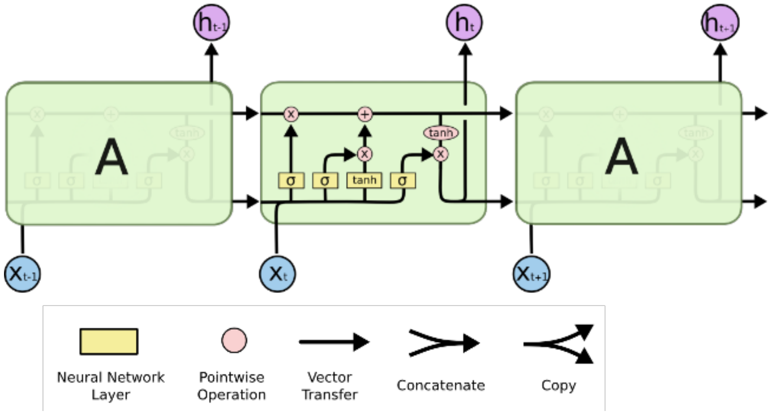
- Core idea: maintain separate state h_t and cell c_t (memory)
- h_t: full update every step
- c_t: only *partially* update through gates
  - σ layer outputs importance ($[0,1]$) for each entry and only modify those entries of c_t

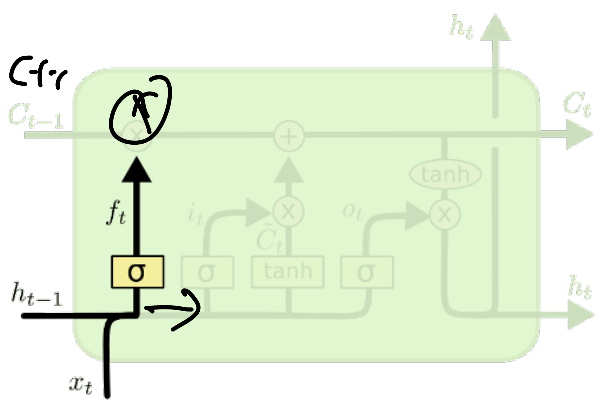


Long Short-Term Memory Network

Forget gate f_t

- f_t outputs whether we want to "forget" things in c_t
  - Compute $c_{t-1} \odot f_t$ (element-wise)
  - $f_t(i) \to 0$: want to forget $c_t(i)$
  - $f_t(i) \to 1$: we want to keep the information in $c_t(i)$



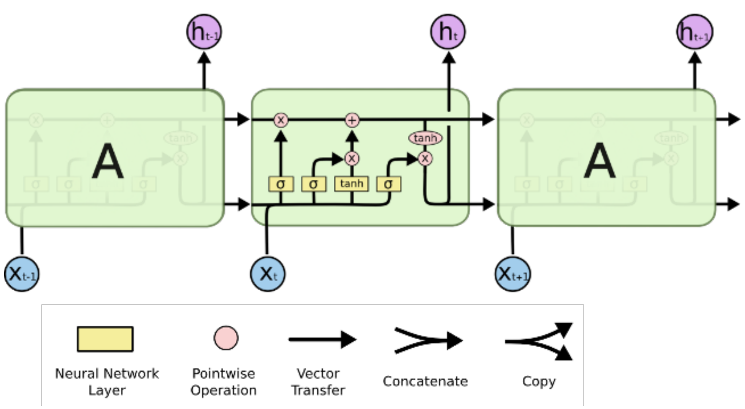


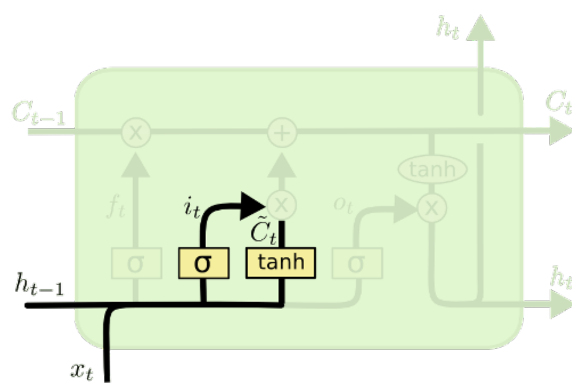
$$f_t = \sigma\left(W_f \cdot [h_{t-1}, x_t] + b_f\right)$$

Long Short-Term Memory Network

Input gate i_t

- i_t extracts useful information from X_t to update memory
    - $\tilde{c}_t$: information from X_t to update memory
    - i_t: which dimension in the memory should be updated by X_t
        - $i_t(j) \rightarrow 1$: we want to use the information in $\tilde{c}_t(j)$ to update memory
        - $i_t(t) \rightarrow 0$: $\tilde{c}_t(j)$ should not contribute to memory





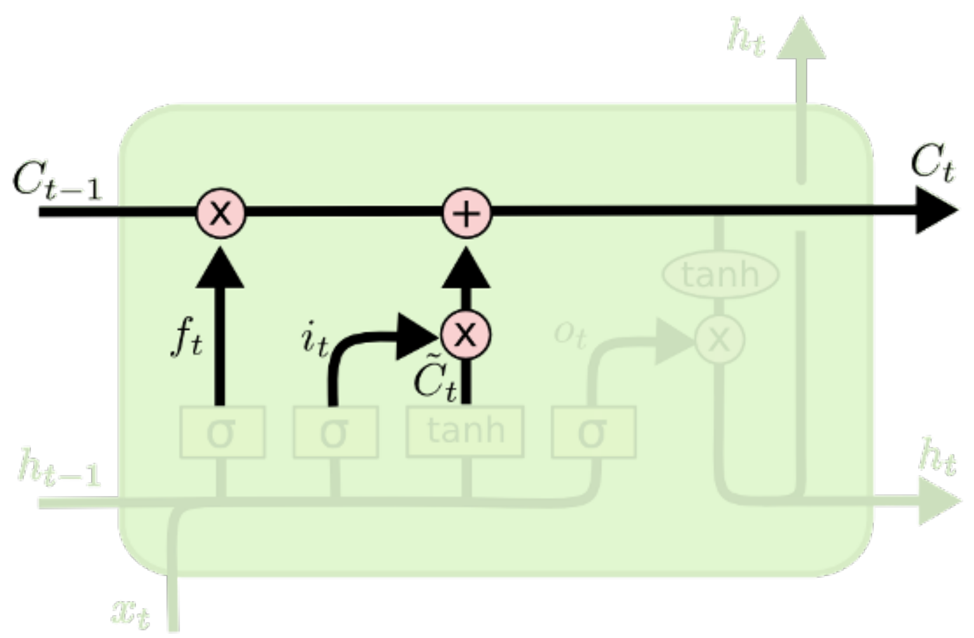
$$i_t = \sigma\left(W_i \cdot [h_{t-1}, x_t] \ + \ b_i\right)$$

$$\tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] \ + \ b_C)$$

Long Short-Term Memory Network

Memory update

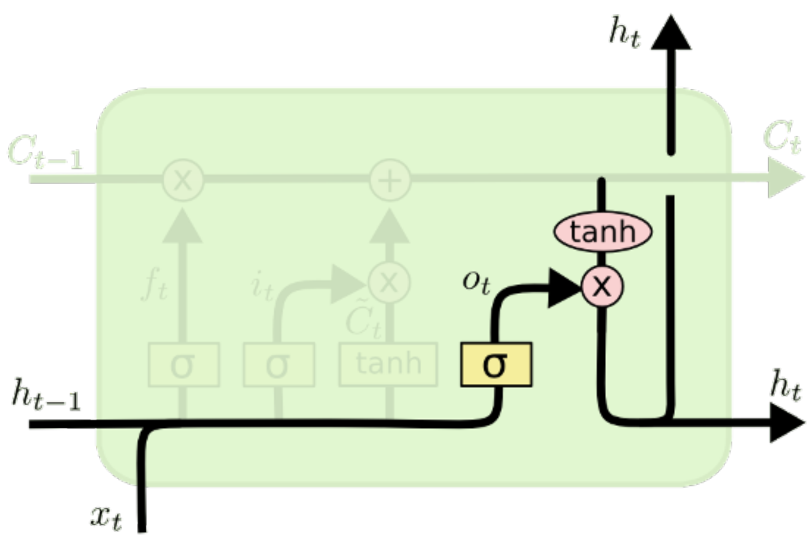
- $c_t = f_t \odot c_{t-1} + i_t \odot \tilde{c}_t$
- f_t forget gate; i_t input date
- $f_t \odot c_{t-1}$: drop useless information in old memory
- $i_t \odot \tilde{c}_t$: add selected new information from current input



Long Short-Term Memory Network

Output gate o_t

- Next hidden state $h_t = o_t \odot \tanh(c_t)$
  - $\tanh(c_t)$: non-linear transformation over all past information
  - o_t: choose important dimensions for the next state
    - $o_t(j) \rightarrow 1$: $\tanh(c_t(j))$ is important for the next state
    - $o_t(j) \rightarrow 0$: $\tanh(c_t(j))$ is not important

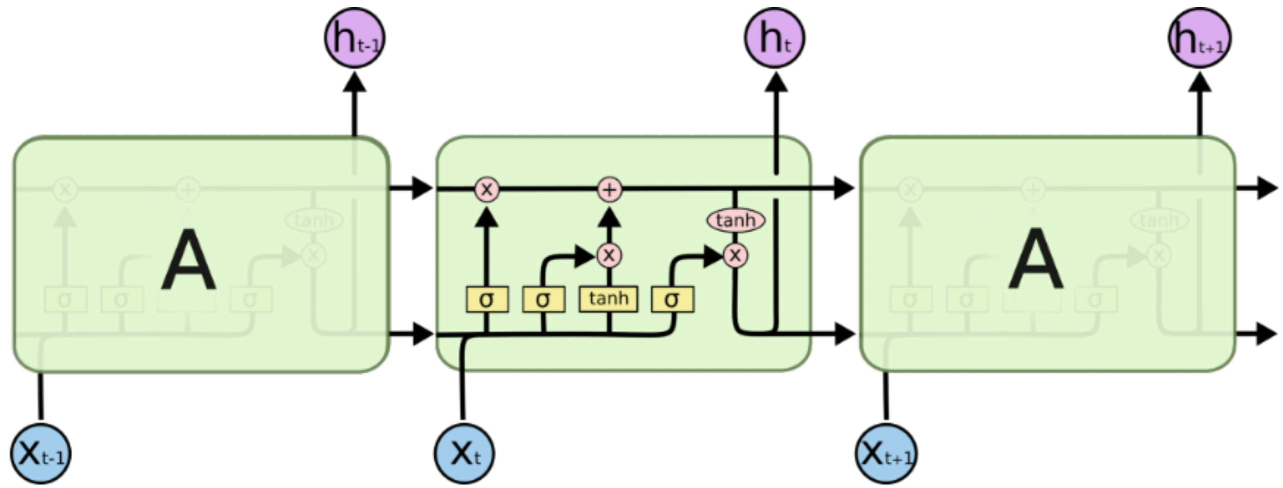


$$o_t = \sigma\left(W_o\ [h_{t-1}, x_t]\ +\ b_o\right)$$

$$h_t = o_t * \tanh\left(C_t\right)$$

Long Short-Term Memory Network

- $h_t = o_t \odot \tanh(c_t)$
- $c_t = f_t \odot c_{t-1} + i_t \odot \tilde{c}_t$
- $Y_t = g(h_t)$



Remarks:

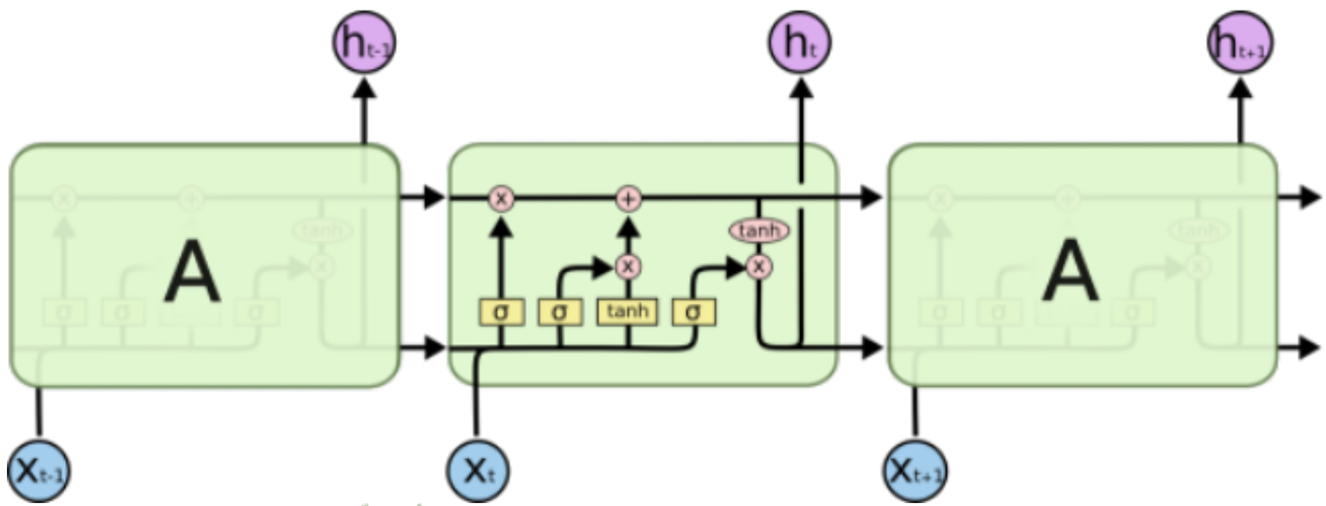
1. No more matrix multiplications for c_t
2. LSTM does not have guarantees for gradient explosion/vanishing
3. LSTM is the dominant architecture for sequence modeling from ’13 - ’16.
4. Why tanh

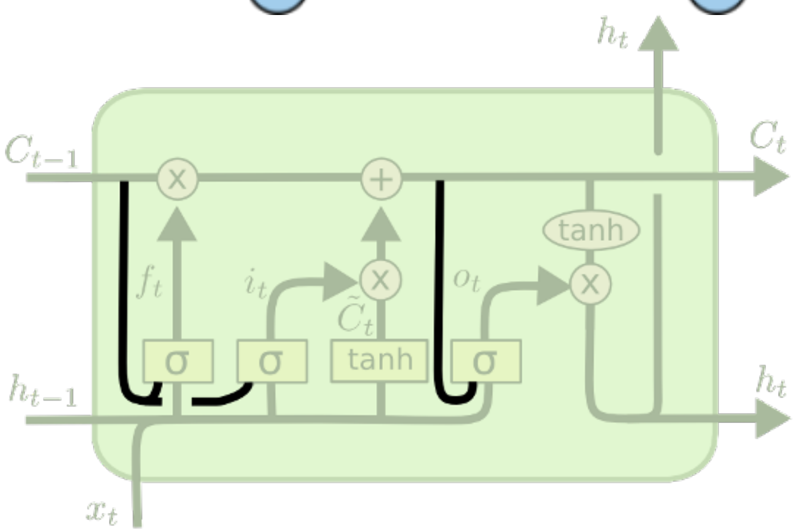
$$\frac{e^x - e^{-x}}{e^x + e^{-x}}$$

LSTM Variant

Peephold Connections (Gers & Schmidhuber ’00)

- Allow gates to take in c_t information





$$f_t = \sigma\left(W_f \cdot [\boldsymbol{C_{t-1}}, h_{t-1}, x_t] \;+\; b_f\right)$$

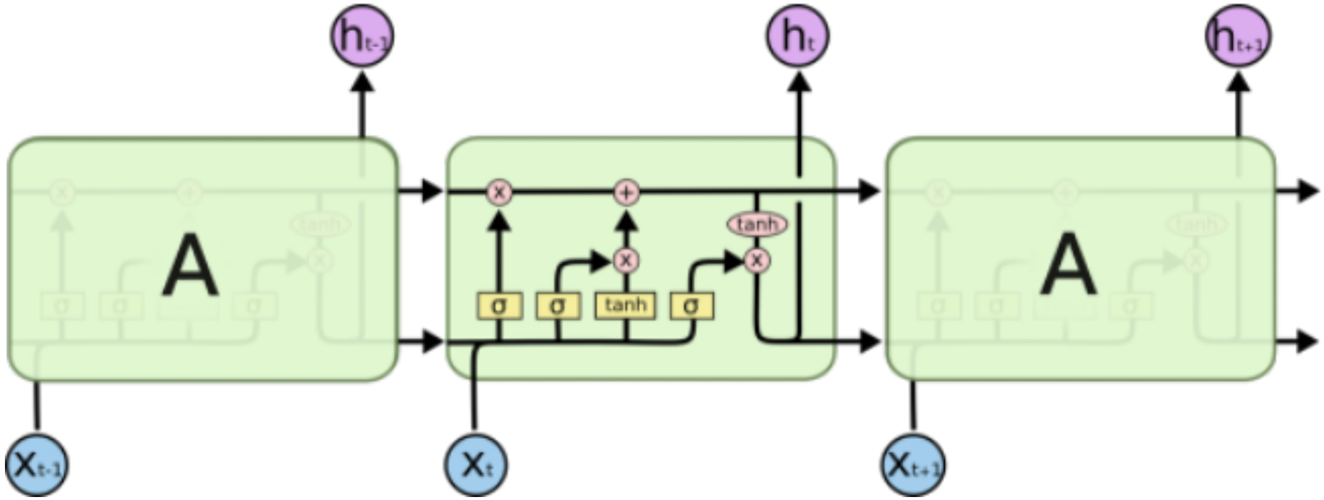
$$i_t = \sigma\left(W_i \cdot [\boldsymbol{C_{t-1}}, h_{t-1}, x_t] \;+\; b_i\right)$$

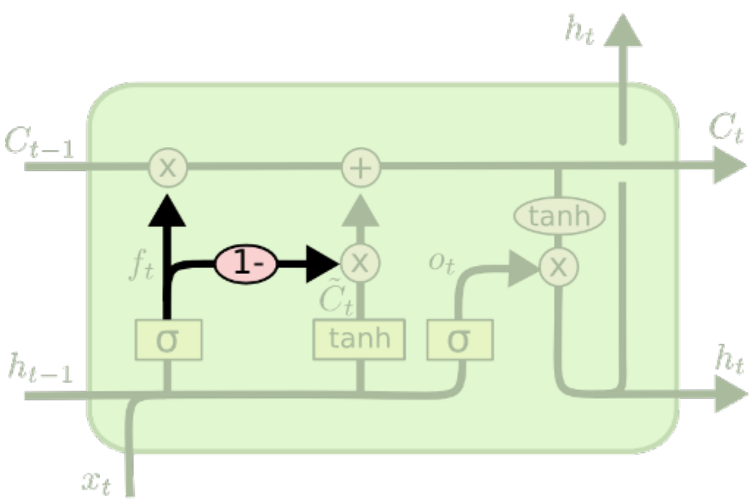
$$o_t = \sigma\left(W_o \cdot [\boldsymbol{C_t}, h_{t-1}, x_t] \;+\; b_o\right)$$

LSTM Variant

Simplified LSTM

- Assume $i_t = 1 - f_t$
- Only two gates are needed: fewer parameters



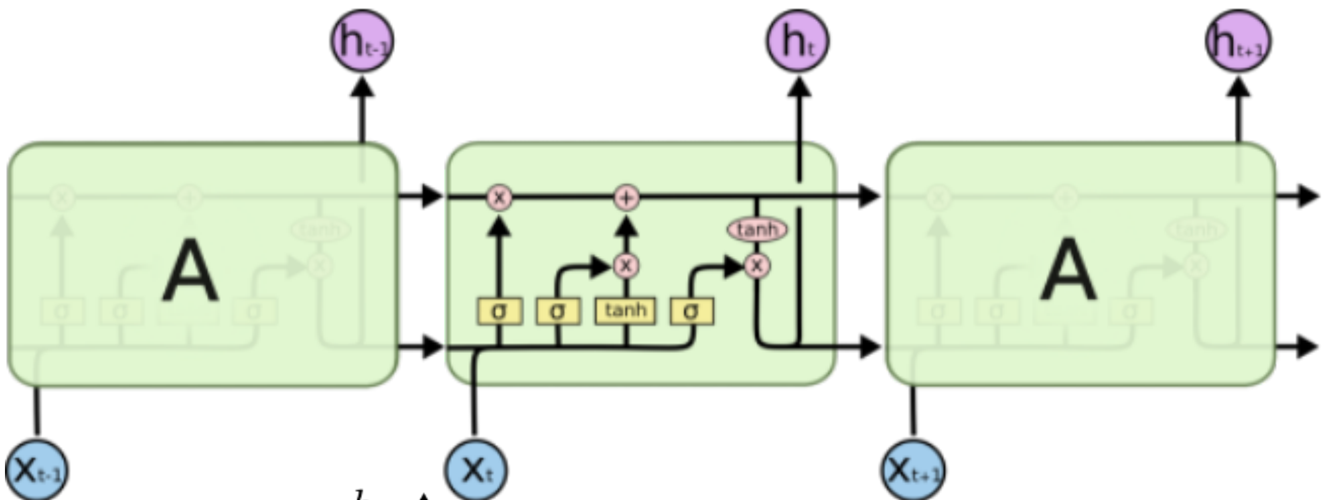


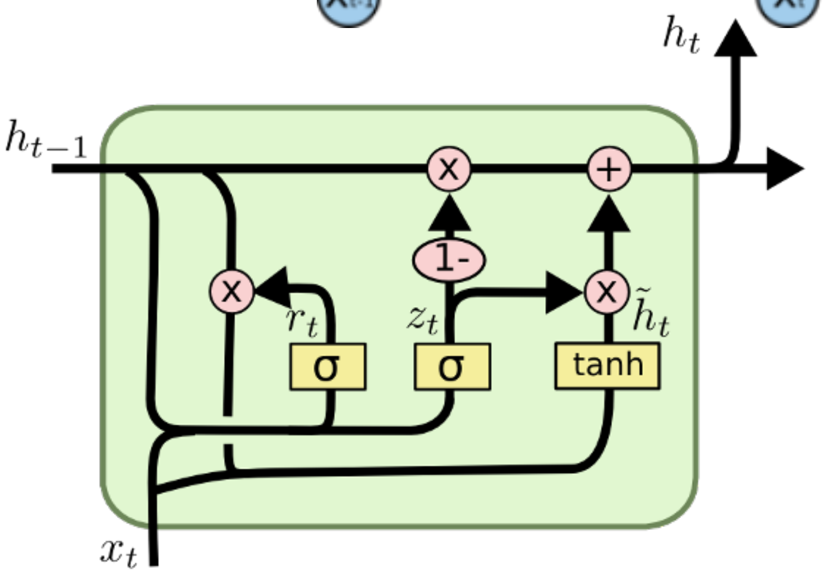
$$C_t = f_t * C_{t-1} + (\mathbf{1} - \boldsymbol{f_t}) * \tilde{C}_t$$

LSTM Variant

Gated Recurrent Unit (GRU, Cho et al. ’14)

- Merge h_t and c_t: much fewer parameters





$$z_t = \sigma\left(W_z \cdot [h_{t-1}, x_t]\right)$$

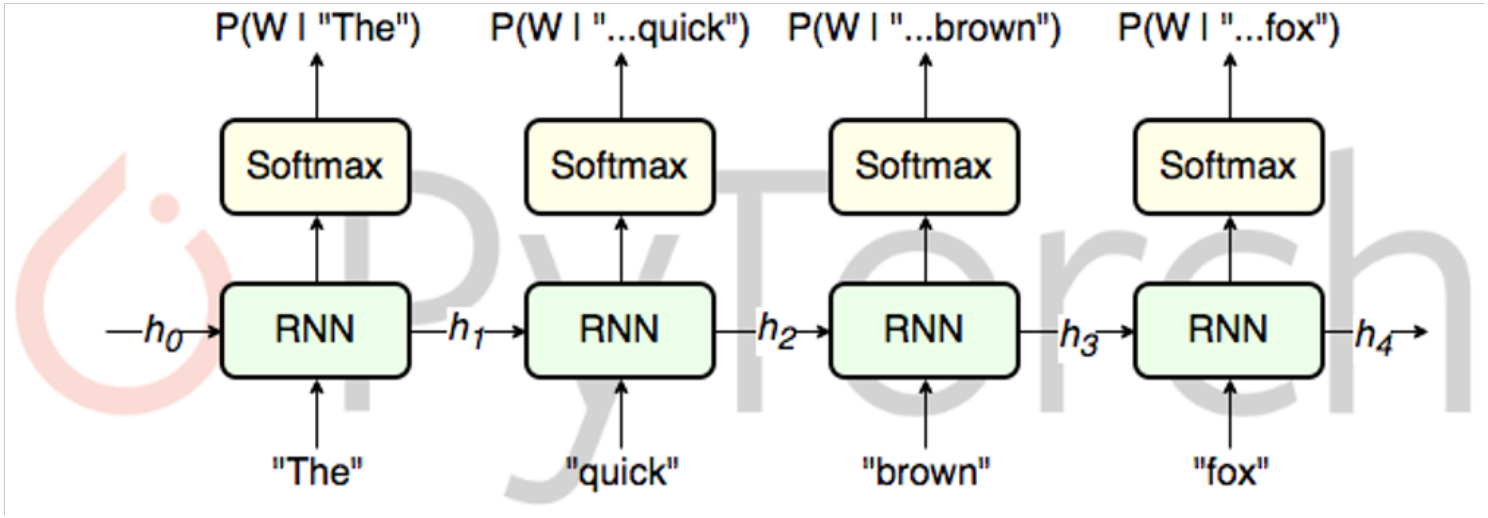
$$r_t = \sigma\left(W_r \cdot [h_{t-1}, x_t]\right)$$

$$\tilde{h}_t = \tanh\left(W \cdot [r_t * h_{t-1}, x_t]\right)$$

$$h_t = (1 - z_t) * h_{t-1} + z_t * \tilde{h}_t$$

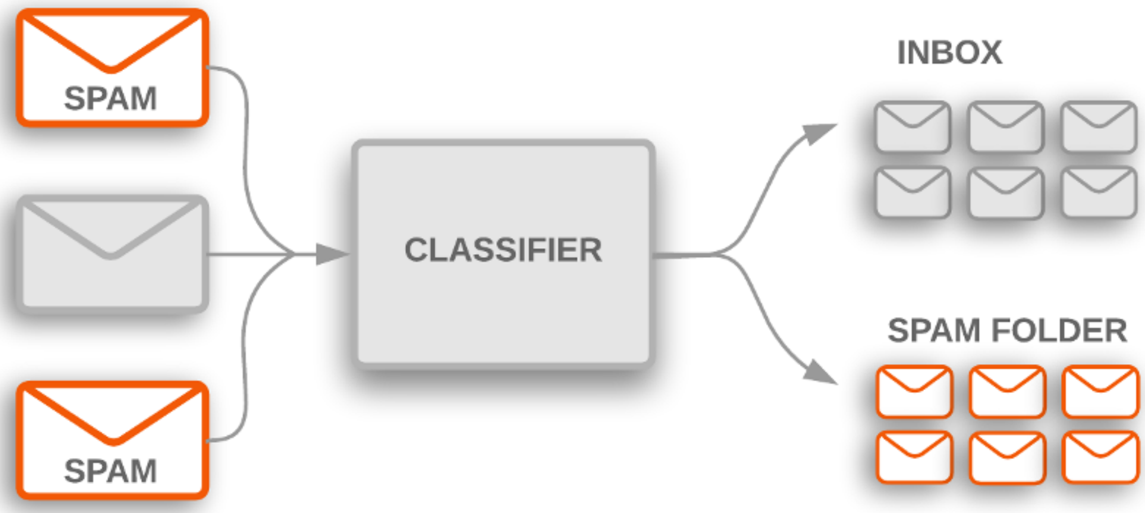
LSTM application: language model

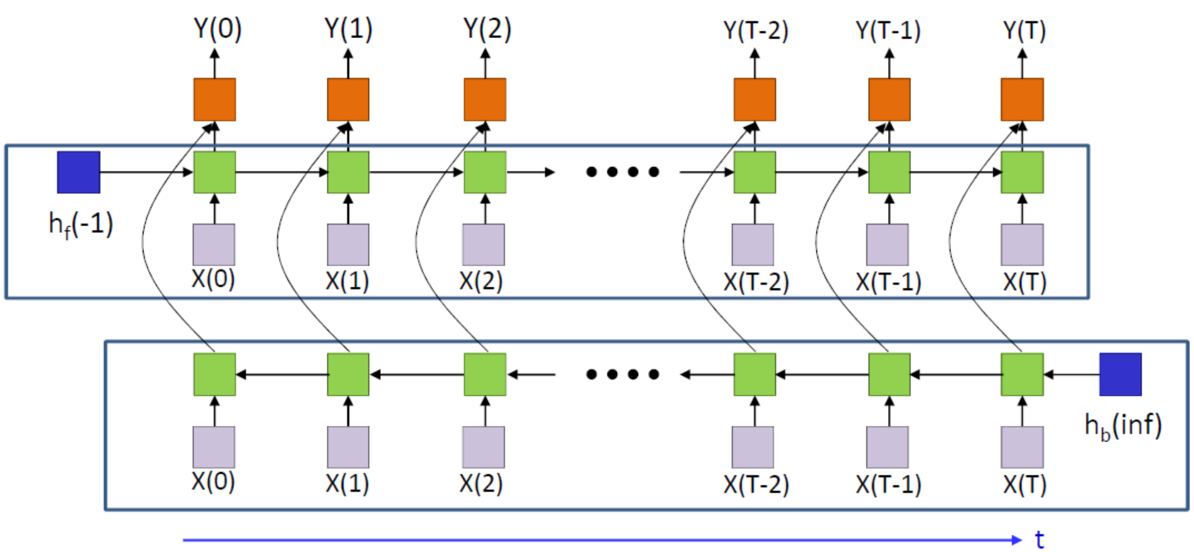
- Autoregressive language model: $P(X;\theta) = \Pi_{t=1}^{L} P(X_t \mid X_{i<t};\theta)$
  - X: a sentence
  - Sequential generation
- LSTM language model
  - X_t: word at position t.
  - Y_t: softmax over all words
- Data: a collection of texts:
  - Wiki



LSTM application: text classification

Bi-directional LSTM and them run softmax on the final hidden state.





Attention Mechanism

Machine Translation

- Before 2014: Statistical Machine Translation (SMT)
  - Extremely complex systems that require massive human efforts
  - Separately designed components
  - A lot of feature engineering
  - Lots of linguistic domain knowledge and expertise

- Before 2016:
  - Google Translate is based on statistical machine learning

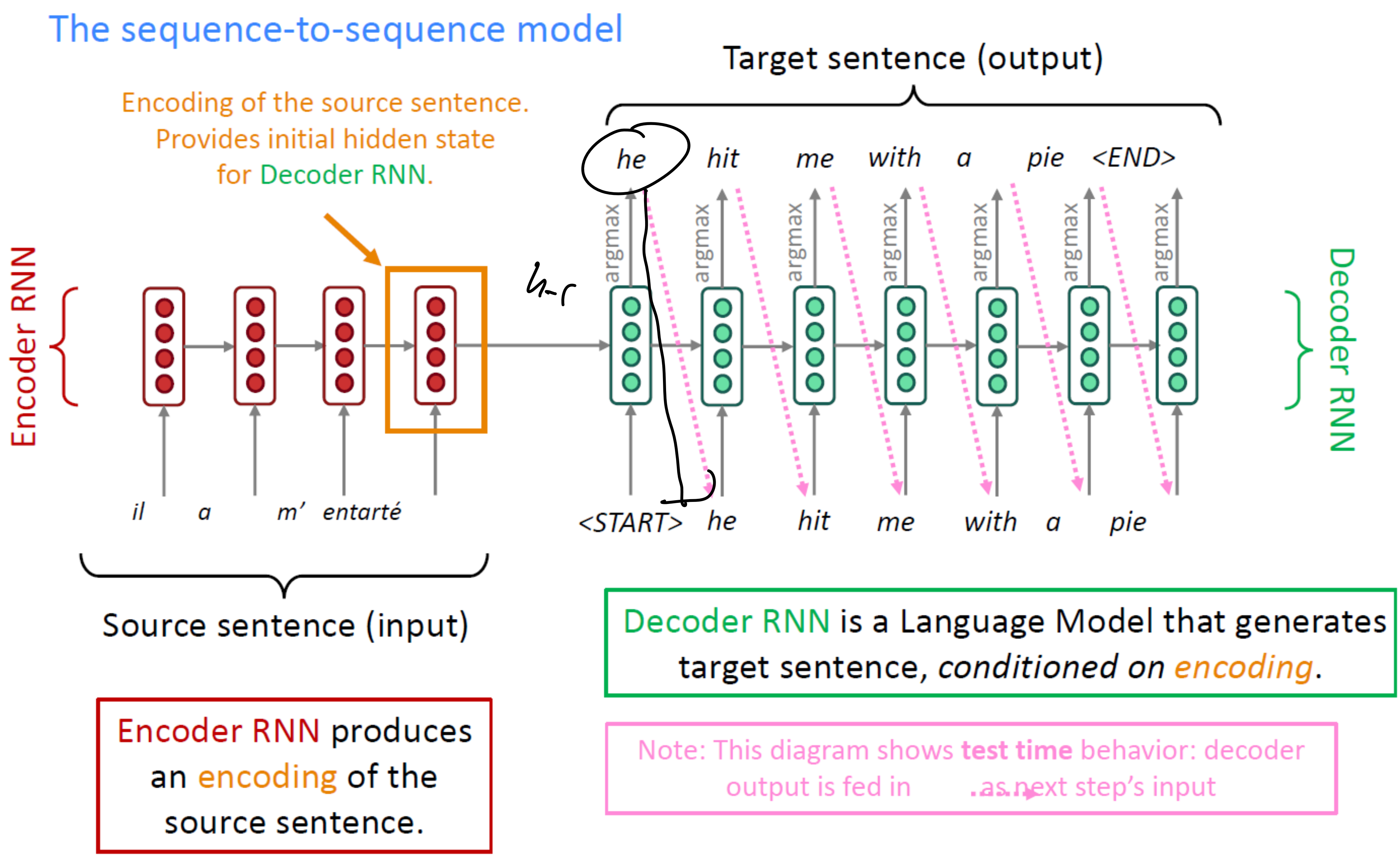
- What happened in 2014?
  - Neural machine translation (NMT)

Sequence to Sequence Model

- Neural Machine Translation (NMT)
  - Learning to translate via a **single end-to-end** neural network.
  - Source language sentence X, target language sentence $Y = f(X;\theta)$

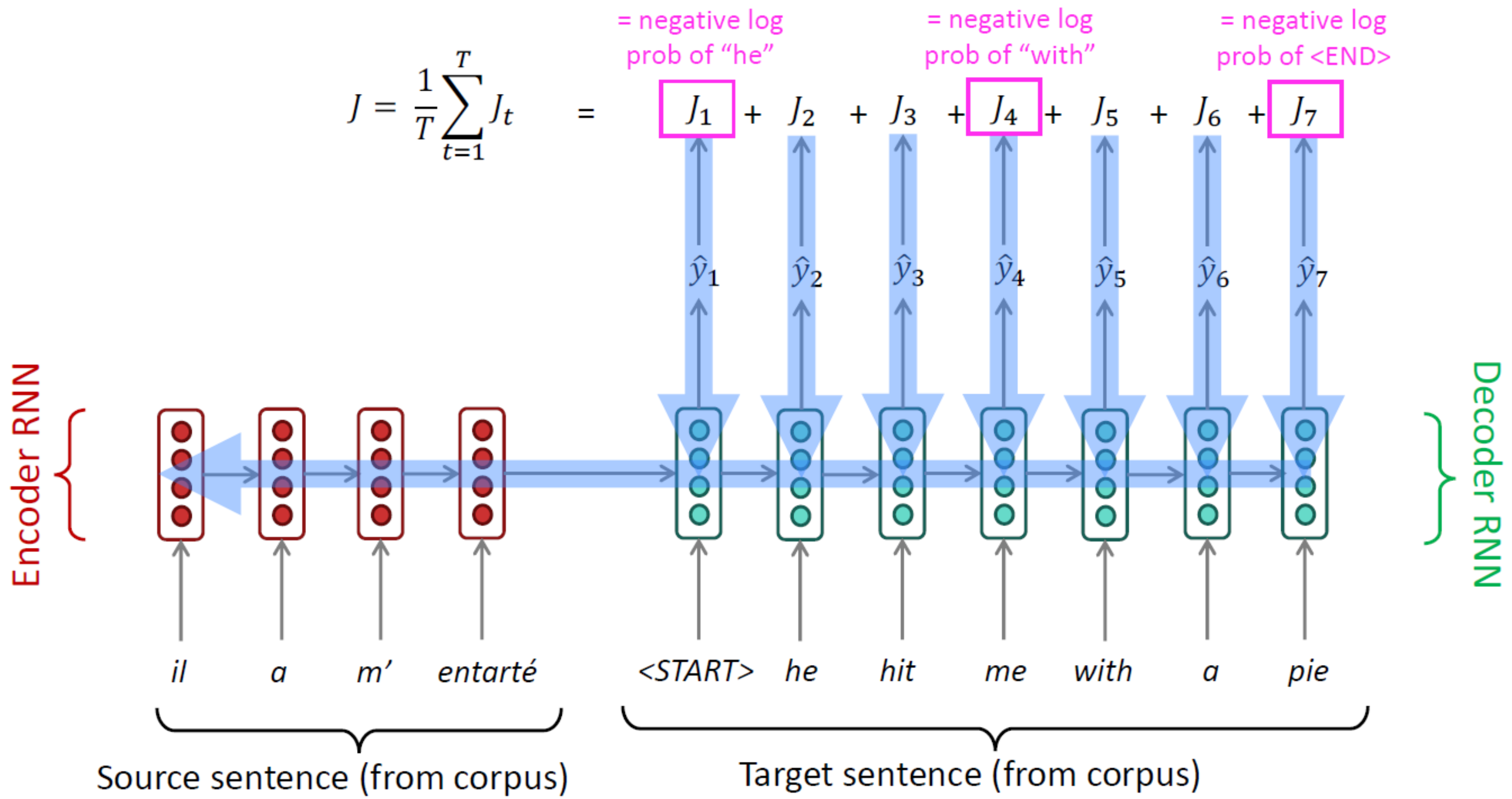
- Sequence to Sequence Model (Seq2Seq, Sutskever et al. , '14)
  - Two RNNs: f_{enc} and f_{dec}
  - Encoder f_{enc}:
    - Takes X as input, and output the initial hidden state for decoder
    - Can use bidirectional RNN
  - Decoder f_{dec}:
    - It takes in the hidden state from f_{enc} to generate Y
    - Can use autoregressive language model

Sequence to Sequence Model



Training Sequence to Sequence Model

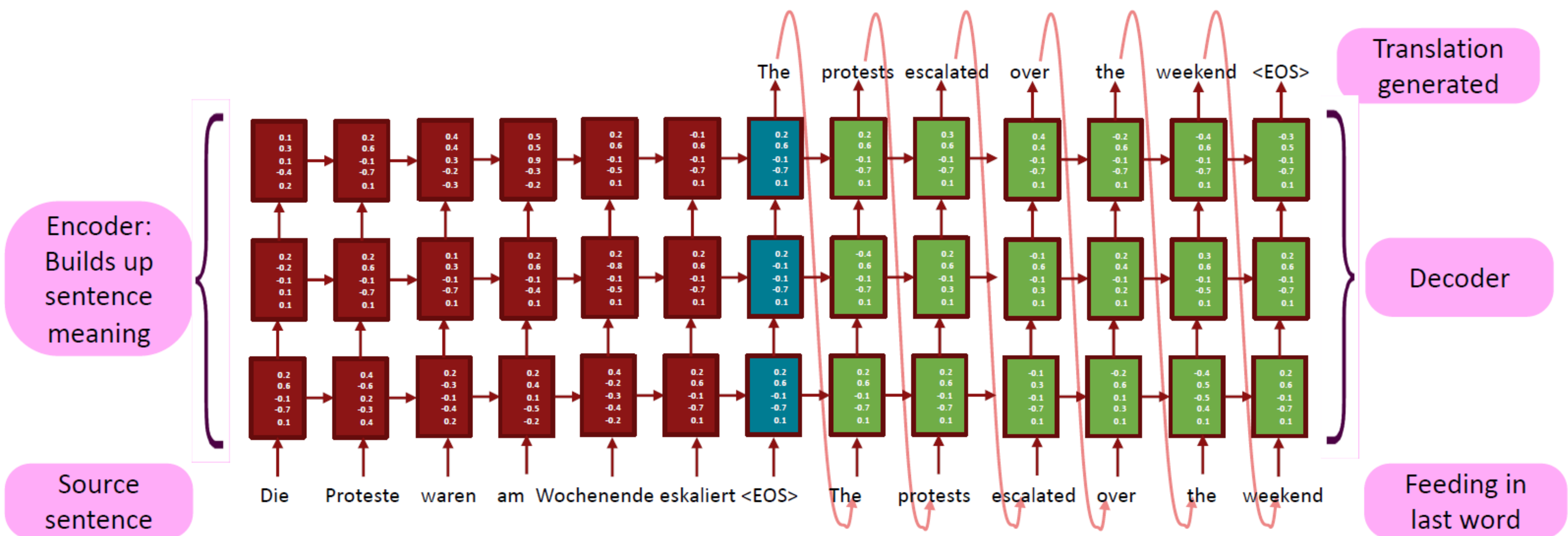
- Collect a huge paired dataset and train it end-to-end via BPTT
- Loss induced by MLE $P(Y|X) = P(Y|f_{enc}(X))$



Seq2seq is optimized as a **single system.** Backpropagation operates *"end-to-end"*.

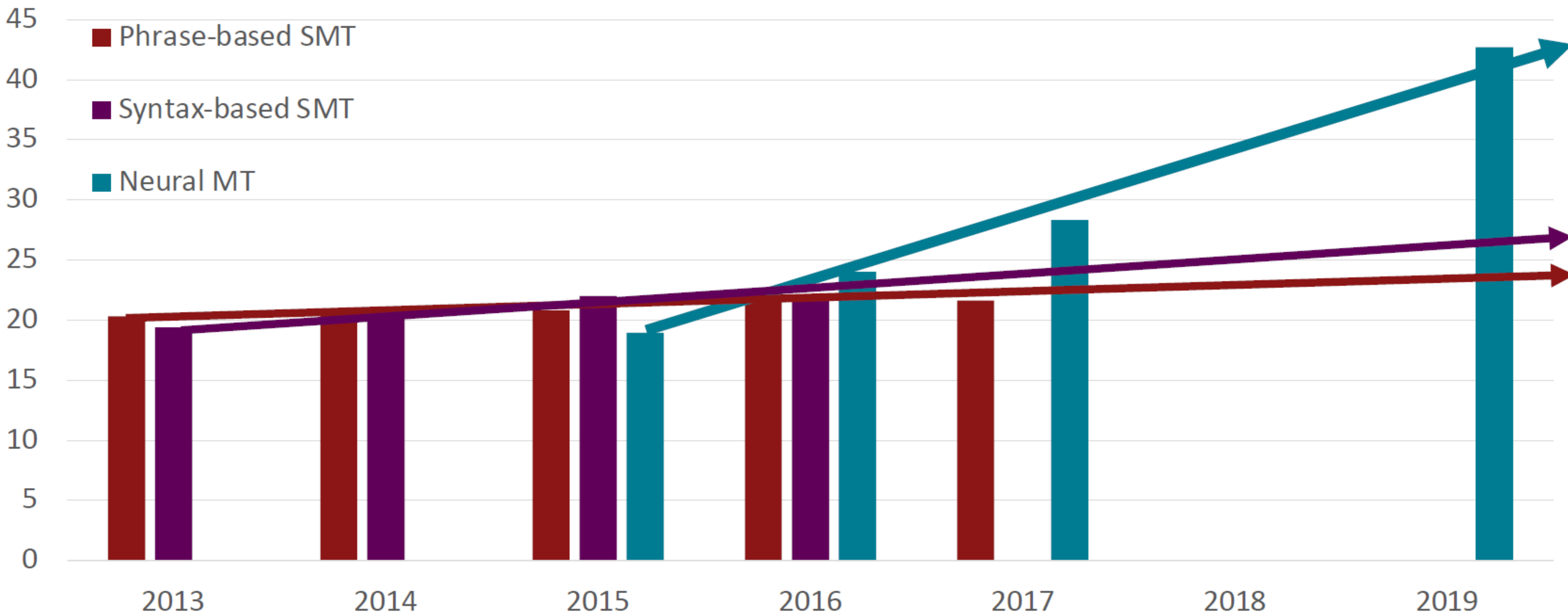
Deep Sequence to Sequence Model

- Stacked seq2seq model



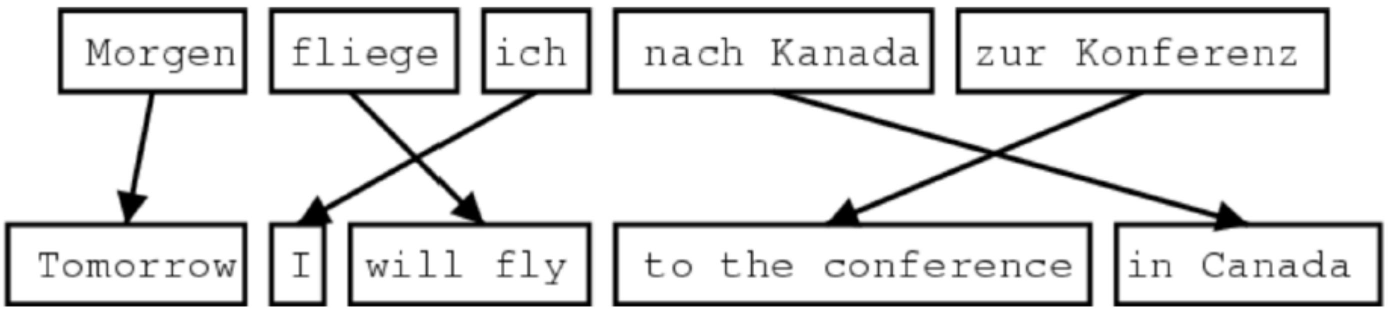
Machine Translation

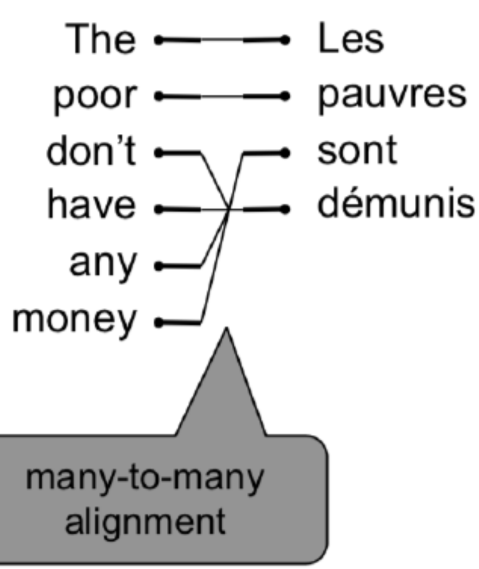
- 2016: Google switched Google Translate from SMT to NMT

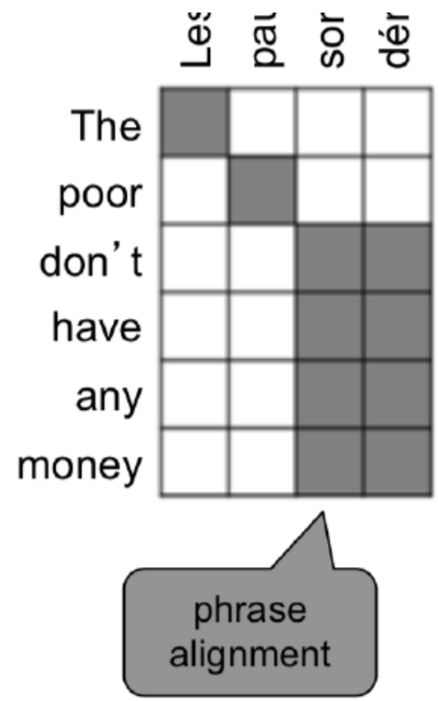


Alignment

- Alignment: the word-level correspondence between X and Y
- Can have complex long-term dependencies

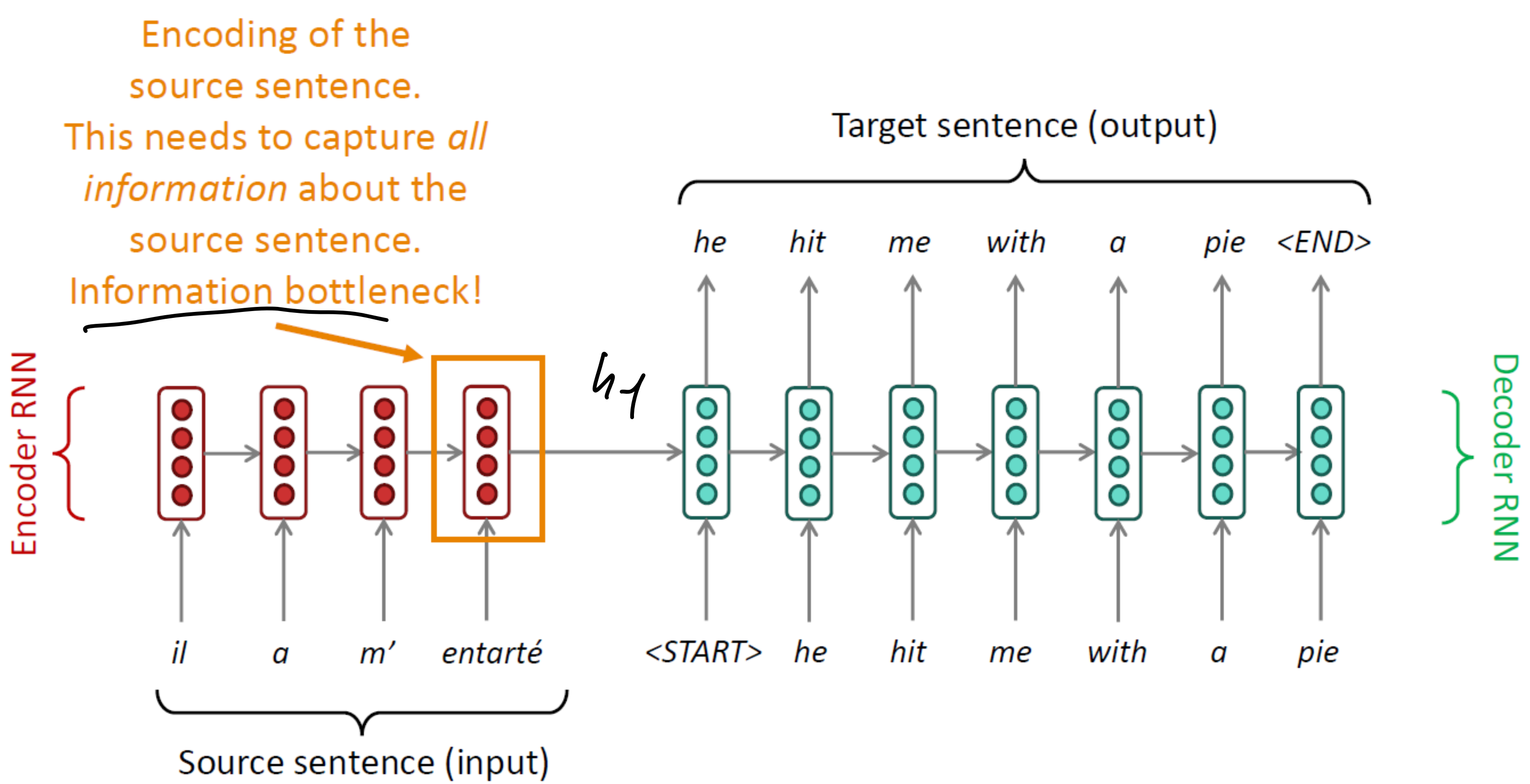






Issue in Seq2Seq

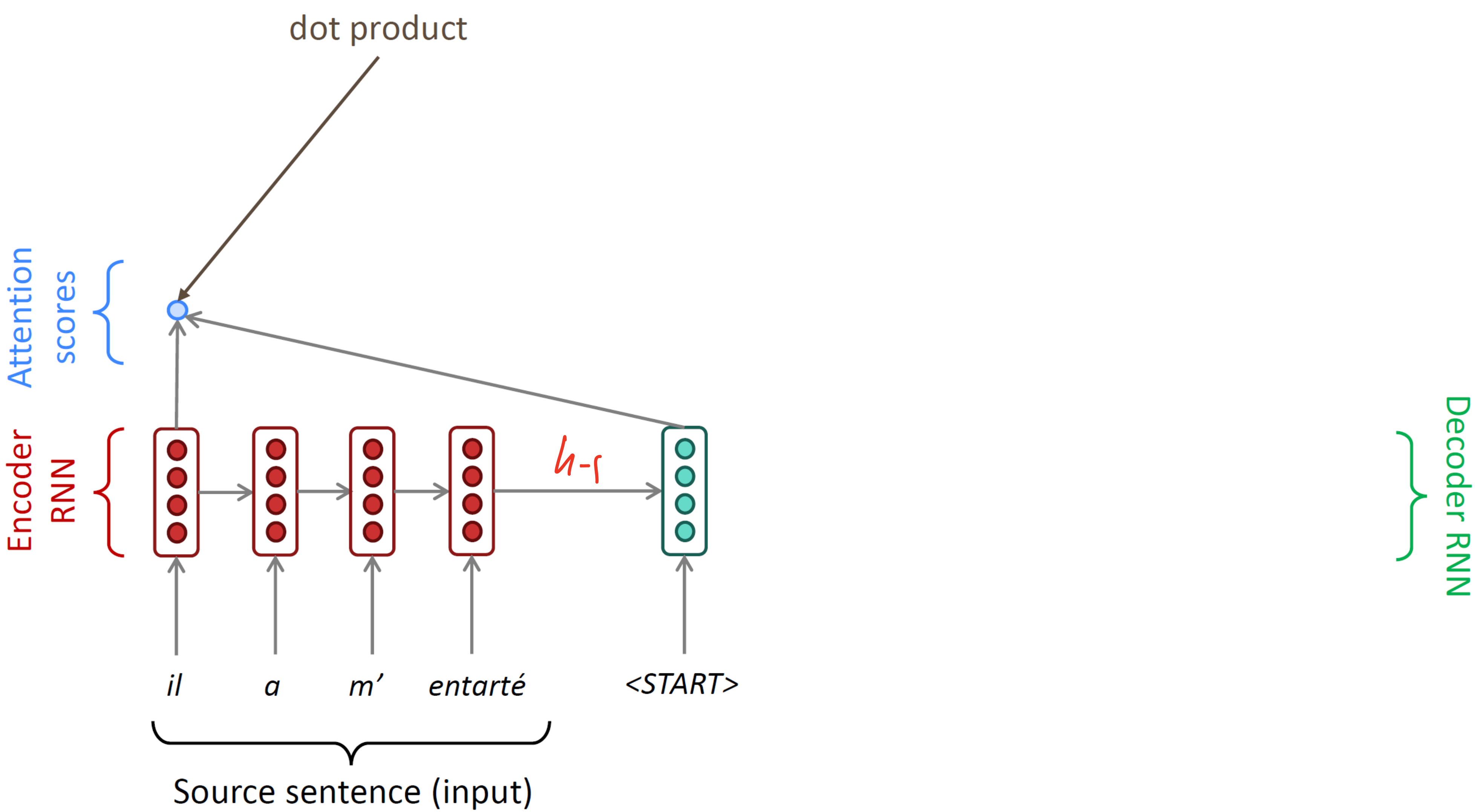
- Alignment: the word-level correspondence between X and Y
  - The information bottleneck due to the hidden state h
  - We want each Y_t to also focus on some X_i that it is aligned with



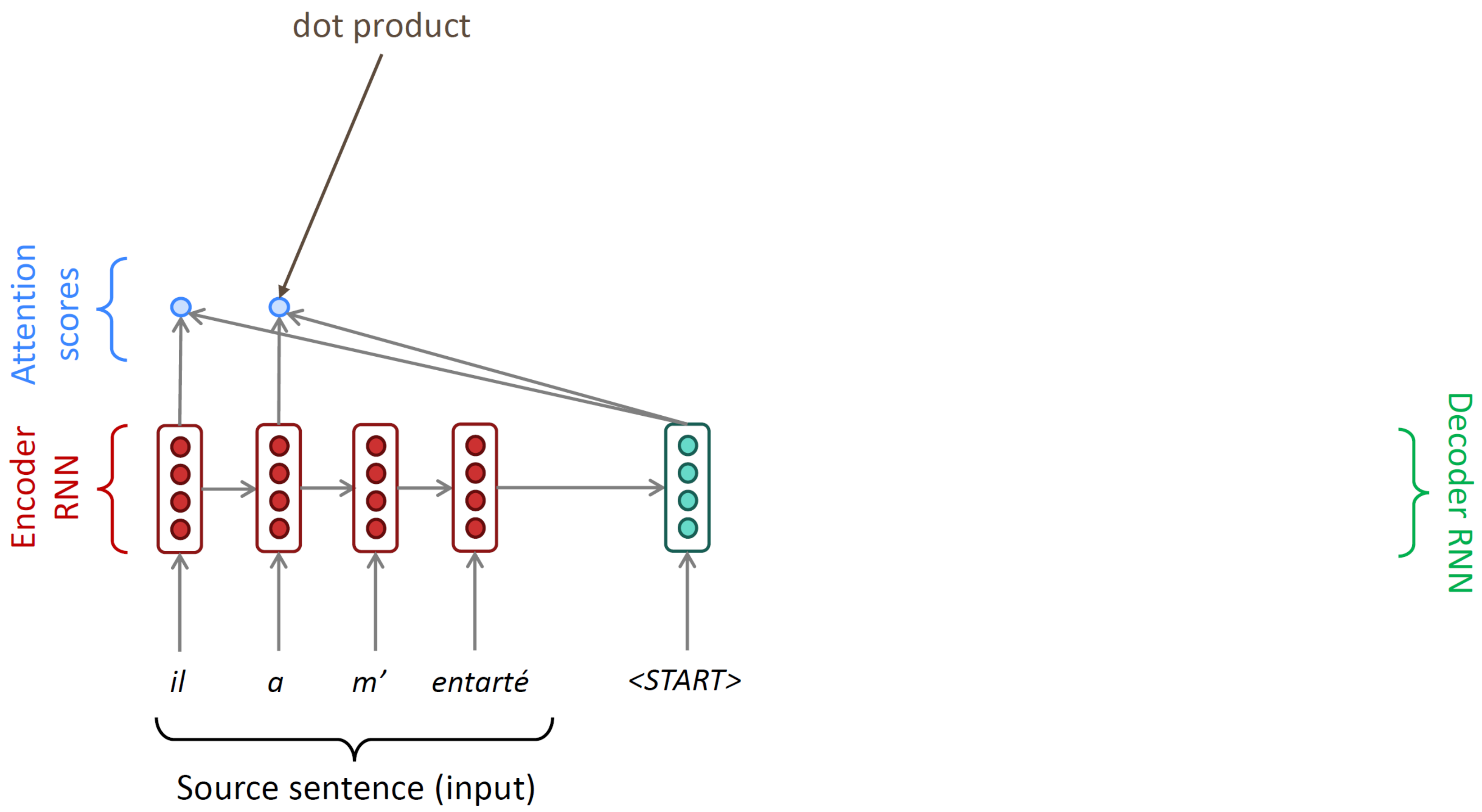
Seq2Seq with Attention

- NMT by jointly learning to align and translate (Bahdanau, Cho, Bengio, ’15)
- Core idea:
  - When decoding Y_t, consider both hidden states and alignment:
    - Hidden state: $h_t = f_{dec}(Y_{i<t})$
    - Alignment: connect to a portion of X
  - When portion of X to focus on?
    - Learn a softmax weight over X: attention distribution P_{att}
    - $P_{att}(X_i \mid h_t)$: how much attention to put on word X_i
    - Attention output $h_{att} = \sum_i f_{enc}(X_i \mid X_{j<i}) \cdot P_{att}(X_i \mid h_{t-1})$
    - Use h_{t-1} and h_{att} to compute Y_t

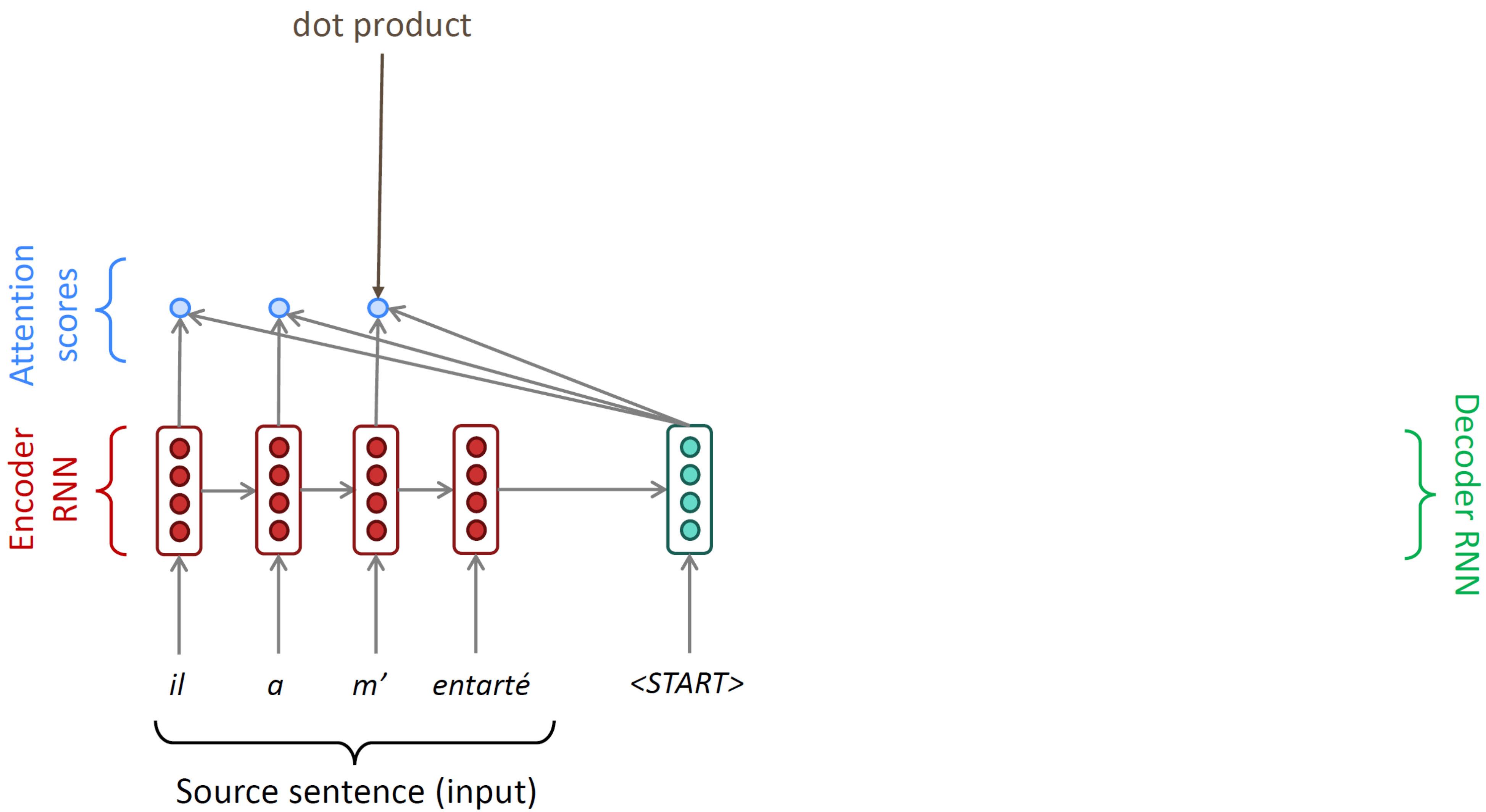
Seq2Seq with Attention



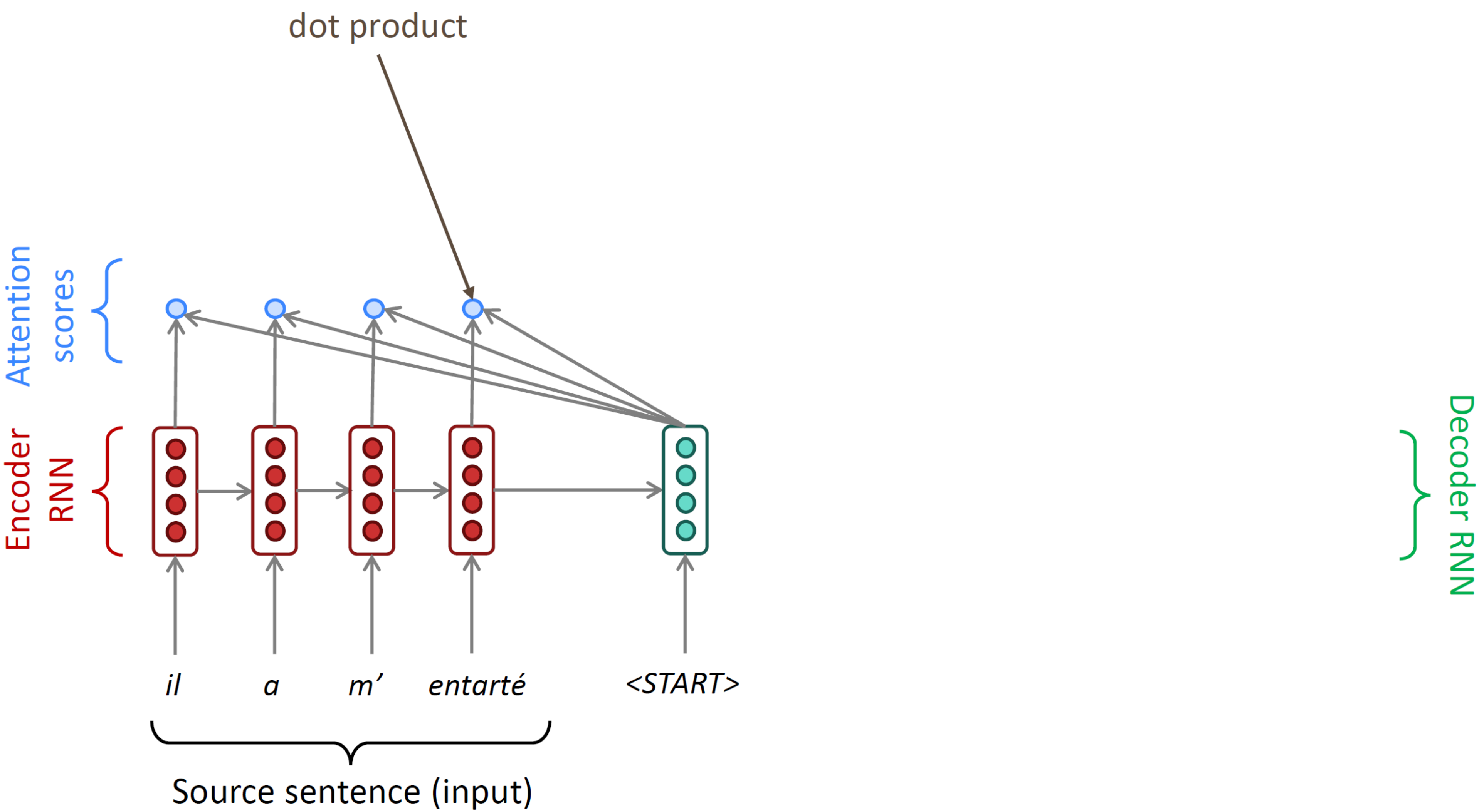
Seq2Seq with Attention



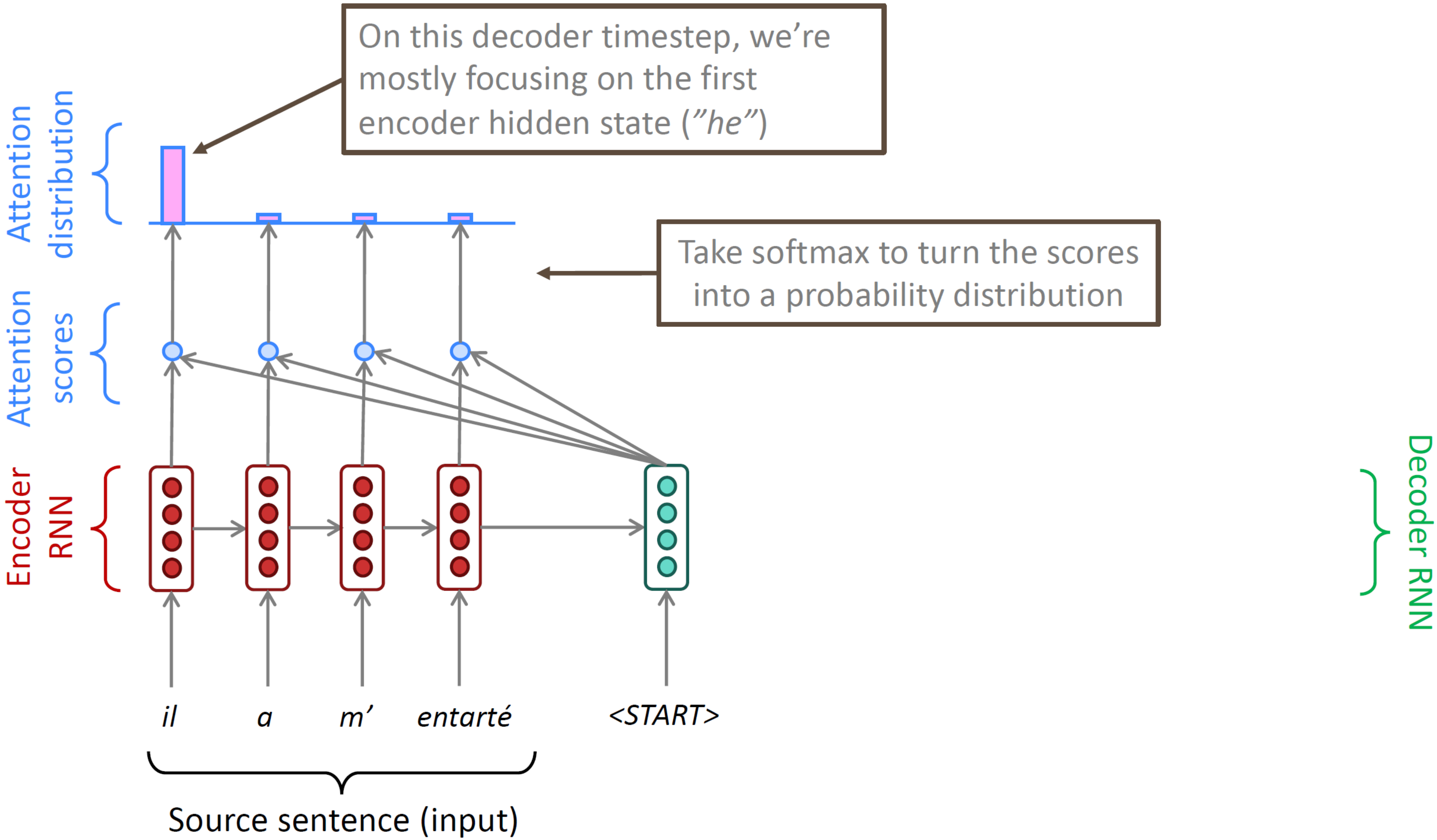
Seq2Seq with Attention



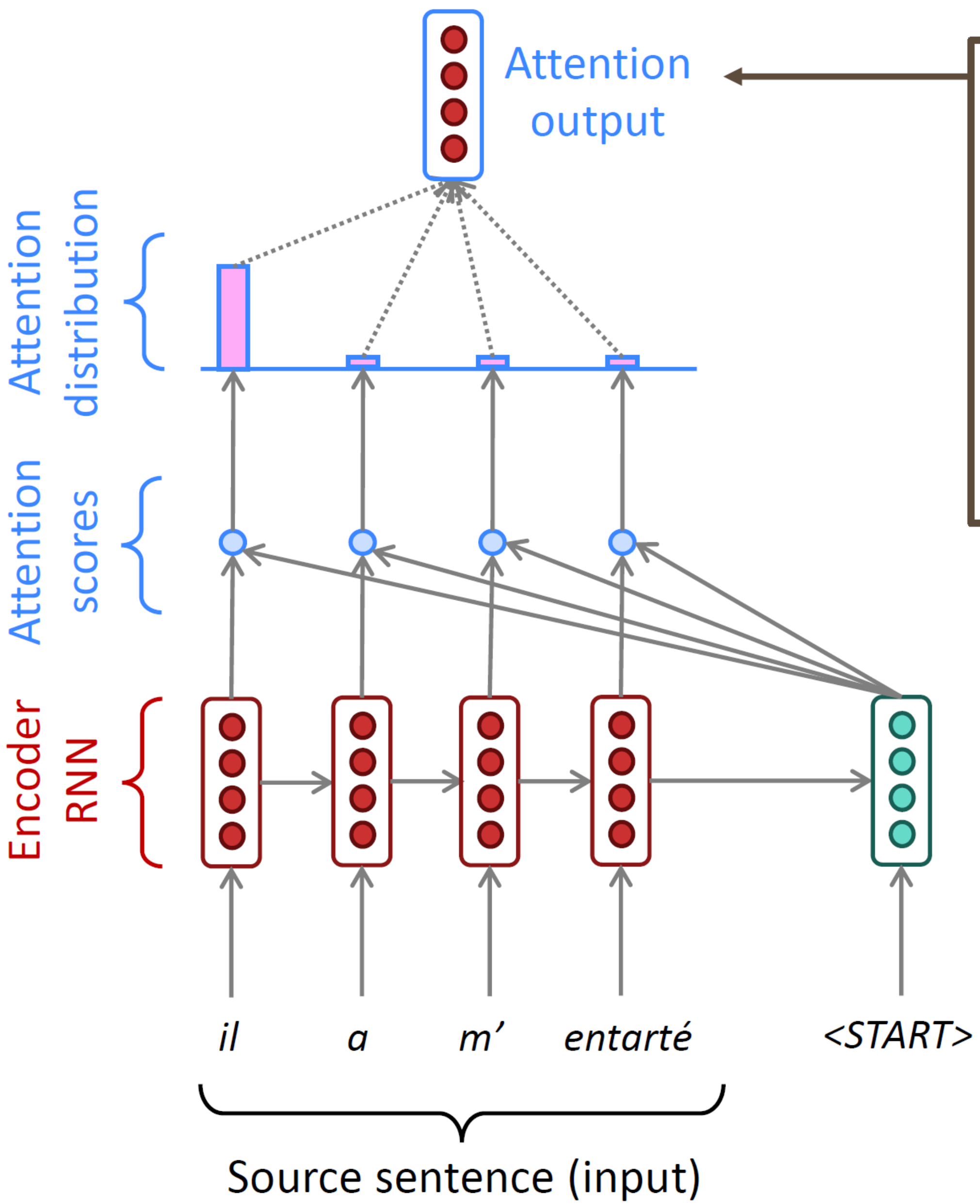
Seq2Seq with Attention



Seq2Seq with Attention



Seq2Seq with Attention

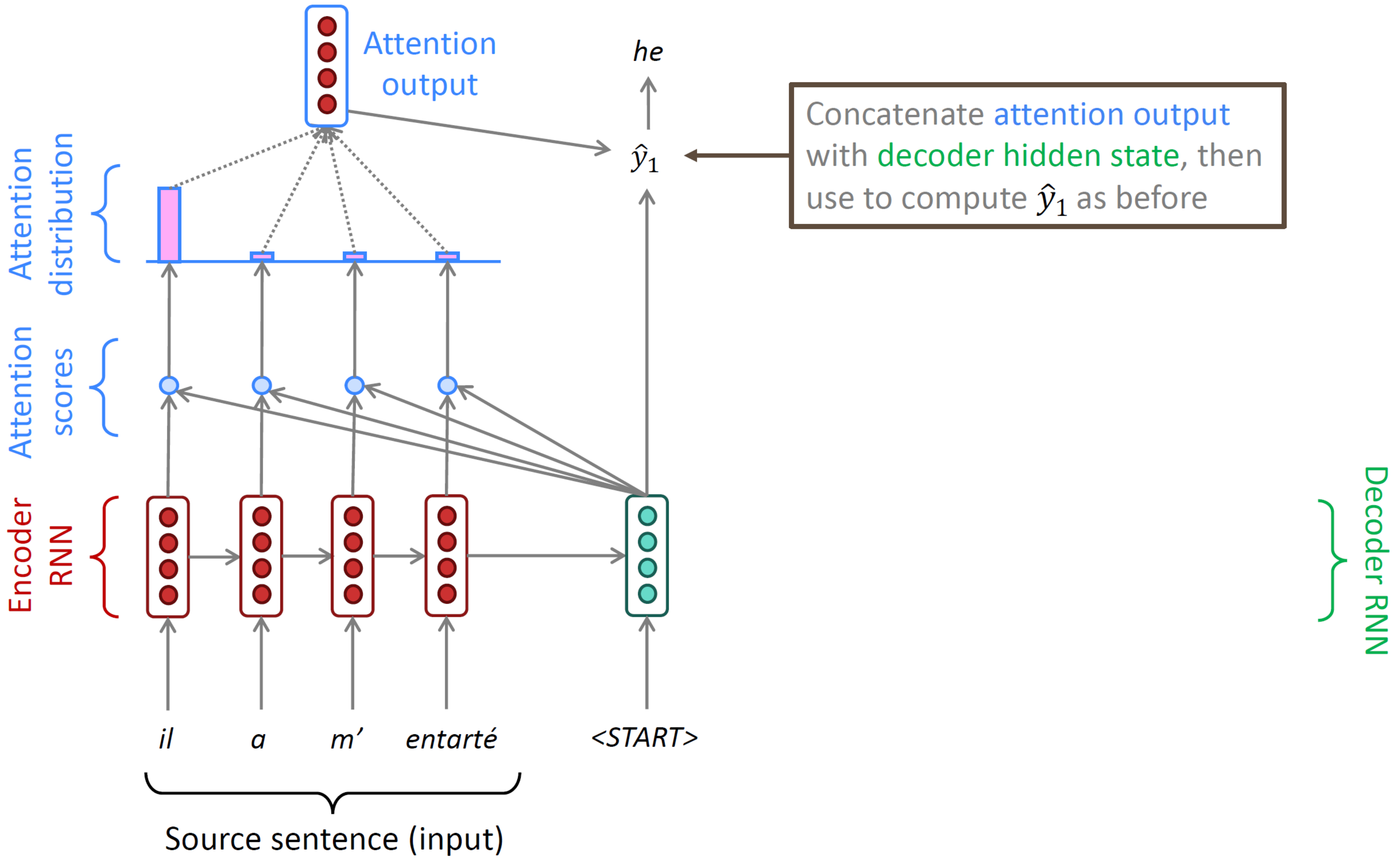


Use the attention distribution to take a **weighted sum** of the encoder hidden states.

The attention output mostly contains information from the hidden states that received high attention.

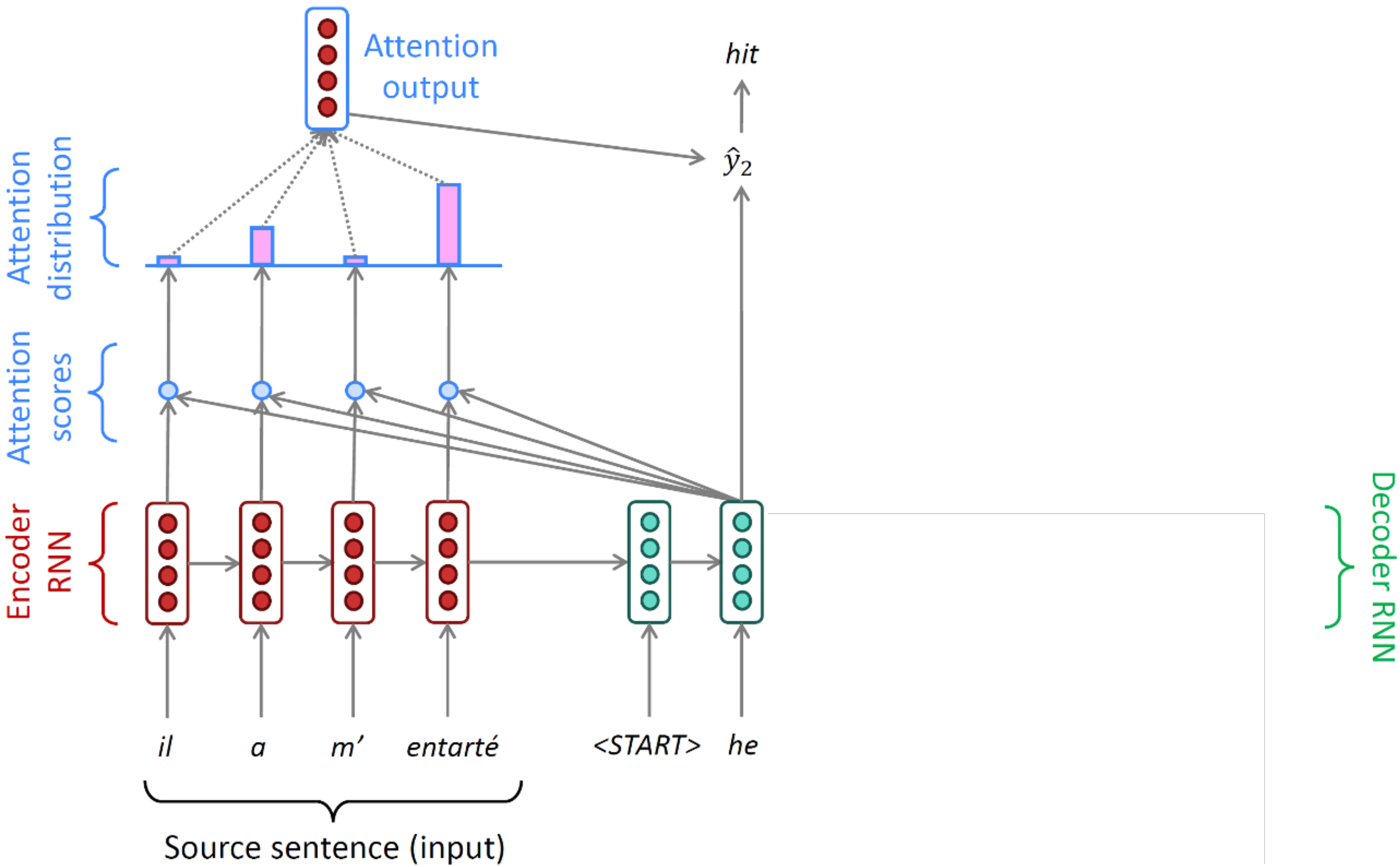
$\sum \beta_i \cdot h_i^{end}$

Seq2Seq with Attention

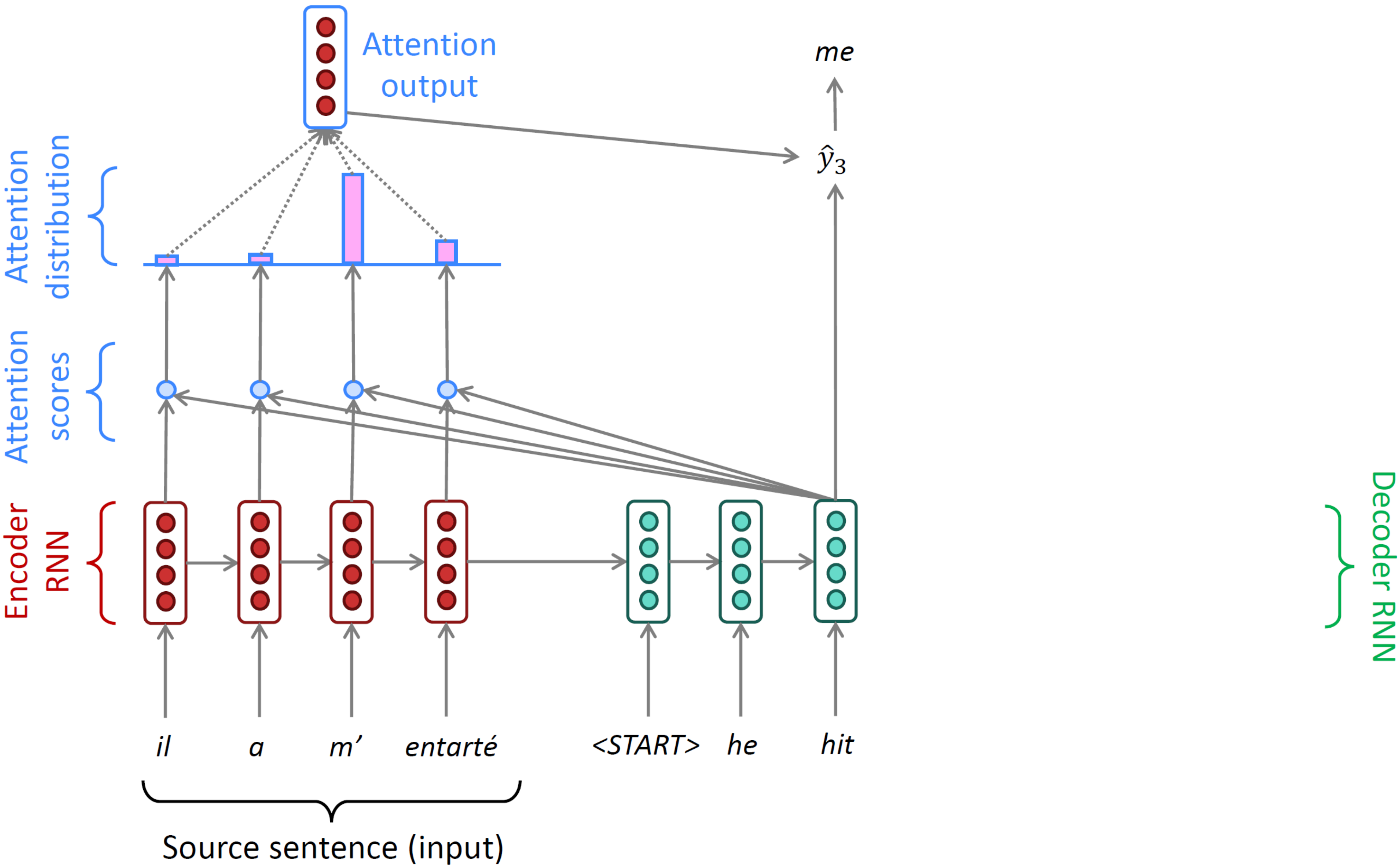


Concatenate attention output with decoder hidden state, then use to compute $\hat{y}_1$ as before

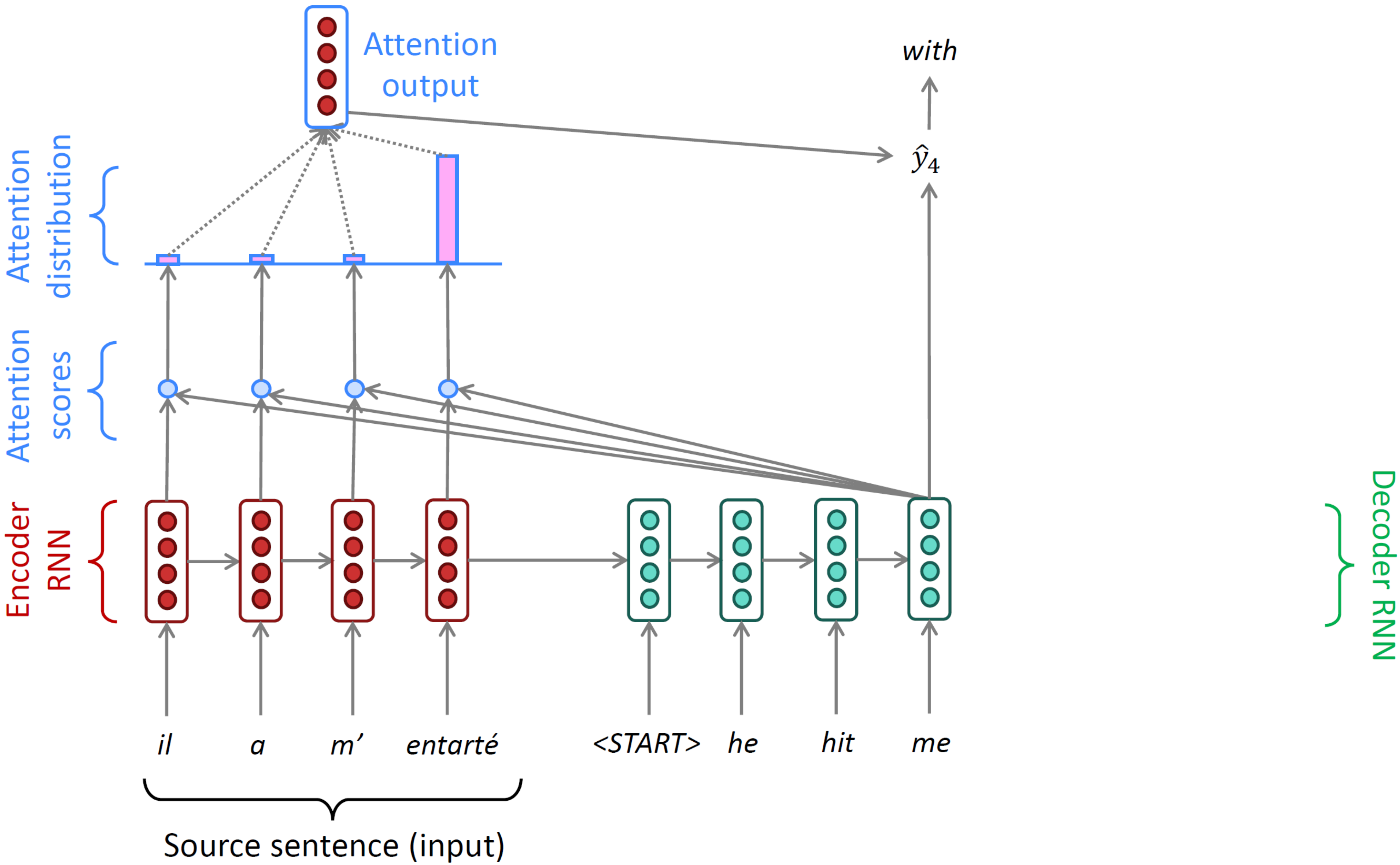
Seq2Seq with Attention



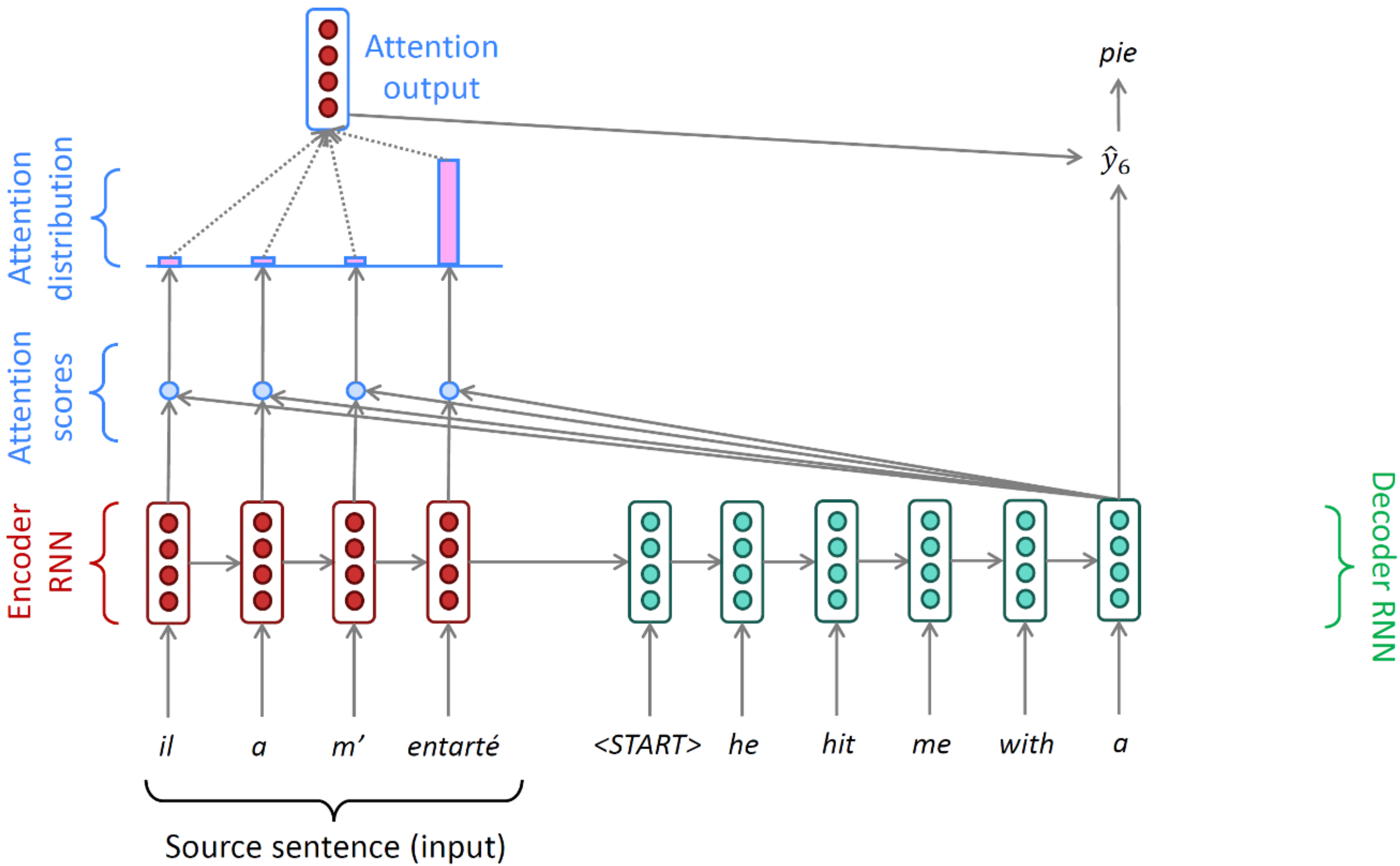
Seq2Seq with Attention



Seq2Seq with Attention



Seq2Seq with Attention



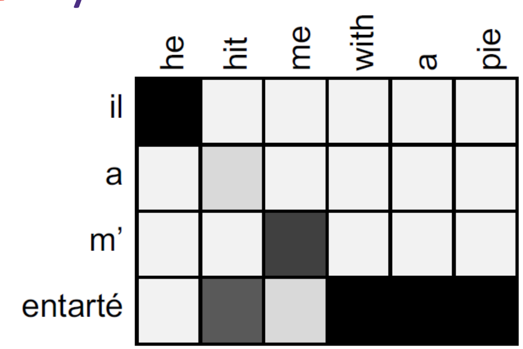
Seq2Seq with Attention

Summary

- Input sequence X, encoder f_{enc}, and decoder f_{dec}
- $f_{enc}(X)$ produces hidden states $h_1^{enc}, h_2^{enc}, \ldots, h_N^{enc}$
- On time step t, we have decoder hidden state h_t
- Compute attention score $e_i = h_t^\top h_i^{enc}$
- Compute attention distribution $\alpha_i = P_{att}(X_i) = \text{softmax}(e_i)$
- Attention output: $h_{att}^{enc} = \sum_i \alpha_i h_i^{enc}$
- $Y_t \sim g(h_t, h_{att}^{enc}; \theta)$
    - Sample an output using both h_t and h_{att}^{enc}

Attention

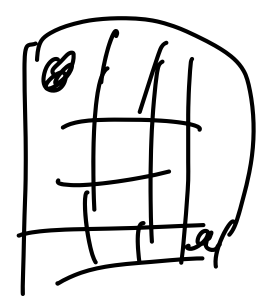
- It significantly improves NMT.
- It solves the bottleneck problem and the long-term dependency issue.
- Also helps gradient vanishing problem.
- Provides some interpretability
  - Understanding which word the RNN encoder focuses on



- Attention is a general technique
  - Given a set of vector values V_i and vector query q
  - Attention computes a weighted sum of values depending on q

Other use cases:

- Attention can be viewed as a module.
- In encoder and decoder (more on this later)
- A representation of a set of points
  - Pointer network (Vinyals, Forunato, Jaitly ’15)
  - Deep Sets (Zaheer et al., ’17)
- Convolutional neural networks
  - To include non-local information in CNN (Non-local network, ’18)



Attention

- Representation learning:
  - A method to obtain a fixed representation corresponding to a query q from an arbitrary set of representations $\{V_i\}$
  - Attention distribution: $\alpha_i = \text{softmax}(\underline{f(v_i, q)})$
  - Attention output: $v_{att} = \sum_i \alpha_i v_i$

$f(v_i, q) = v_i^\top q$

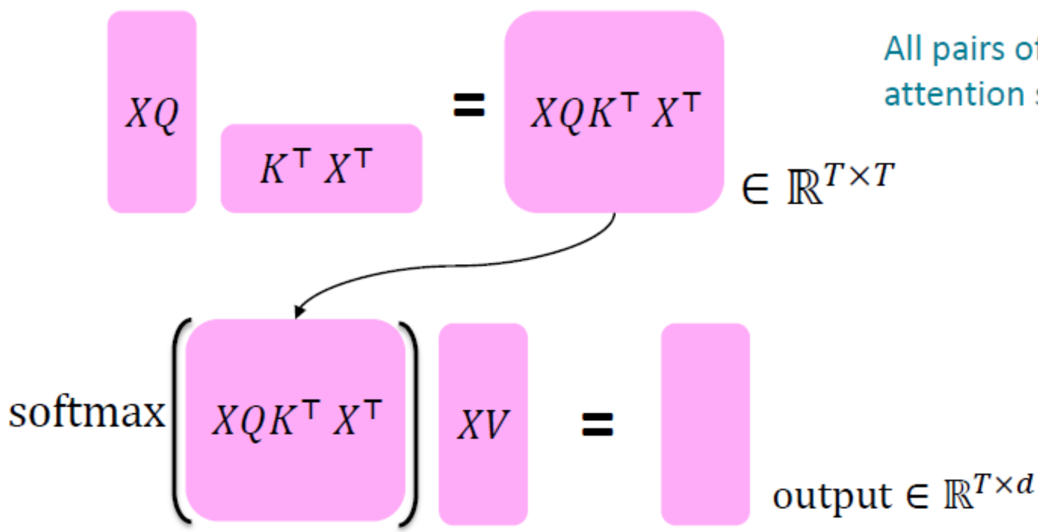
- Attent variant: $f(v_i, q)$
  - Multiplicative attention: $f(v_i, q) = q^\top W h_i$, W is a weight matrix
  - Additive attention: $f(v_i, q) = u^\top \tanh(W_1 v_i + W_2 q)$

Key-query-value attention

$X_t \in \mathbb{R}^d$

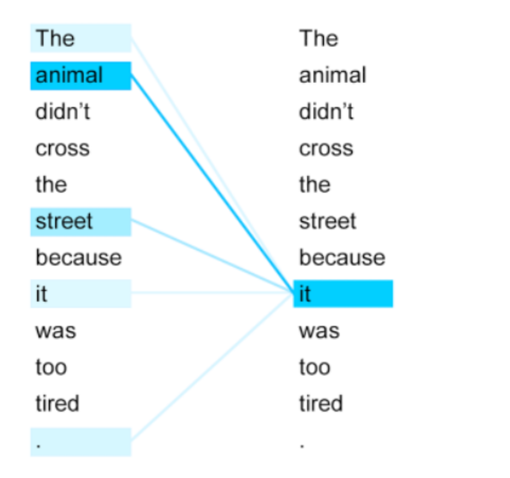
$W^q, W^k : \mathbb{R}^{4\times d}$, $W^v \in \mathbb{R}^{5\times d}$

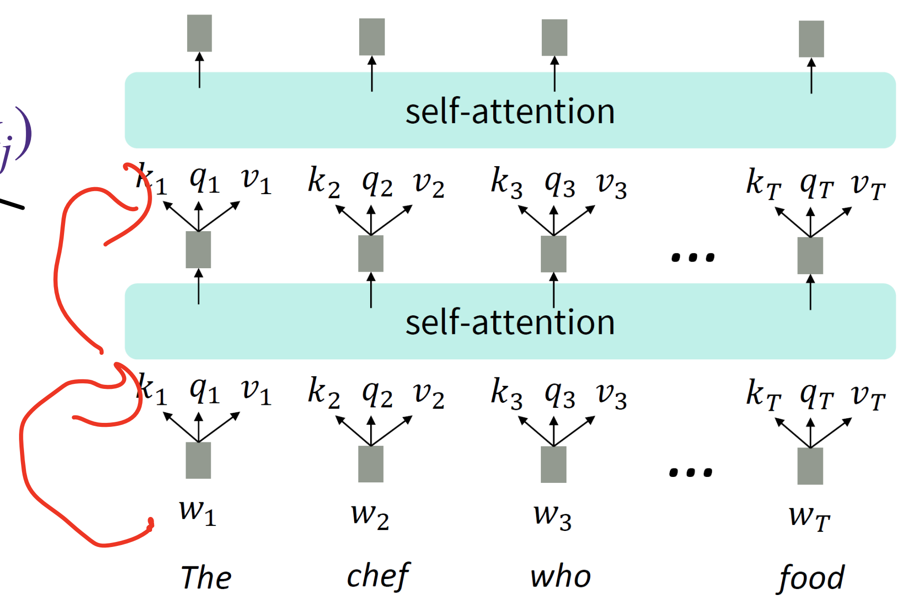
- Obtain q_t, v_t, k_t from X_t
- $q_t = W^q X_t$; $v_t = W^v X_t$; $k_t = W^k X_t$ (position encoding omitted)
  - W^q, W^v, W^k are learnable weight matrices
- $\alpha_{i,j} = \text{softmax}(q_i^\top k_j)$; $out_i = \sum_k \alpha_{i,j} v_j$
- Intuition: key, query, and value can focus on different parts of input



Attention is all you need (Vsawani '17)

- A pure attention-based architecture for sequence modeling
  - No RNN at all!
- Basic component: self-attention, $Y = f_{SA}(X;\theta)$
  - X_t uses attention on entire X sequence
  - Y_t computed from X_t and the attention output
- Computing Y_t
  - Key k_t, value v_t, query q_t from X_t
    - $(k_t, v_t, q_t) = g_1(X_t;\theta)$
  - Attention distribution $\alpha_{t,j} = \text{softmax}(q_t^\top k_j)$
    - Attention output $out_t = \sum_j \alpha_{t,j} v_j$
    - $Y_t = g_2(out_t;\theta)$





Issues of Vanilla Self-Attention

- Attention is order-invariant
- Lack of non-linearities
  - All the weights are simple weighted average
- Capability of autoregressive modeling
  - In generation tasks, the model cannot "look at the future"
  - e.g. Text generation:
    - Y_t can only depend on $X_{i<t}$
    - But vanilla self-attention requires the entire sequence

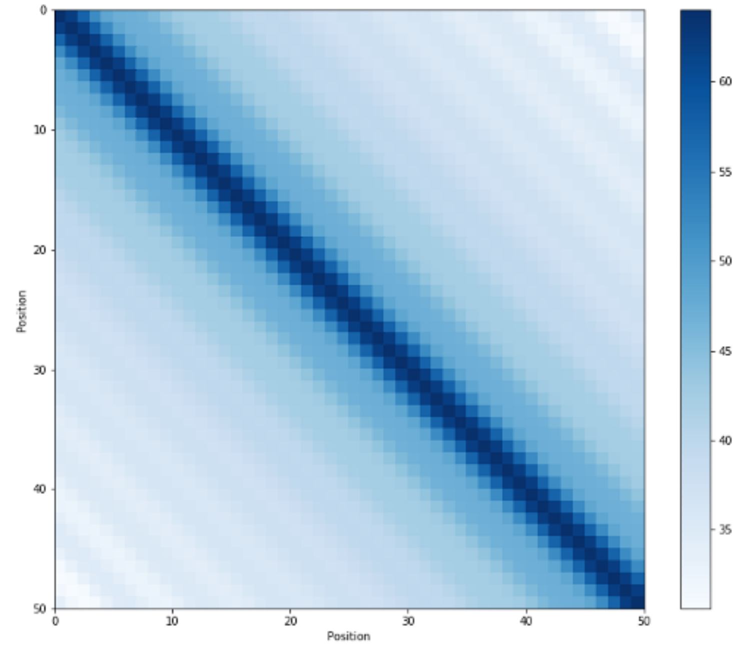
Position Encoding

- Vanilla self-attention
  - $(k_t, v_t, q_t) = g_1(X_t; \theta)$
  - $\alpha_{t,j} = \text{softmax}(q_t^\top k_j)$
  - Attention output $out_t = \sum_j \alpha_{t,j} v_j$
- Idea: position encoding:
  - p_i: an embedding vector (feature) of position i
  - $(k_t, v_t, q_t) = g_1([X_t, p_t]; \theta)$
- In practice: Additive is sufficient: $k_t \leftarrow \tilde{k}_t + p_t, q_t \leftarrow \tilde{q}_t + p_t, v_t \leftarrow \tilde{v}_t + p_t;$ $(\tilde{k}_t, \tilde{v}_t, \tilde{q}_t) = g_1(X_t; \theta)$
- p_t is only included in the first layer

Position Encoding

p_t design 1: **Sinusoidal position representation**

- Pros:
  - simple
  - naturally models "relative position"
  - Easily applied to long sequences
- Cons:
  - Not learnable
  - Generalization poorly to sequences longer than training data



Heatmap of $p_i^T p_j$

$$p_i = \begin{pmatrix} \sin(i/10000^{2*1/d}) \\ \cos(i/10000^{2*1/d}) \\ \vdots \\ \sin(i/10000^{2*\frac{d}{2}/d}) \\ \cos(i/10000^{2*\frac{d}{2}/d}) \end{pmatrix}$$

Position Encoding

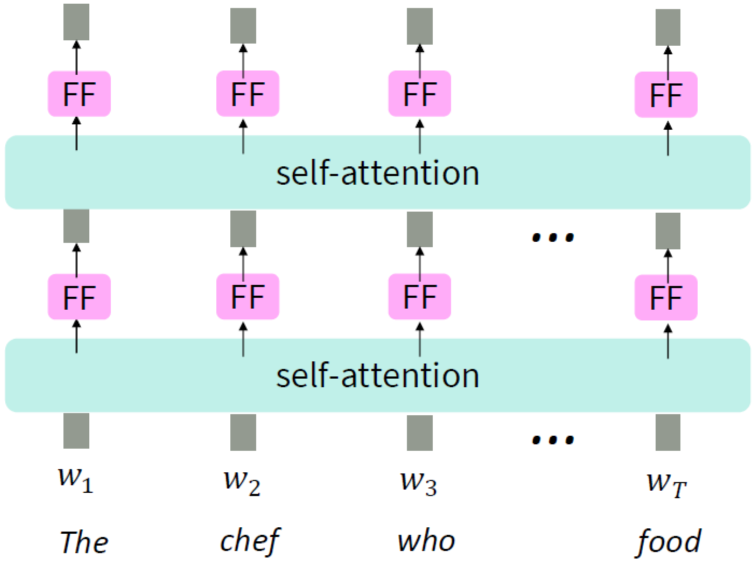
p_t design 2: **Learned representation**

- Assume maximum length L, learn a matrix $p \in \mathbb{R}^{d \times T}$, p_t is a column of p
- Pros:
  - Flexible
  - Learnable and more powerful
- Cons:
  - Need to assume a fixed maximum length L
  - Does not work at all for length above L

Combine Self-Attention with Nonlinearity

- Vanilla self-attention
  - No element-wise activation (e.g., ReLU, tanh)
  - Only weighted average and softmax operator

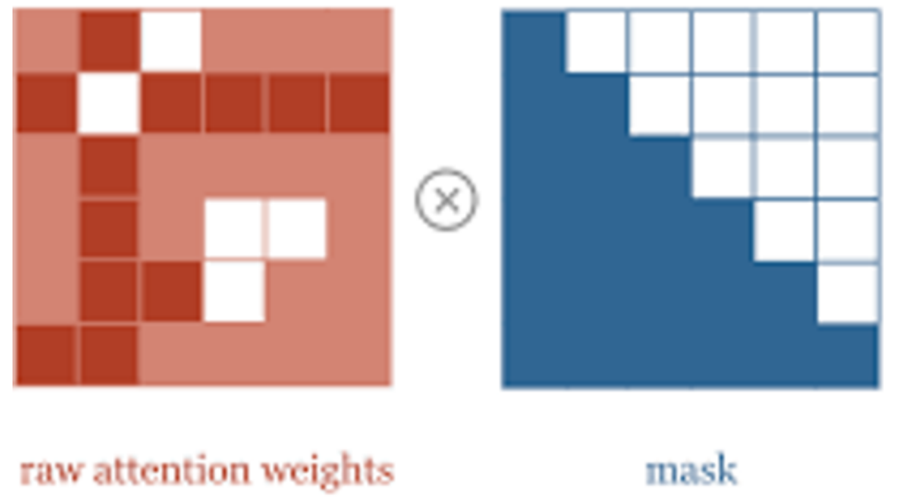
- Fix:
  - Add an MLP to process out_i
  - $m_i = MLP(out_i) = W_2 \text{ReLU}(W_1 out_i + b_1) + b_2$
  - Usually do not put activation layer before softmaax

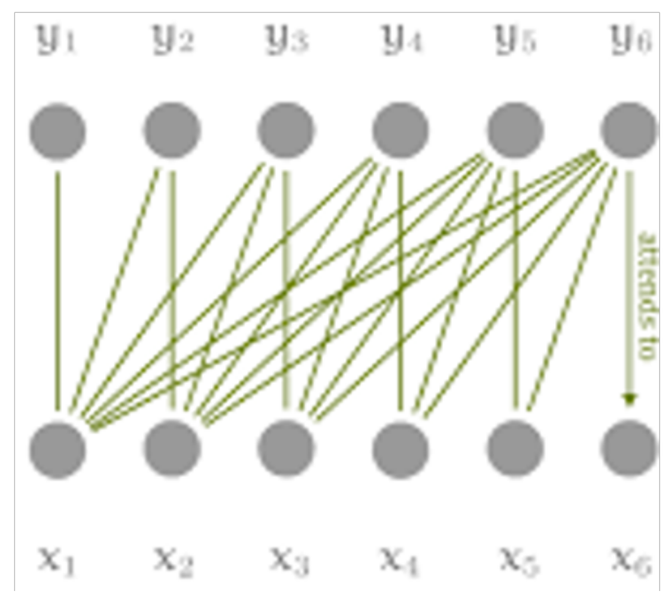


Masked Attention

- In language model decoder: $P(Y_t \mid X_{i<t})$
  - out_t cannot look at future $X_{i>t}$

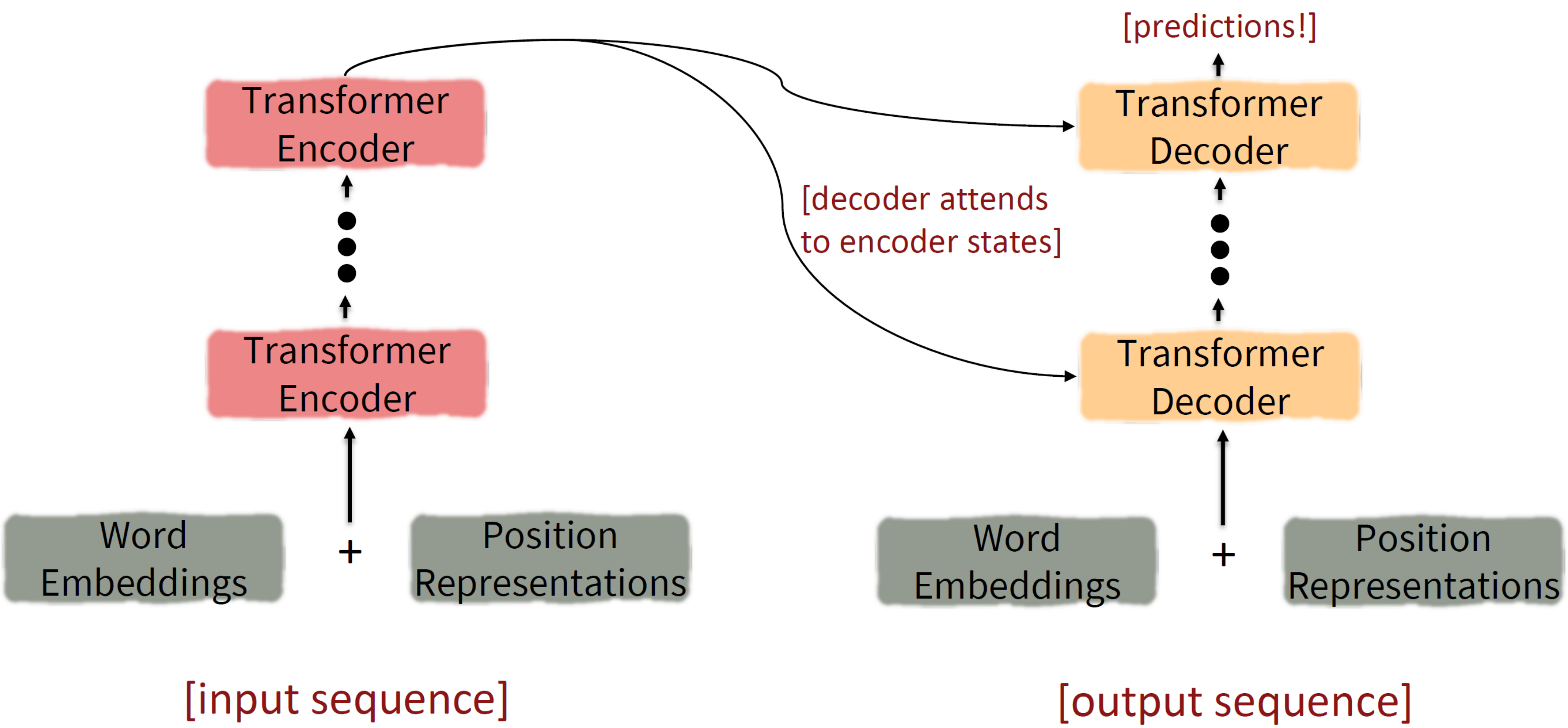
- Masked attention
  - Compute $e_{i,j} = q_i^\top k_j$ as usuall
  - Mask out $e_{i>j}$ by setting $e_{i>j} = -\infty$
    - $e \odot (1 - M) \leftarrow -\infty$
    - M is a fixed 0/1 mask matrix
  - Then compute $\alpha_i = \text{softmax}(e_i)$
  - Remarks:
    - $M = 1$ for full self-attention
    - Set M for arbitrary dependency ordering





Transformer

Transformer-based sequence-to-sequence modeling



Key-query-value attention

- Obtain q_t, v_t, k_t from X_t
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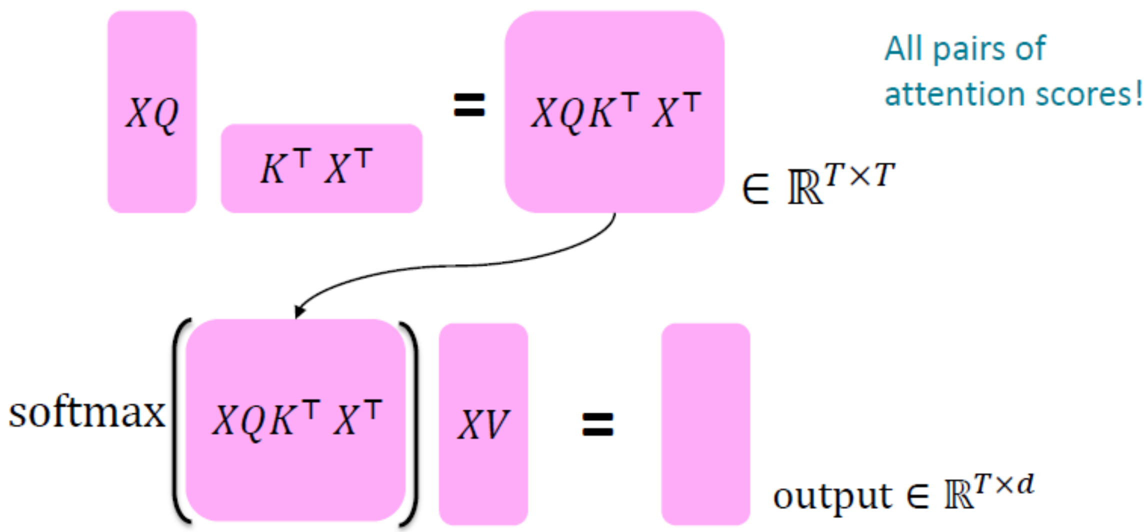
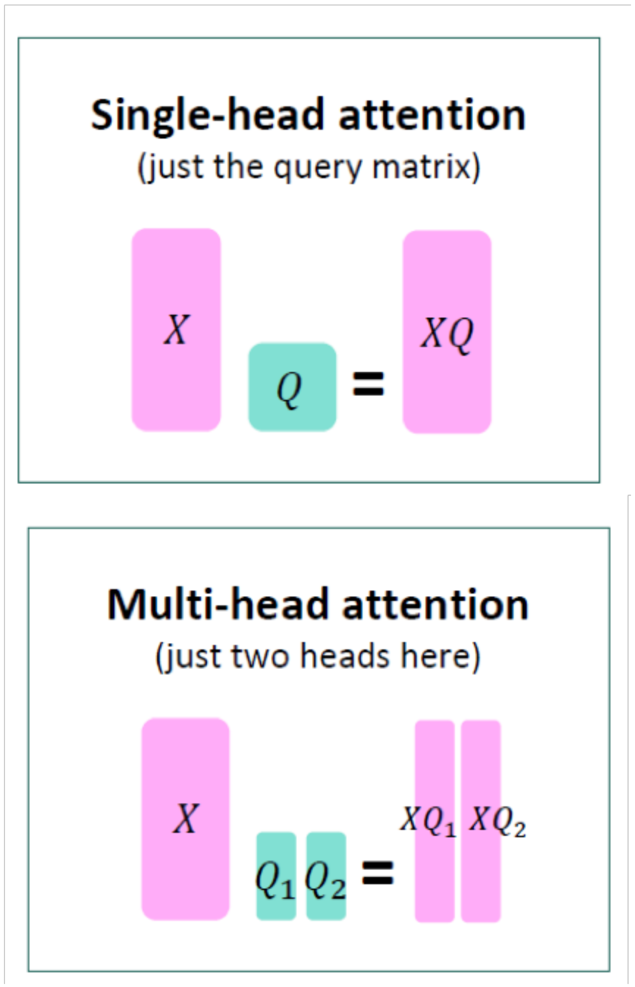


Multi-headed attention

- Standard attention: single-headed attention
  - $X_t \in \mathbb{R}^d, Q, K, V \in \mathbb{R}^{d \times d}$
  - We only look at a single position j with high $\alpha_{i,j}$
  - What if we want to look at different j for different reasons?
- Idea: define h separate attention heads
  - h different attention distributions, keys, values, and queries
  - $Q^\ell, K^\ell, V^\ell \in \mathbb{R}^{d \times \frac{d}{h}}$ for $1 \leq \ell \leq h$
  - $\alpha_{i,j}^\ell = \text{softmax}((q_i^\ell)^\top k_j^\ell); out_i^\ell = \sum_j \alpha_{i,j}^\ell v_j^\ell$

#Params Unchanged!



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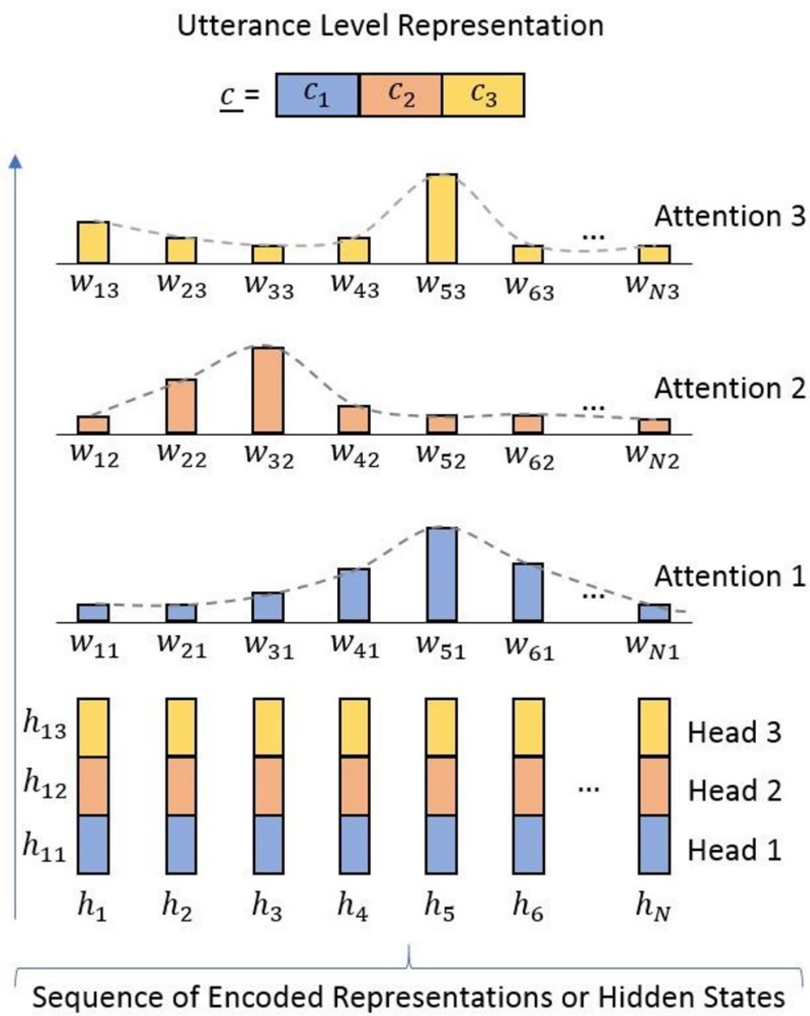
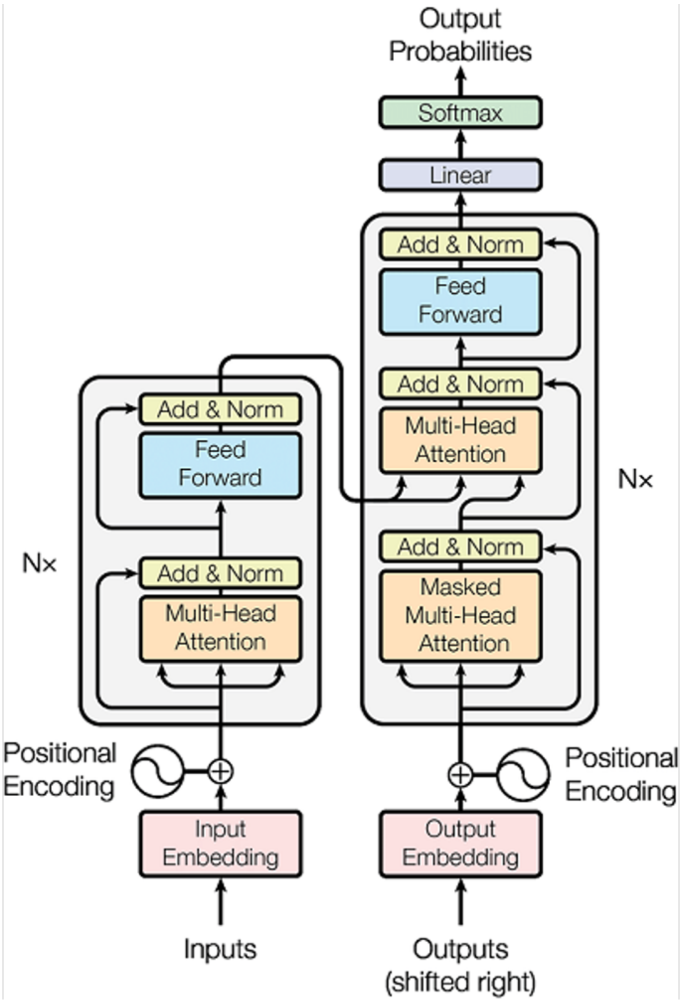


Transformer

Transformer-based sequence-to-sequence model

- Basic building blocks: self-attention
  - Position encoding
  - Post-processing MLP
  - Attention mask

- Enhancements:
  - Key-query-value attention
  - Multi-headed attention
  - Architecture modifications:
    - Residual connection
    - Layer normalization



Transformer

Machine translation with transformer

Model	BLEU		Training Cost (FLOPs)	
	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	$2.3 \cdot 10^{19}$	$1.4 \cdot 10^{20}$
ConvS2S [9]	25.16	40.46	$9.6 \cdot 10^{18}$	$1.5 \cdot 10^{20}$
MoE [32]	26.03	40.56	$2.0 \cdot 10^{19}$	$1.2 \cdot 10^{20}$
Deep-Att + PosUnk Ensemble [39]		40.4		$8.0 \cdot 10^{20}$
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**	$7.7 \cdot 10^{19}$	$1.2 \cdot 10^{21}$
Transformer (base model)	27.3	38.1	$\mathbf{3.3 \cdot 10^{18}}$	
Transformer (big)	**28.4**	**41.8**	$2.3 \cdot 10^{19}$	

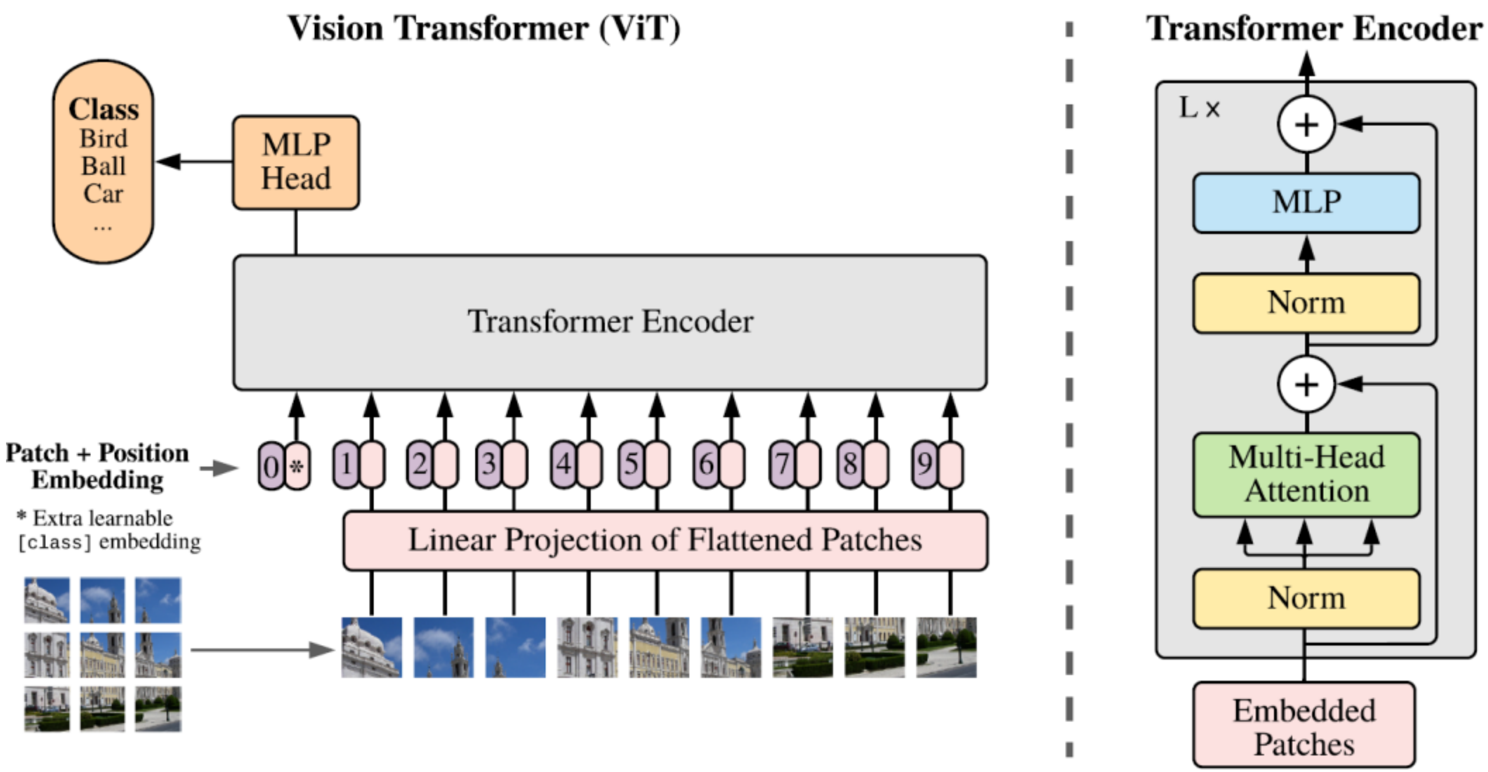
Transformer

- Limitations of transformer: Quadratic computation cost
  - Linear for RNNs
  - Large cost for large sequence length, e.g., $L > 10^4$

- Follow-ups:
  - Large-scale training: transformer-XL; XL-net (‘20)
  - Projection tricks to $O(L)$: Linformer ('20)
  - Math tricks to $O(L)$: Performer (‘20)
  - Sparse interactions: Big Bird (‘20)
  - Deeper transformers: DeepNet (’22)

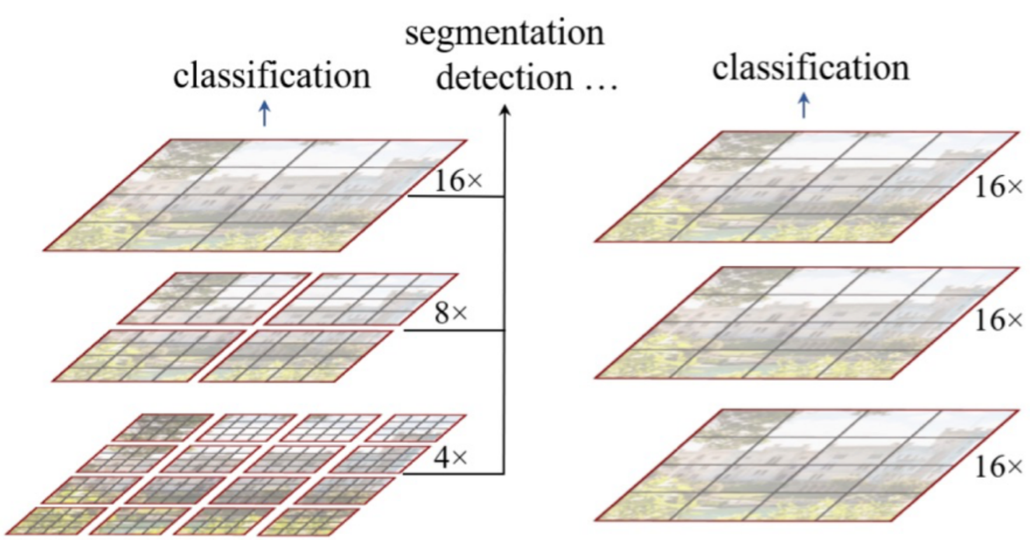
Transformer for Images

- Vision Transformer ('21)
  - Decompose an image to 16x16 patches and then apply transformer encoder



Transformer for Images

- Swin Transformer ('21)
  - Build hierachical feature maps at different resolution
    - Self-attention only within each block
    - Shifted block partitions to encode information between blocks



(a) Swin Transformer (ours)

(b) ViT

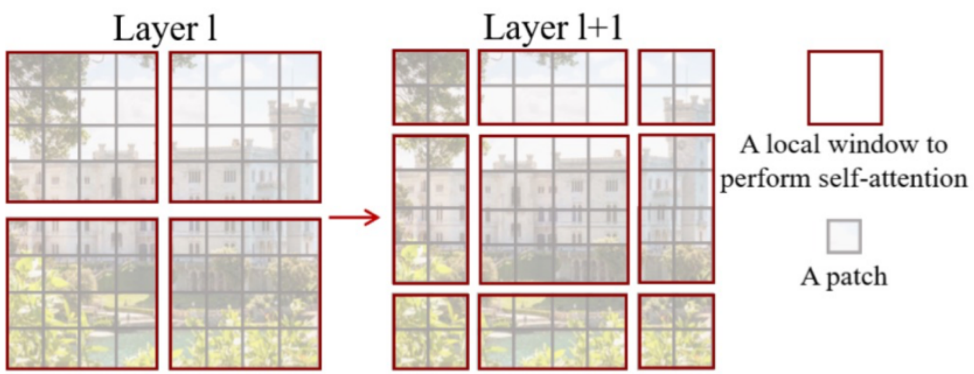
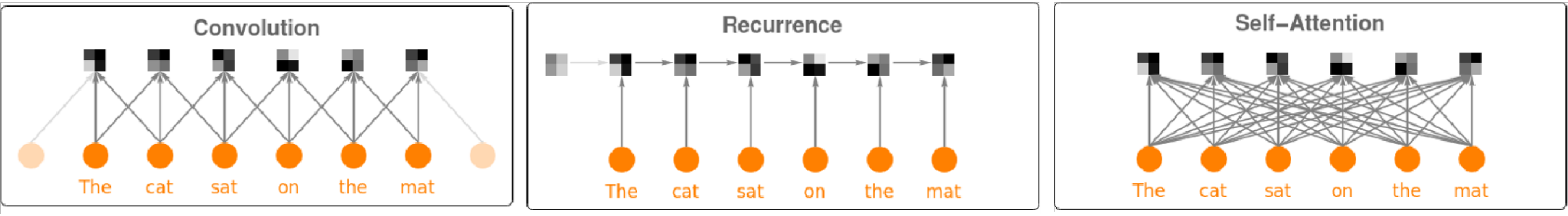


Figure 2. An illustration of the *shifted window* approach for com-

CNN vs. RNN vs. Attention



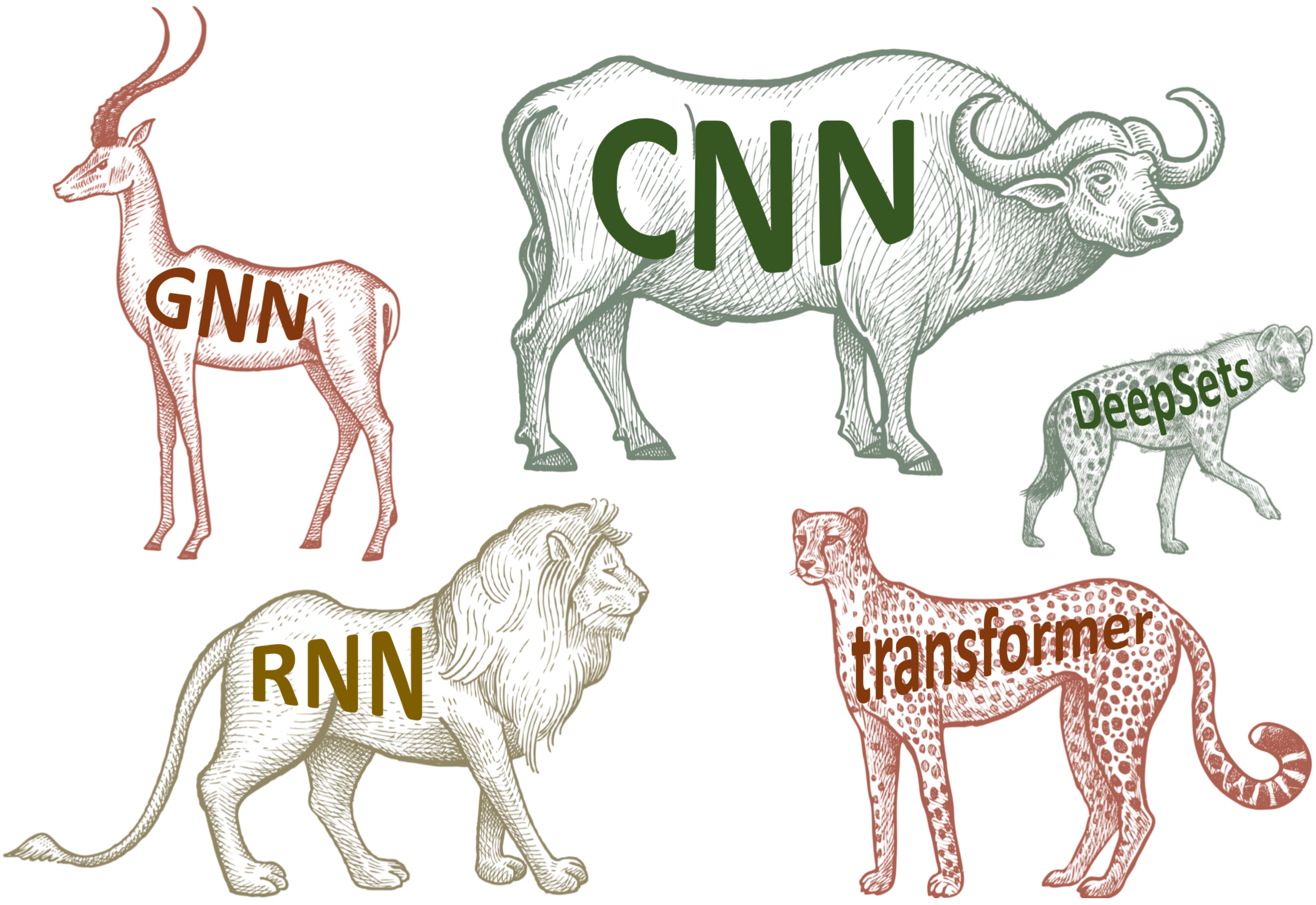
Summary

- Language model & sequence to sequence model:
  - Fundamental ideas and methods for sequence modeling

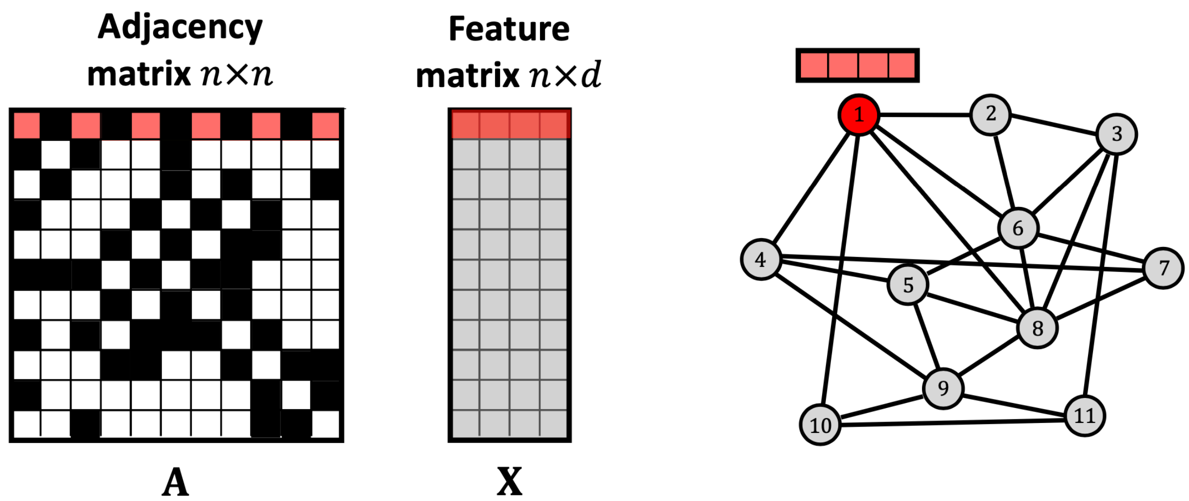
- Attention mechanism
  - So far the most successful idea for sequence data in deep learning
  - A scale/order-invariant representation
  - Transformer: a fully attention-based architecture for sequence data
  - Transformer + Pretraining: the core idea in today's NLP tasks

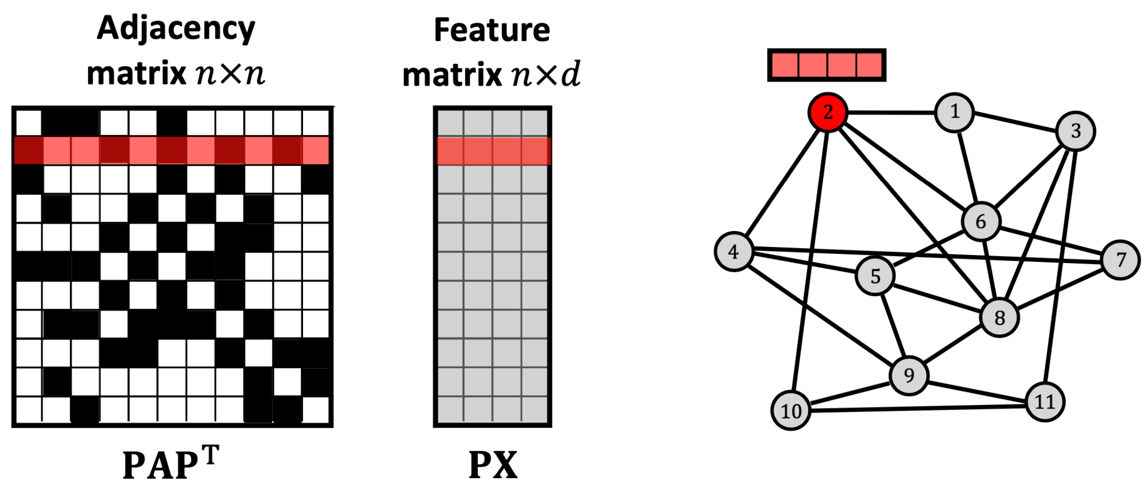
- LSTM is still useful in lightweight scenarios

Other architectures



Graph Neural Networks



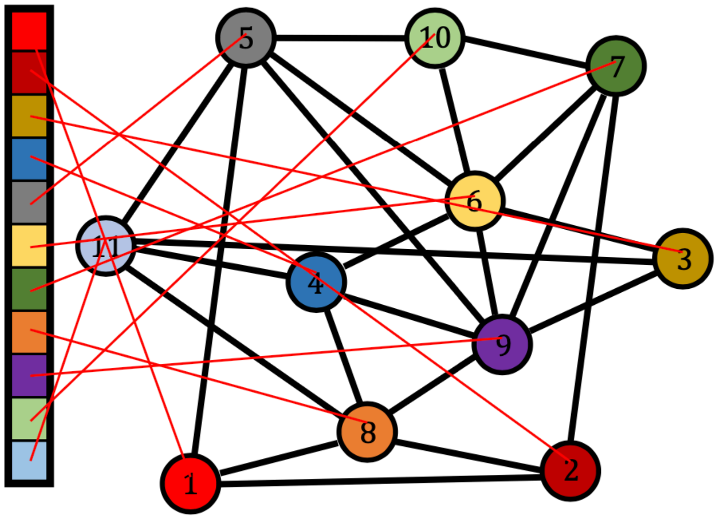


arbitrary ordering of nodes

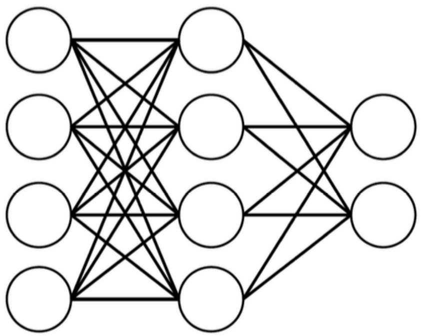
Graph Neural Networks

permutation-equivariant

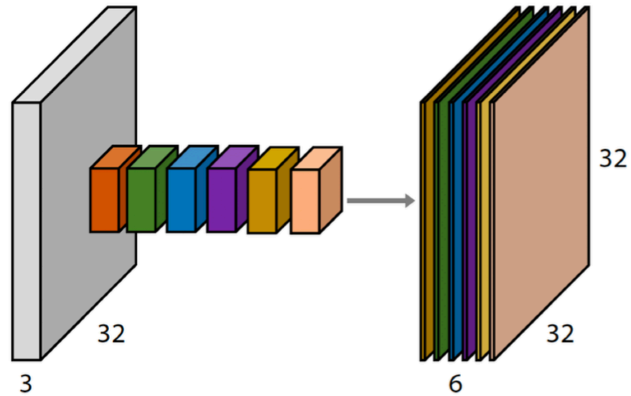
$$\mathbf{F}\left(\mathbf{PX}, \mathbf{PAP}^\top\right) = \mathbf{PF}(\mathbf{X}, \mathbf{A})$$



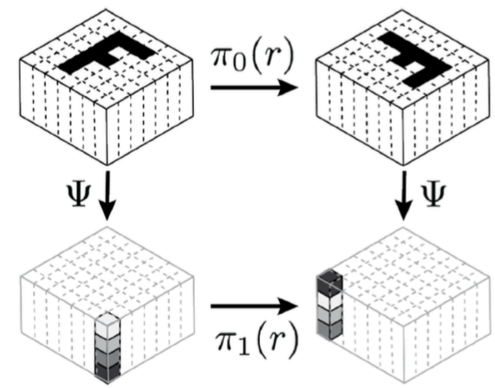
Geometric Deep Learning



Perceptrons
Function regularity

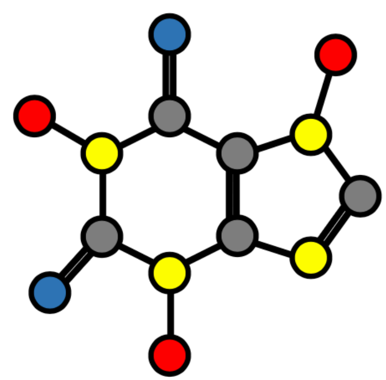


CNNs
Translation



Group-CNNs
Translation+Rotation

DeepSets / Transformers
Permutation



GNNs
Permutation

Intrinsic CNNs
Local frame choice