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

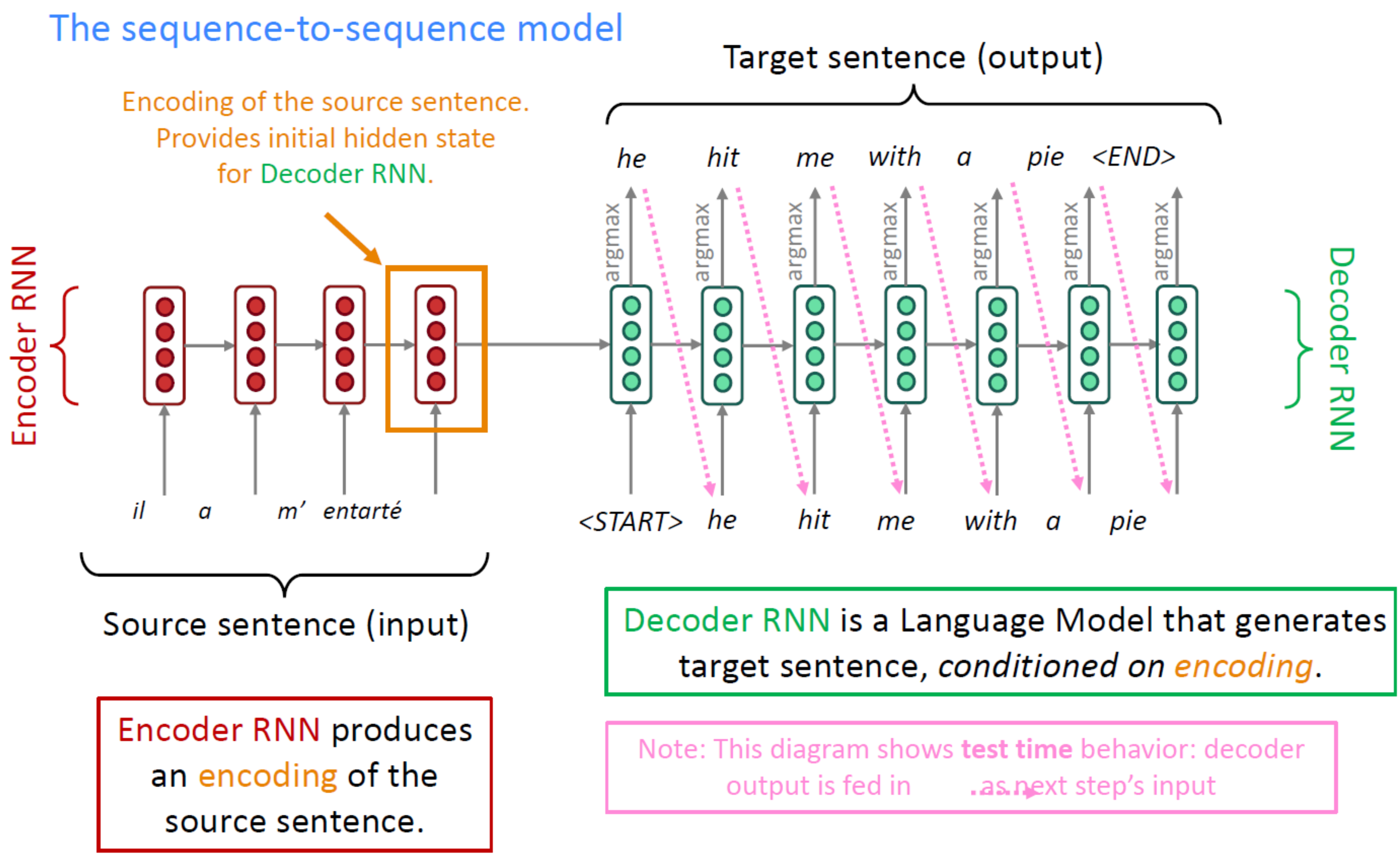
- What happened in 2014?
  - Neural machine translation (NMT)

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 $Y = f(X; \theta)$

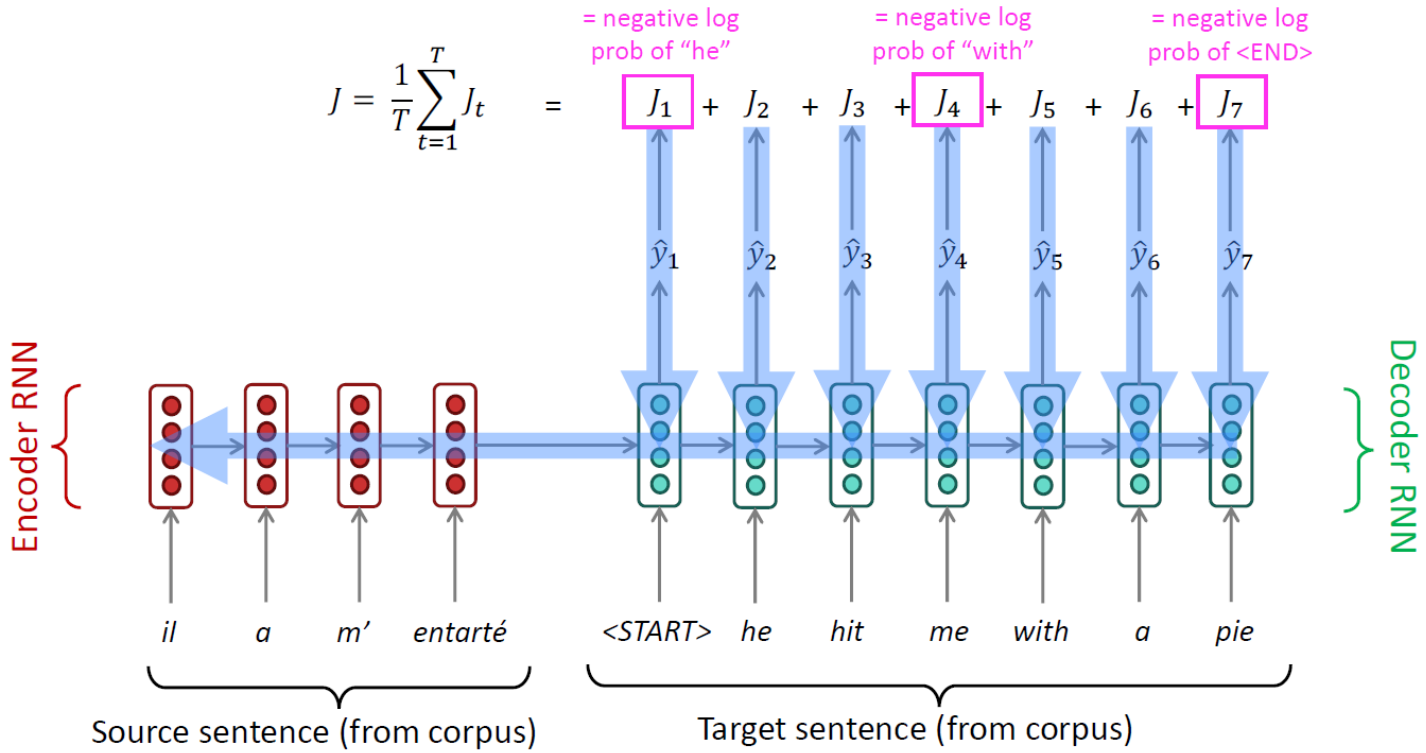
- Sequence to Sequence Model (Seq2Seq, Sutskever et al. , '14)
  - Two RNNs: f_{enc} and f_{dec}
  - Encoder f_{enc}:
    - Takes X as input, and output the initial hidden state for decoder
    - Can use bidirectional RNN
  - Decoder f_{dec}:
    - It takes in the hidden state from f_{enc} to generate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

Sequence to Sequence Model



Training Sequence to Sequence Model

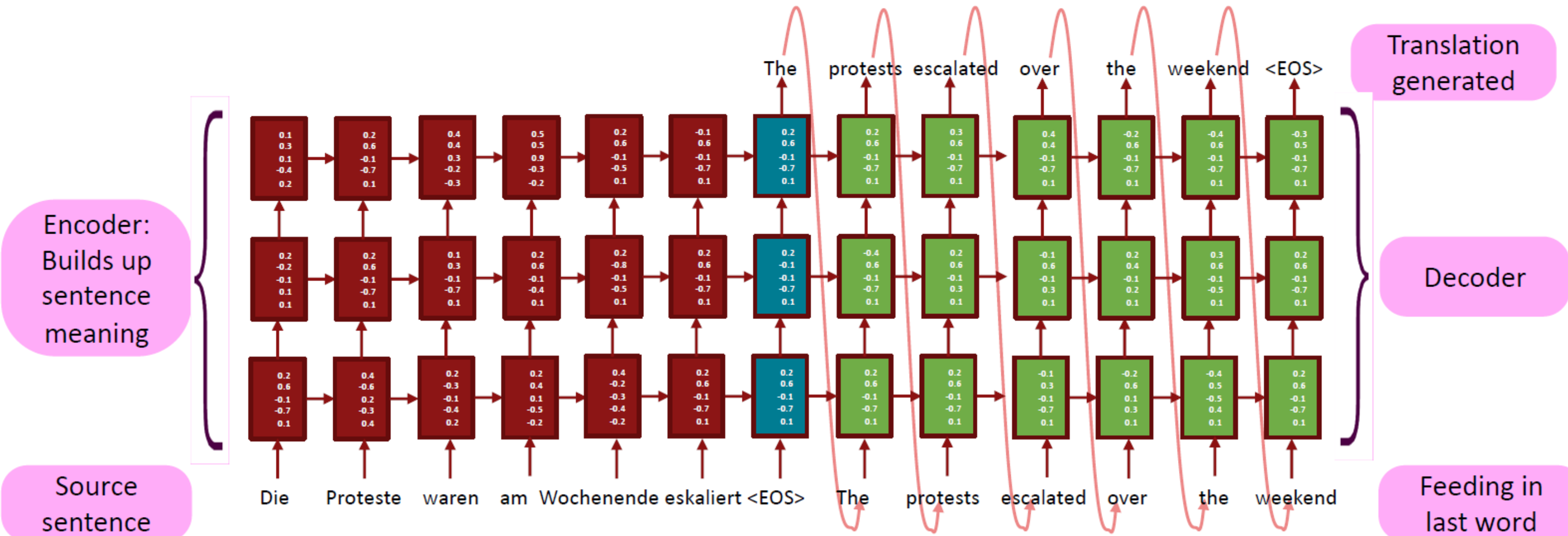
- Collect a huge paired dataset and train it end-to-end via BPTT
- Loss induced by MLE $P(Y|X) = P(Y|f_{enc}(X))$



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

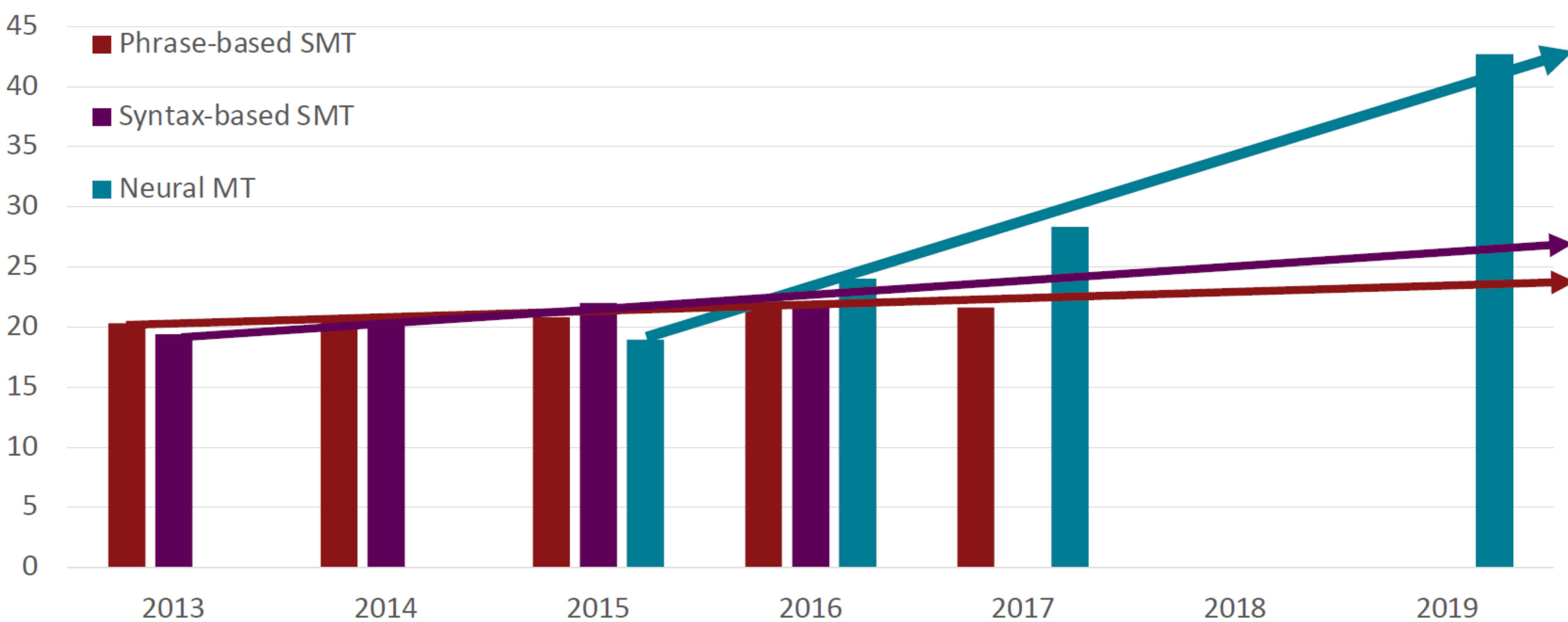
Deep Sequence to Sequence Model

- Stacked seq2seq model



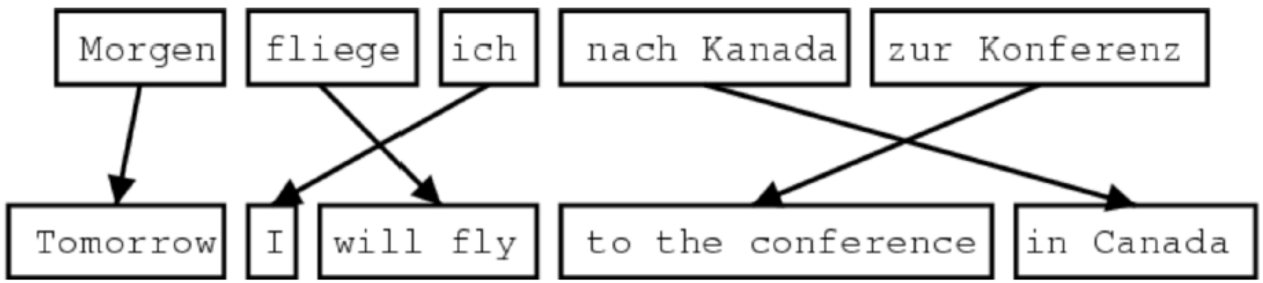
Machine Translation

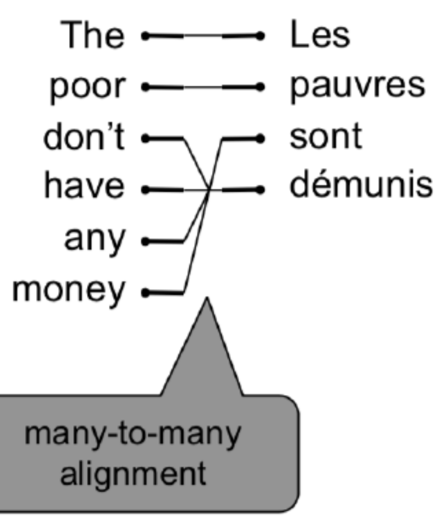
- 2016: Google switched Google Translate from SMT to NMT

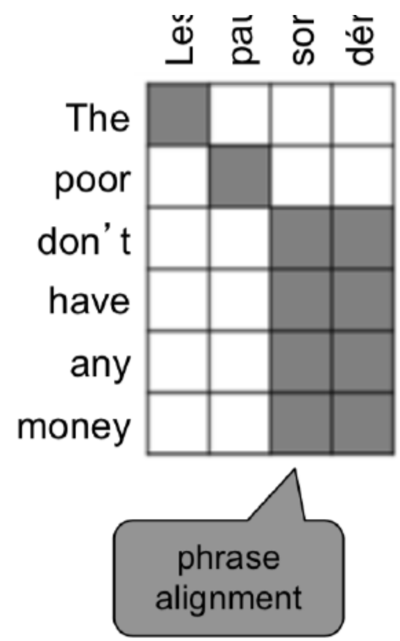


Alignment

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

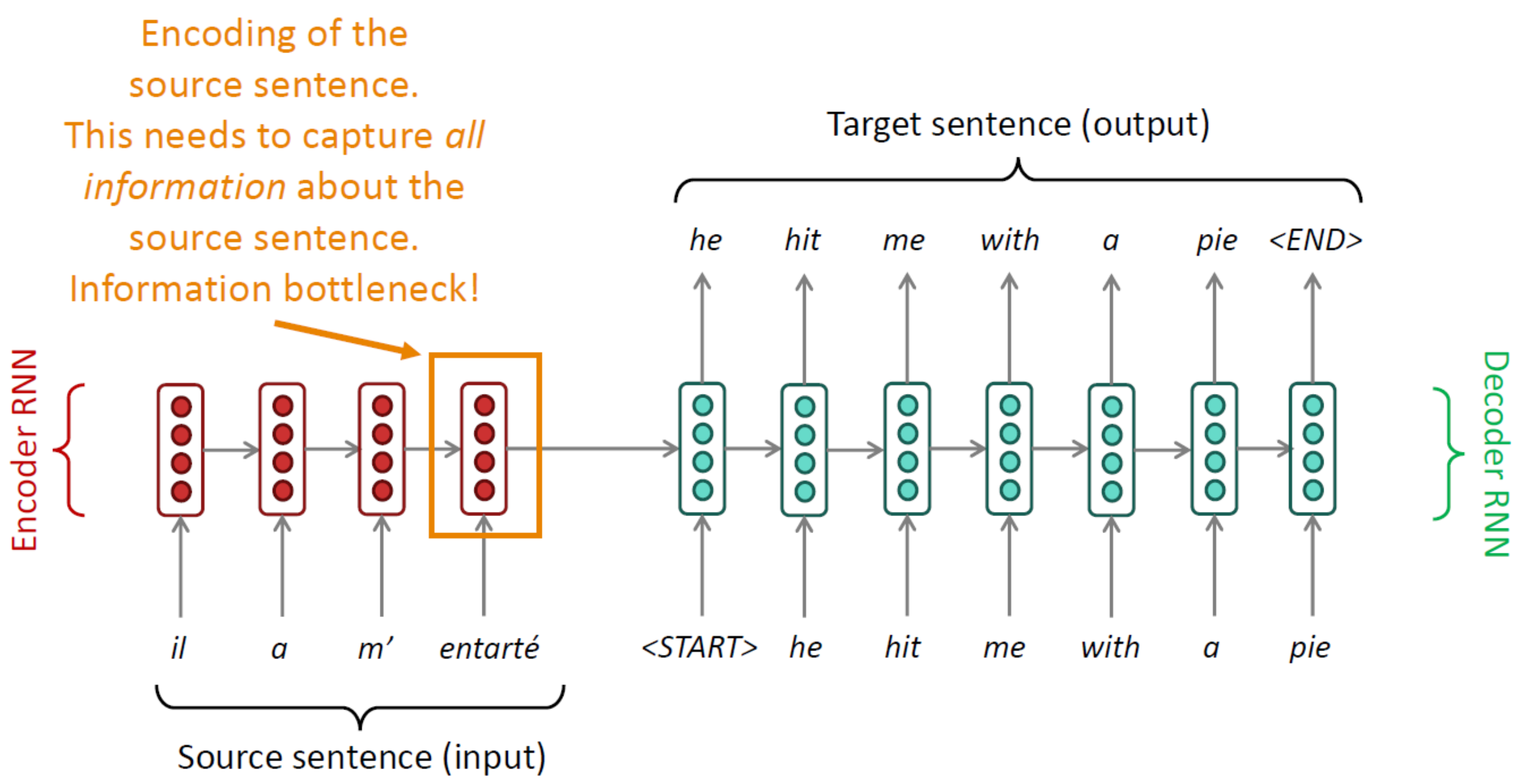






Issue in Seq2Seq

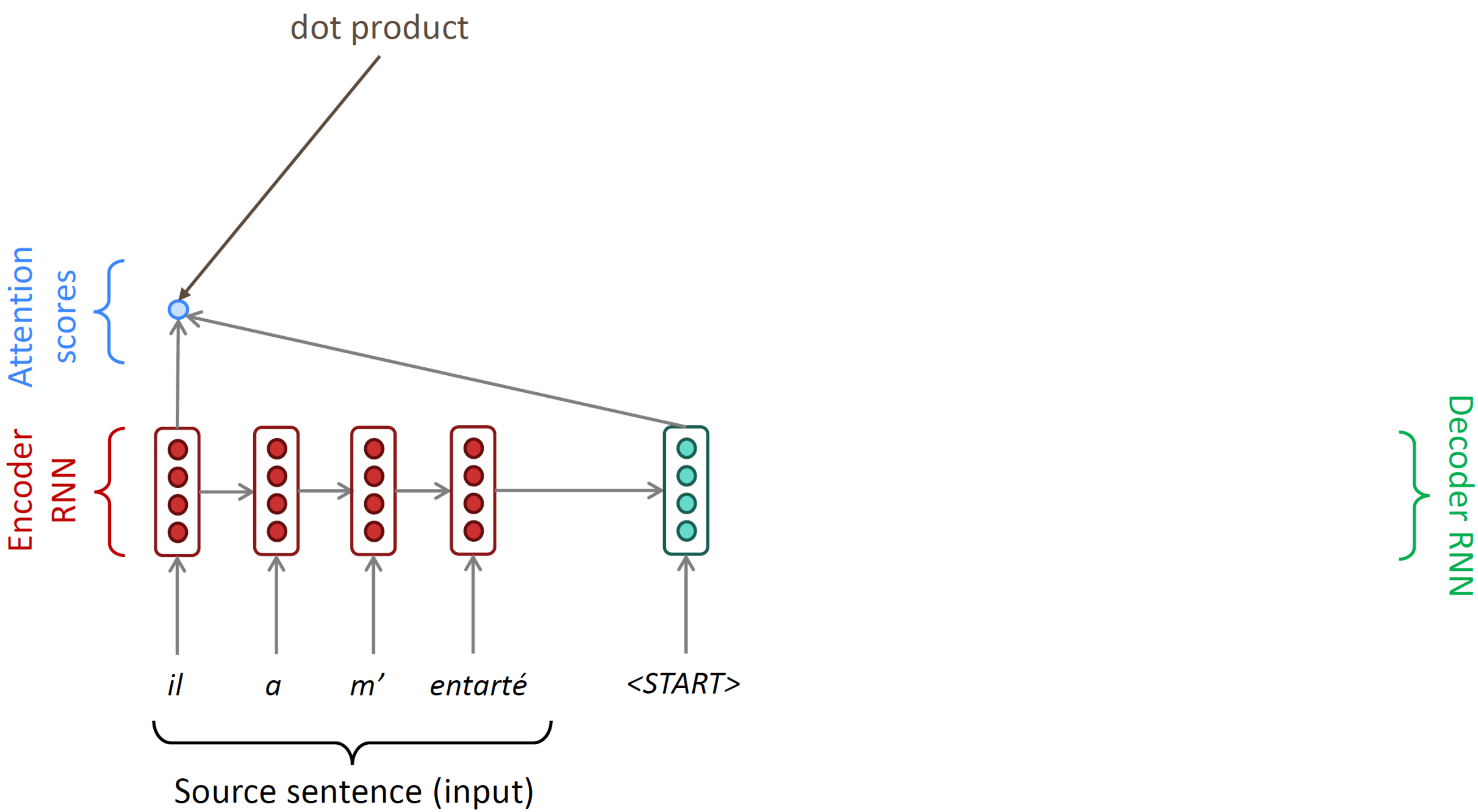
- Alignment: the word-level correspondence between X and Y
  - The information bottleneck due to the hidden state h
  - We want each Y_t to also focus on some X_i that it is aligned with



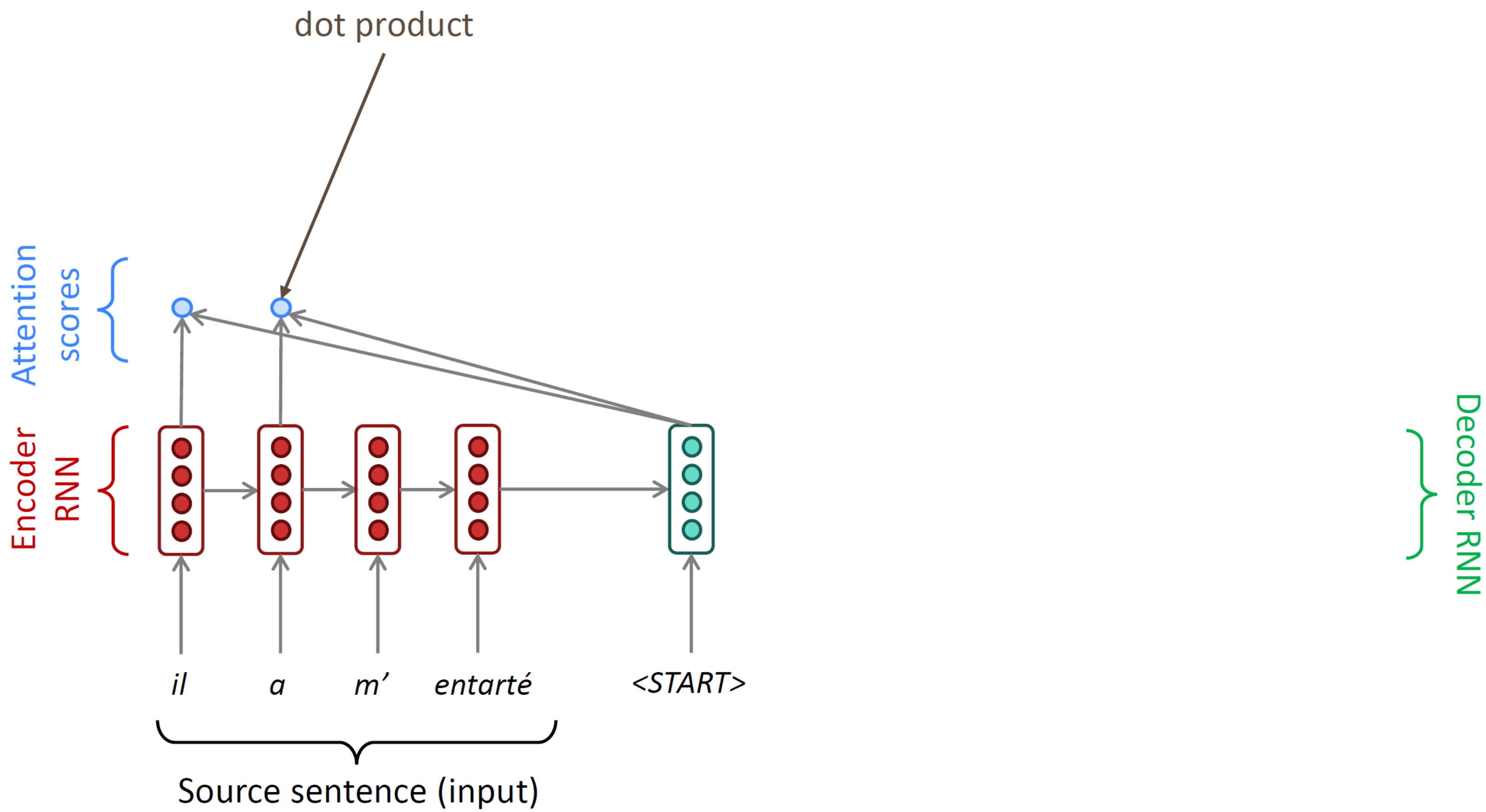
Seq2Seq with Attention

- 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

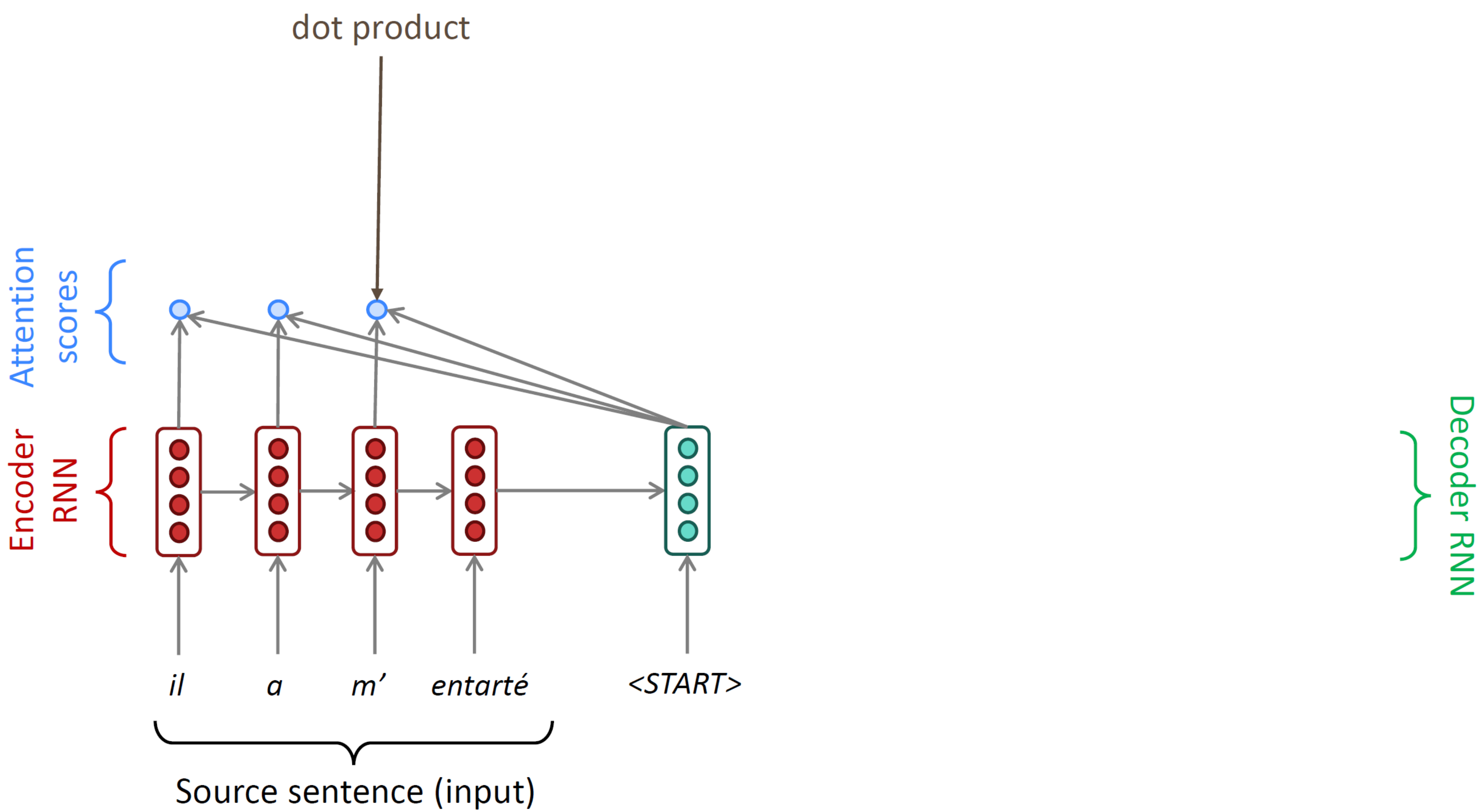
Seq2Seq with Attention



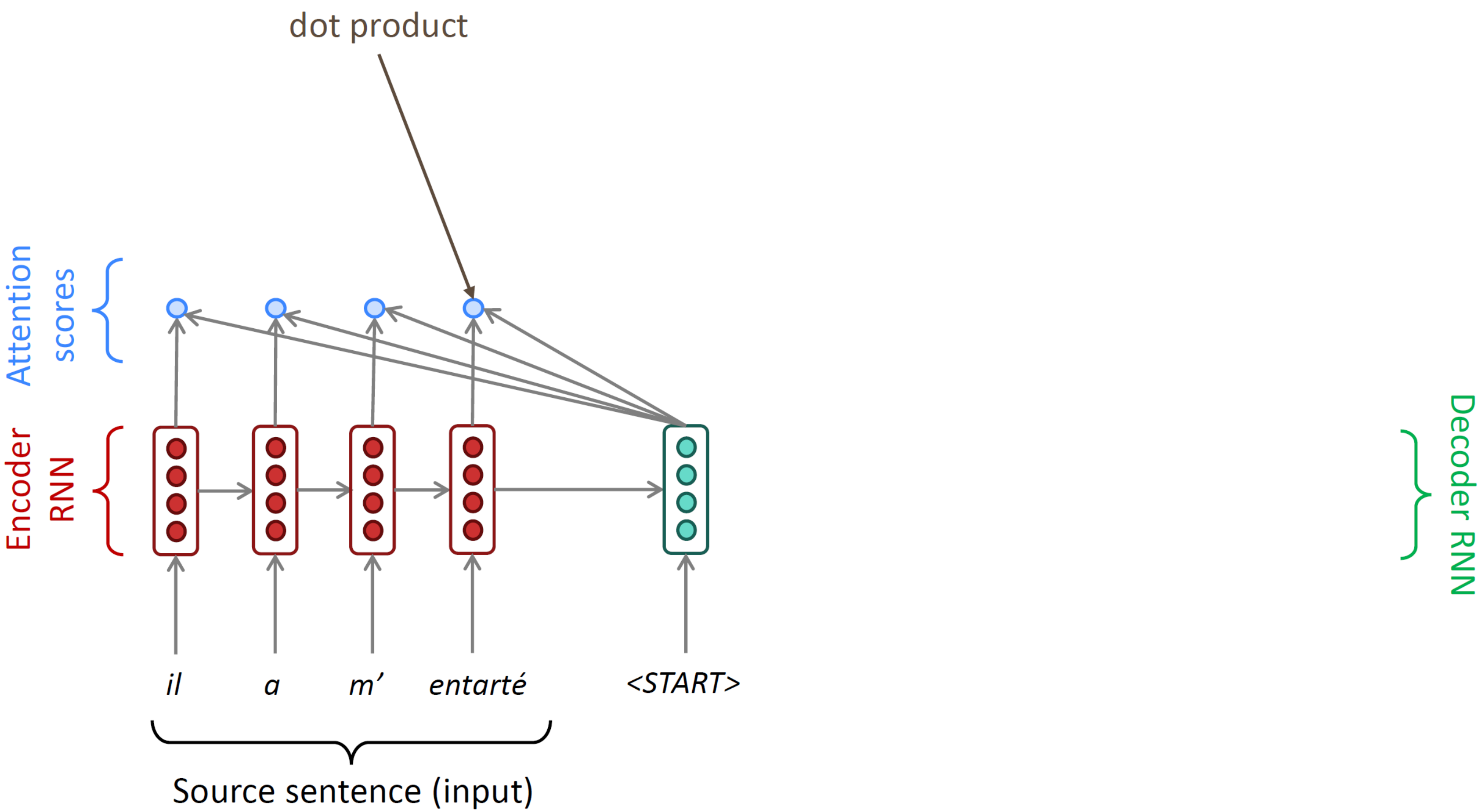
Seq2Seq with Attention



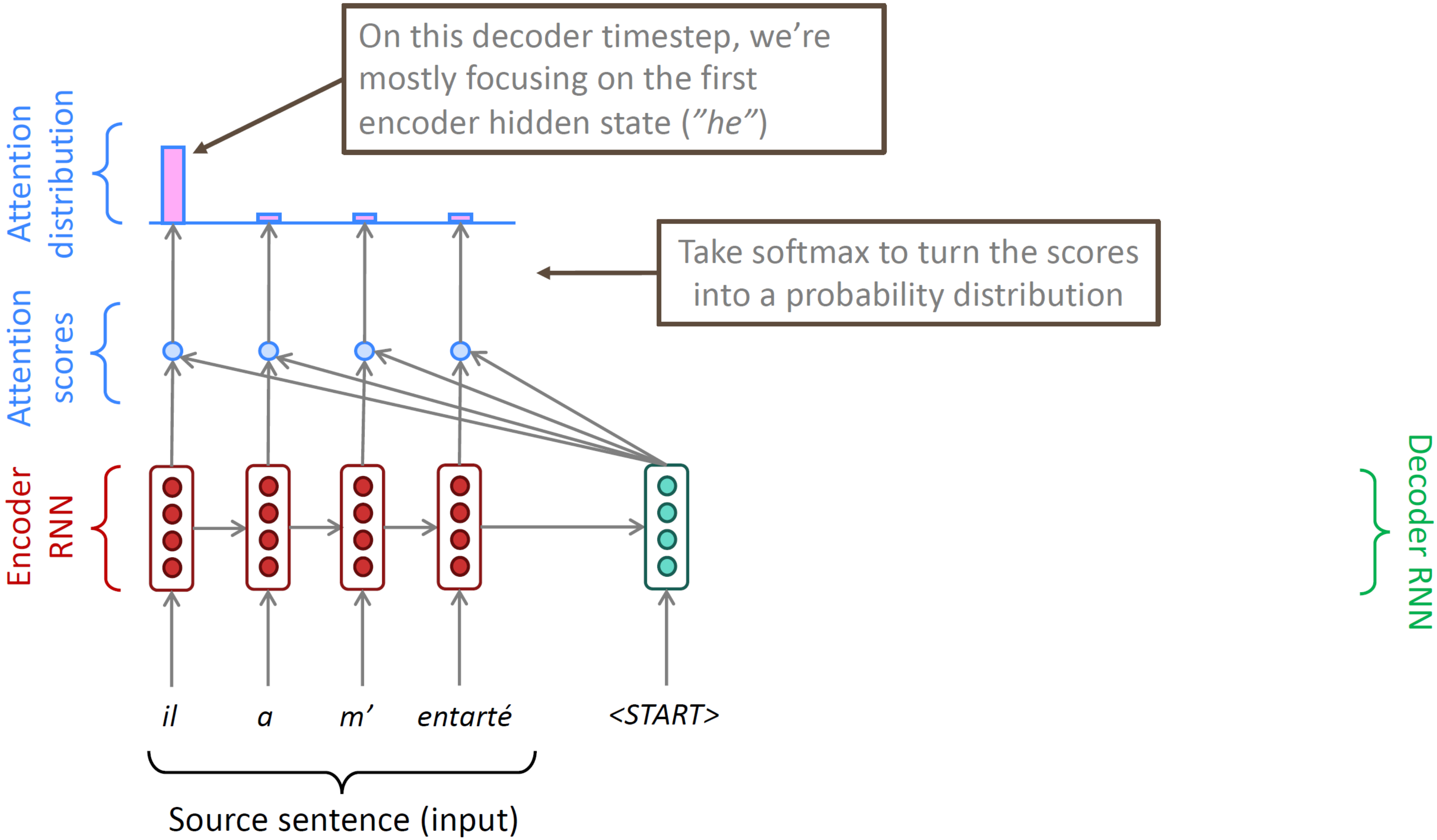
Seq2Seq with Attention



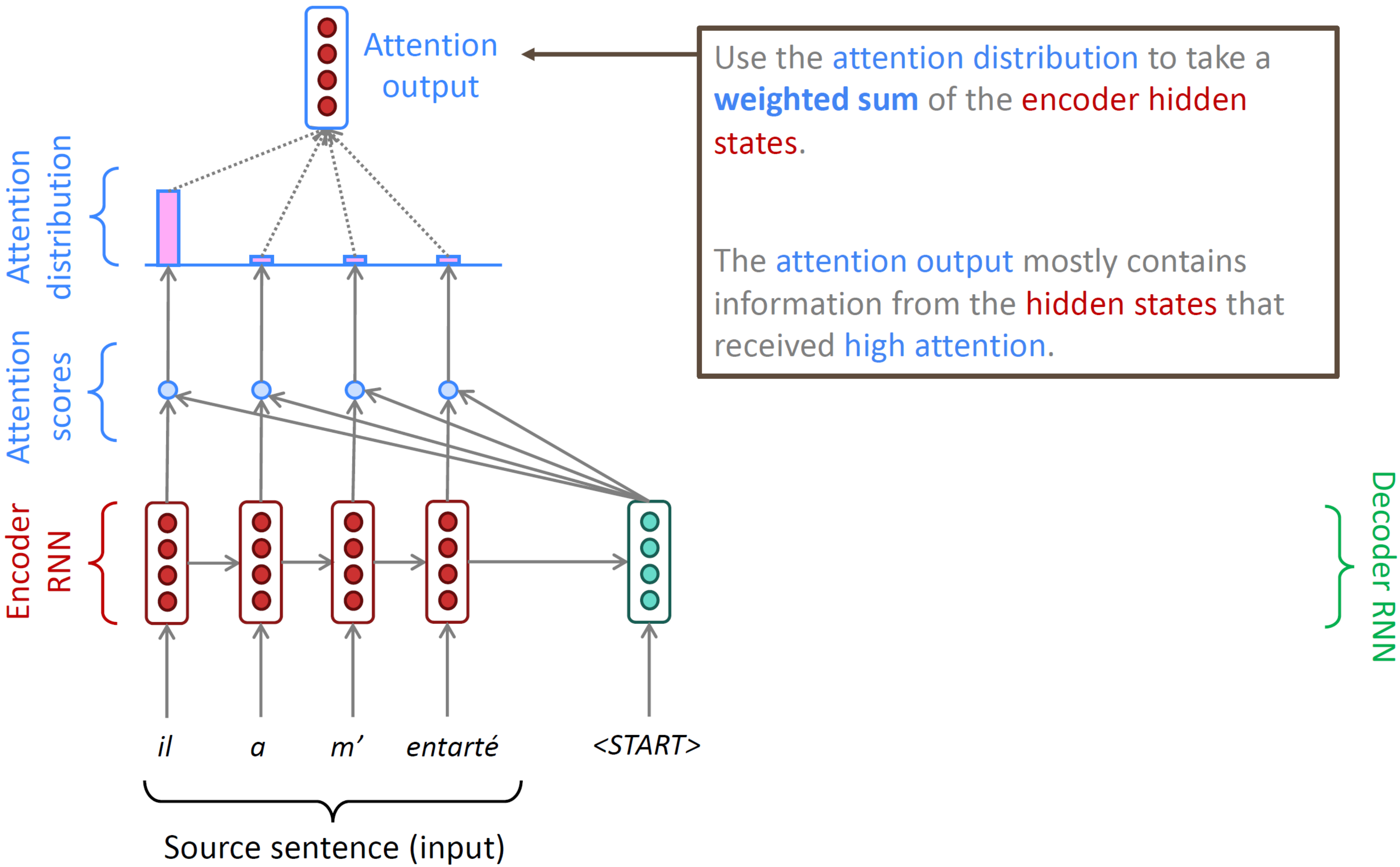
Seq2Seq with Attention



Seq2Seq with Attention



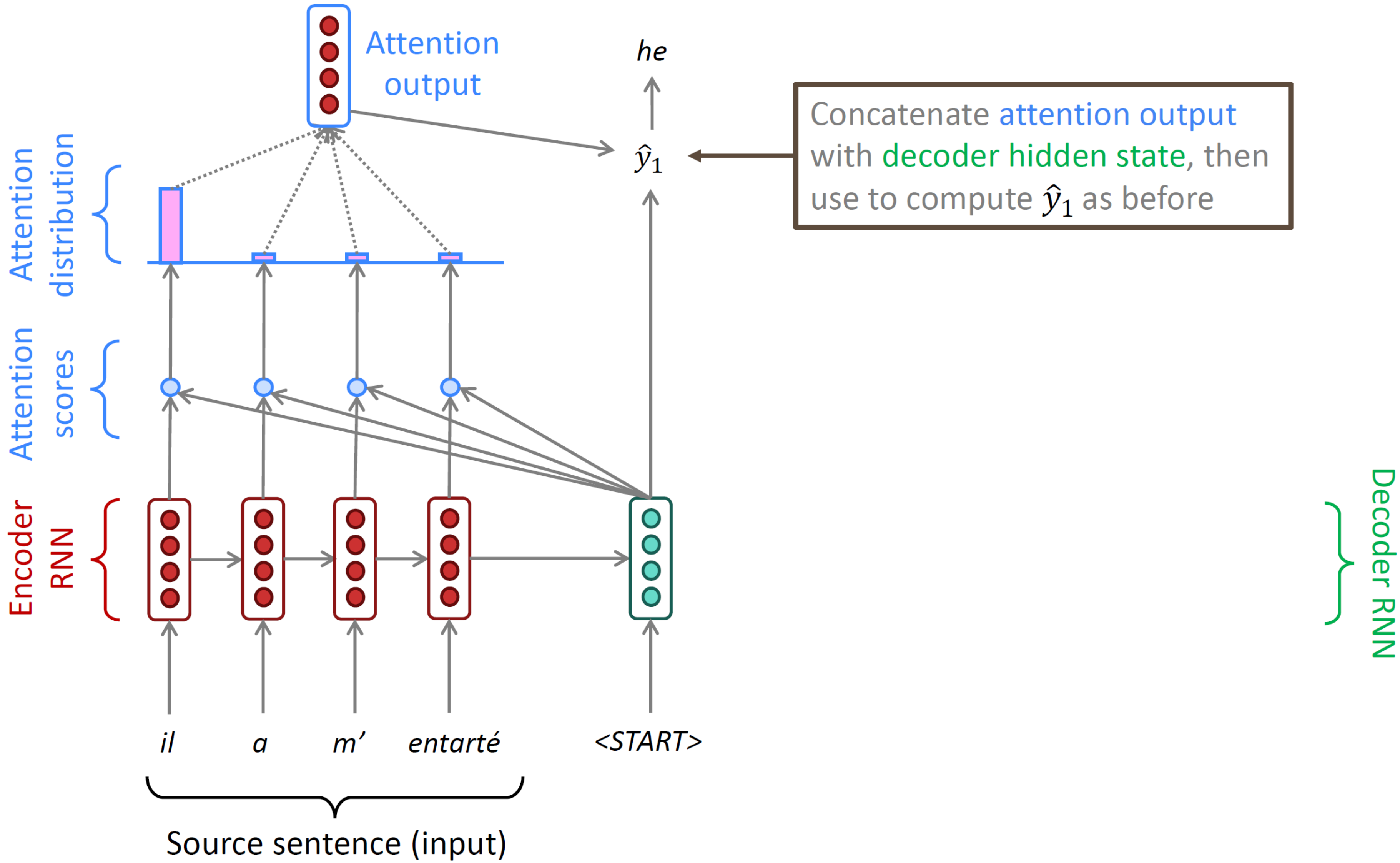
Seq2Seq with Attention



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

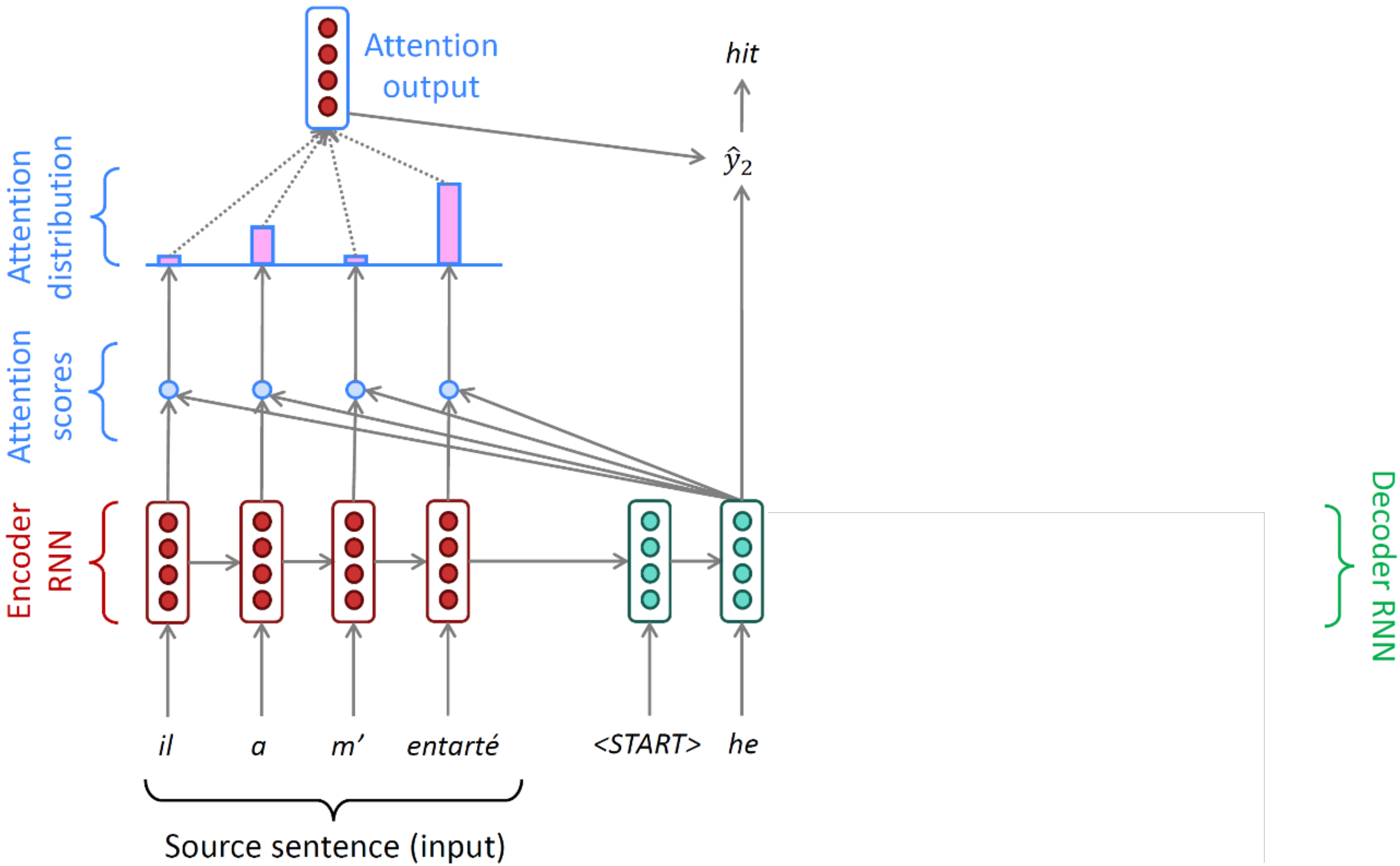
The attention output mostly contains information from the hidden states that received high attention.

Seq2Seq with Attention

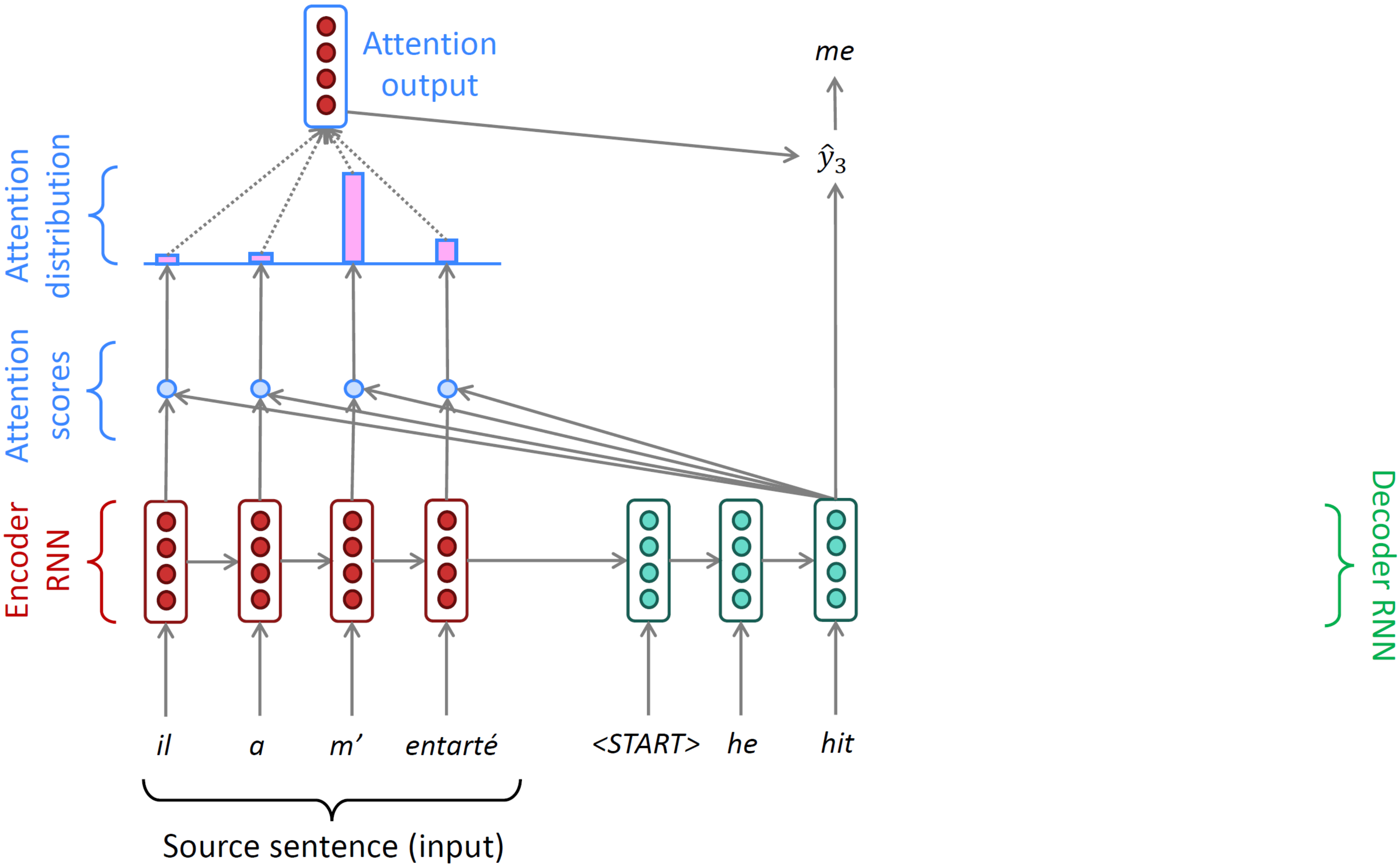


Concatenate attention output with decoder hidden state, then use to compute $\hat{y}_1$ as before

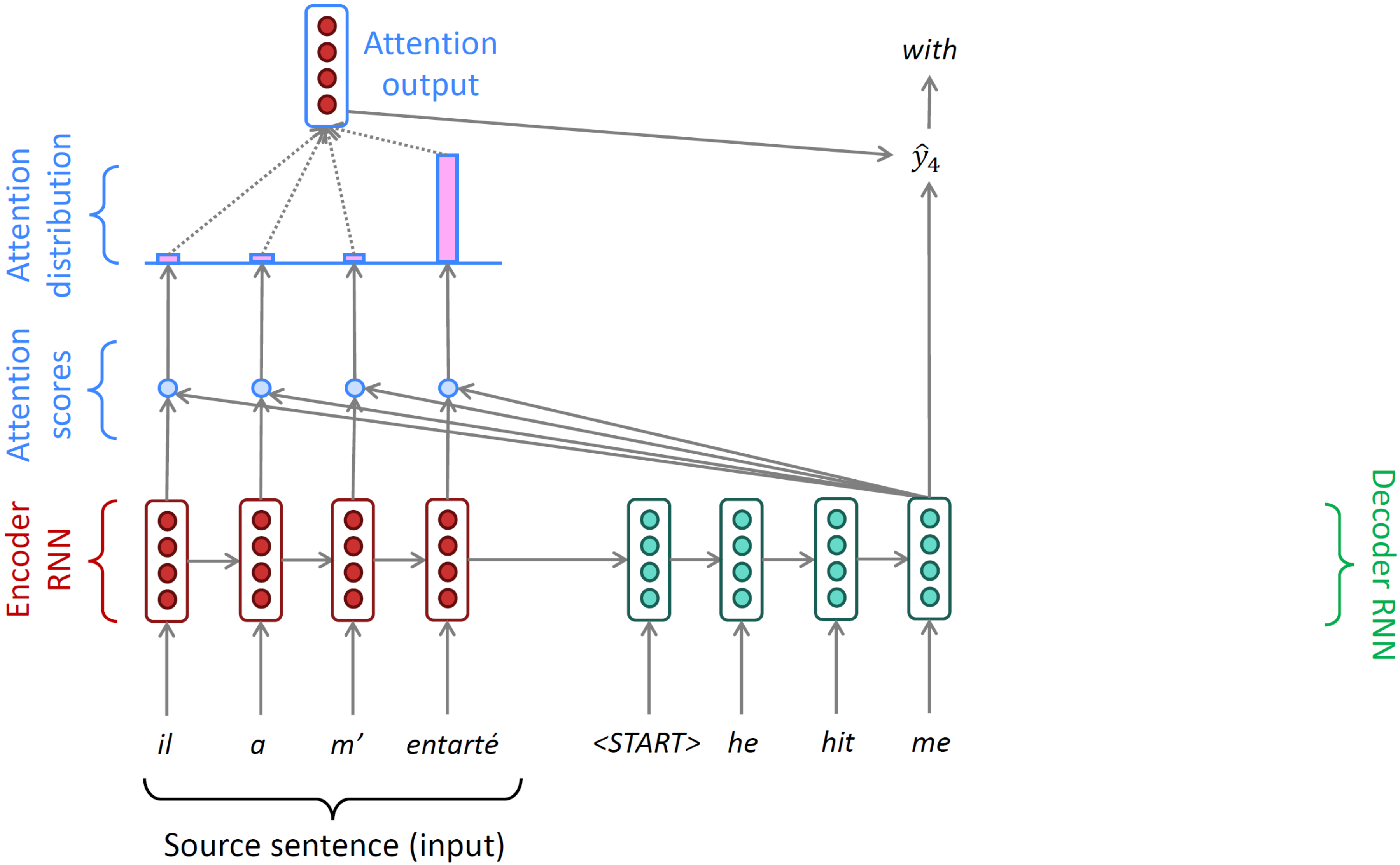
Seq2Seq with Attention



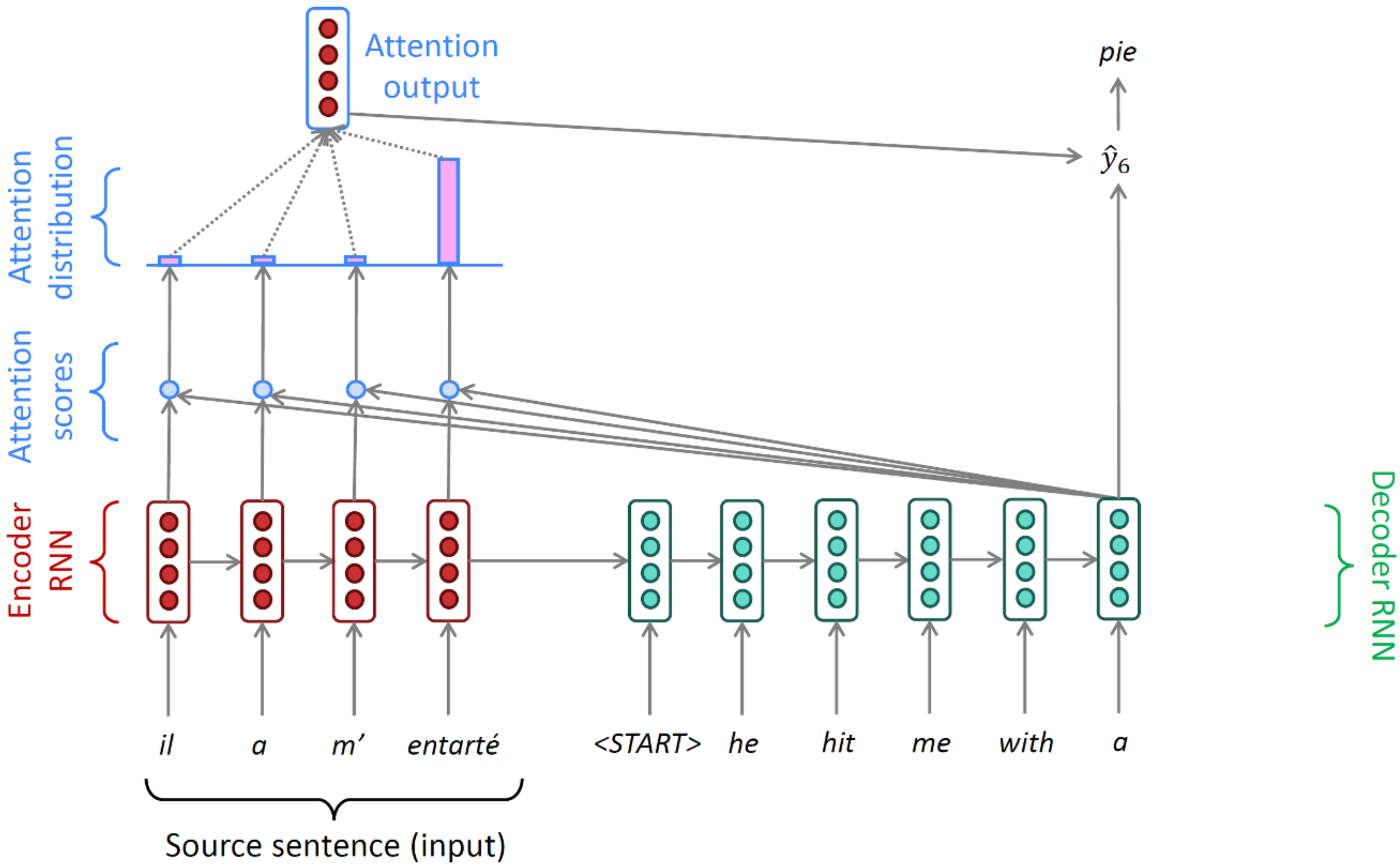
Seq2Seq with Attention



Seq2Seq with Attention



Seq2Seq with Attention



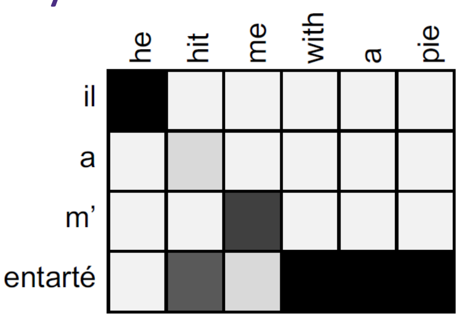
Seq2Seq with Attention

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)

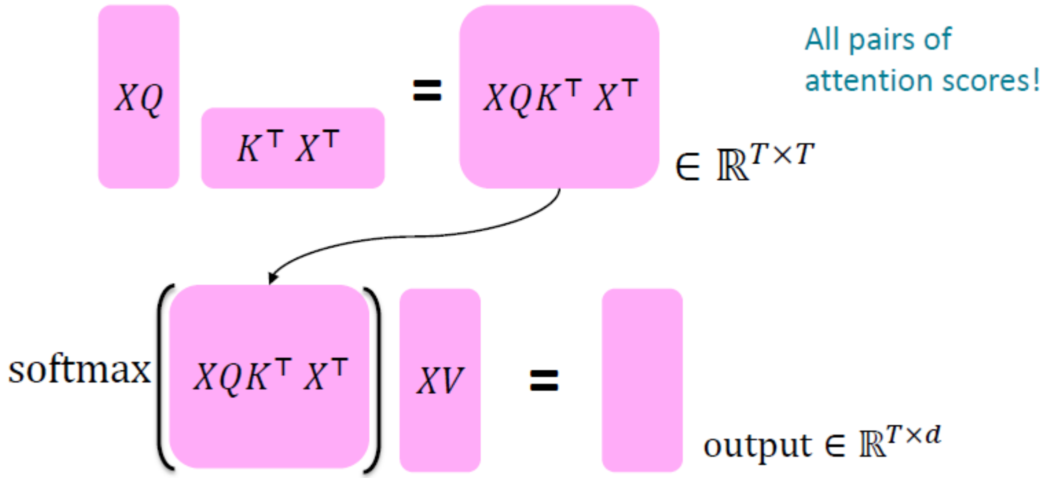
Attention

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

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

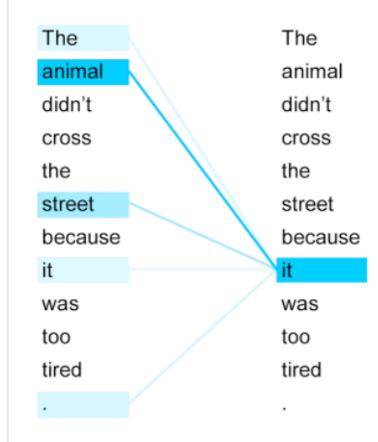
Key-query-value attention

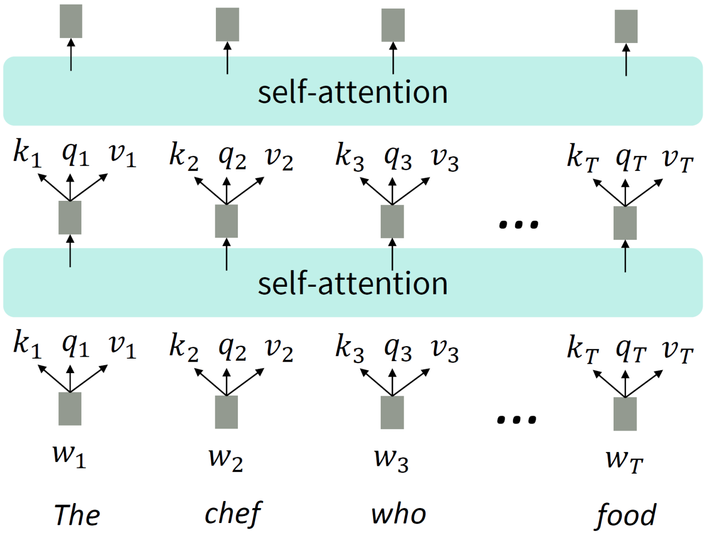
- Obtain q_t, v_t, k_t from X_t
- $q_t = W^q X_t; v_t = W^v X_t; k_t = W^k X_t$ (position encoding omitted)
  - W^q, W^v, W^k are learnable weight matrices
- $\alpha_{i,j} = \text{softmax}(q_i^\top k_j); out_i = \sum_k \alpha_{i,j} v_j$
- Intuition: key, query, and value can focus on different parts 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
  - $(k_t, v_t, q_t) = g_1([X_t, p_t]; \theta)$

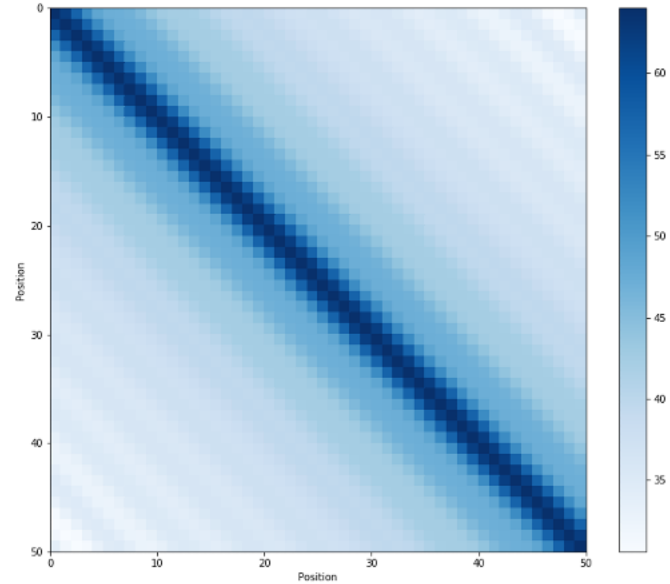
- In practice: Additive is sufficient: $k_t \leftarrow \tilde{k}_t + p_t, q_t \leftarrow \tilde{q}_t + p_t, v_t \leftarrow \tilde{v}_t + p_t;$ $(\tilde{k}_t, \tilde{v}_t, \tilde{q}_t) = g_1(X_t; \theta)$

- 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

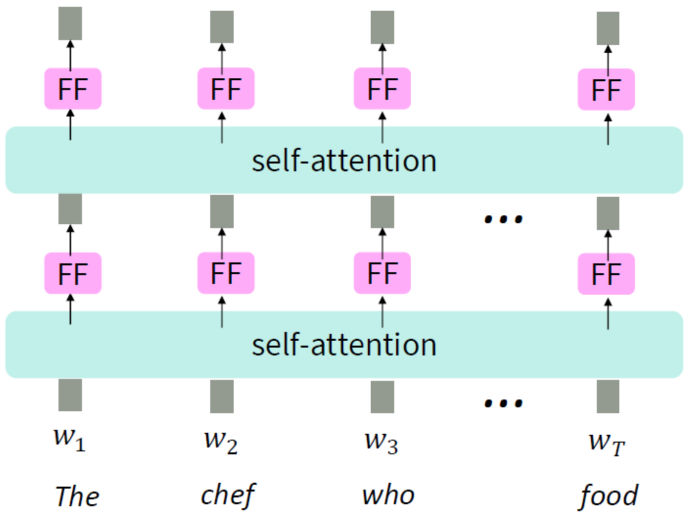
p_t design 2: **Learned representation**

- 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

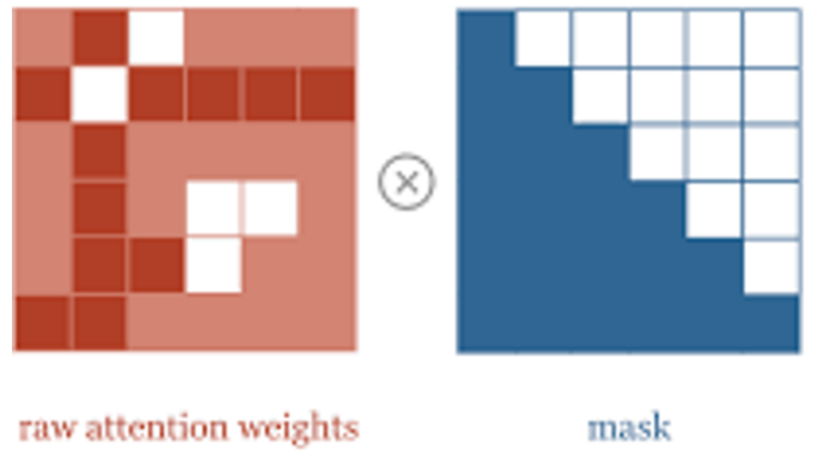
- Fix:
  - Add an MLP to process out_i
  - $m_i = MLP(out_i) = W_2 \text{ReLU}(W_1 out_i + b_1) + b_2$
  - Usually do not put activation layer before softmaax

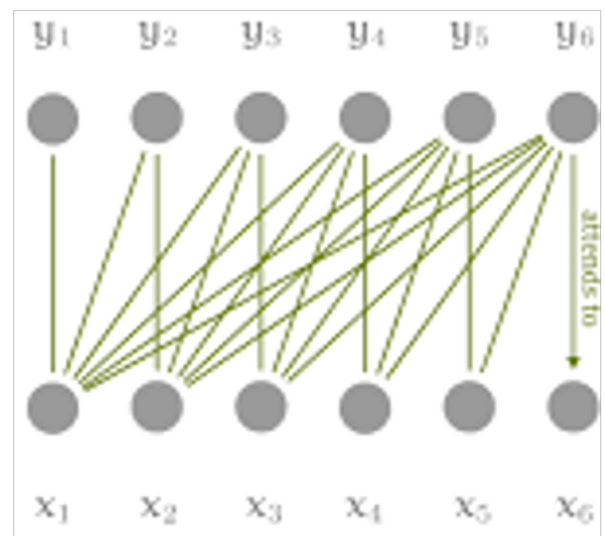


Masked Attention

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

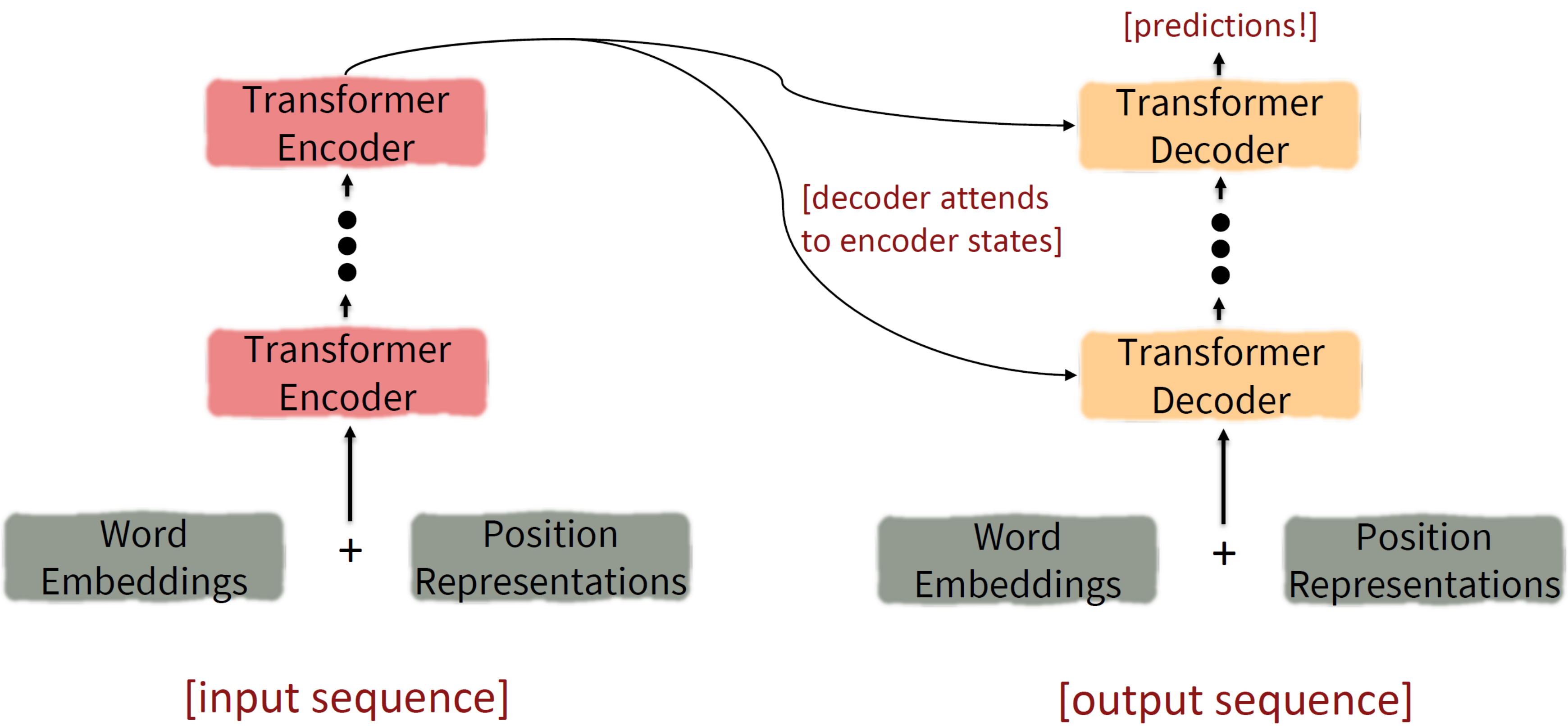
- Masked attention
  - Compute $e_{i,j} = q_i^\top k_j$ as usuall
  - Mask out $e_{i>j}$ by setting $e_{i>j} = -\infty$
    - $e \odot (1 - M) \leftarrow -\infty$
    - M is a fixed 0/1 mask matrix
  - Then compute $\alpha_i = \text{softmax}(e_i)$
  - Remarks:
    - $M = 1$ for full self-attention
 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





Transformer

Transformer-based sequence-to-sequence modeling



Key-query-value attention

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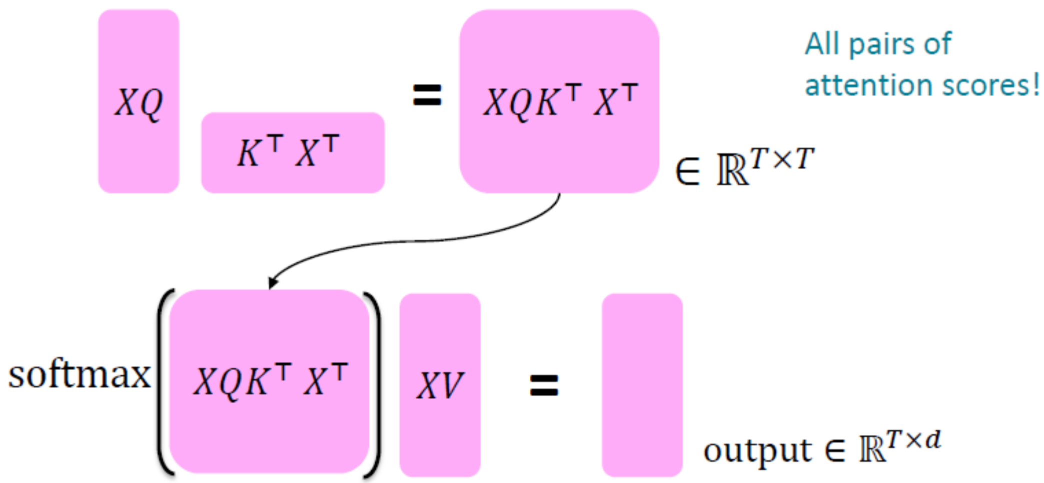
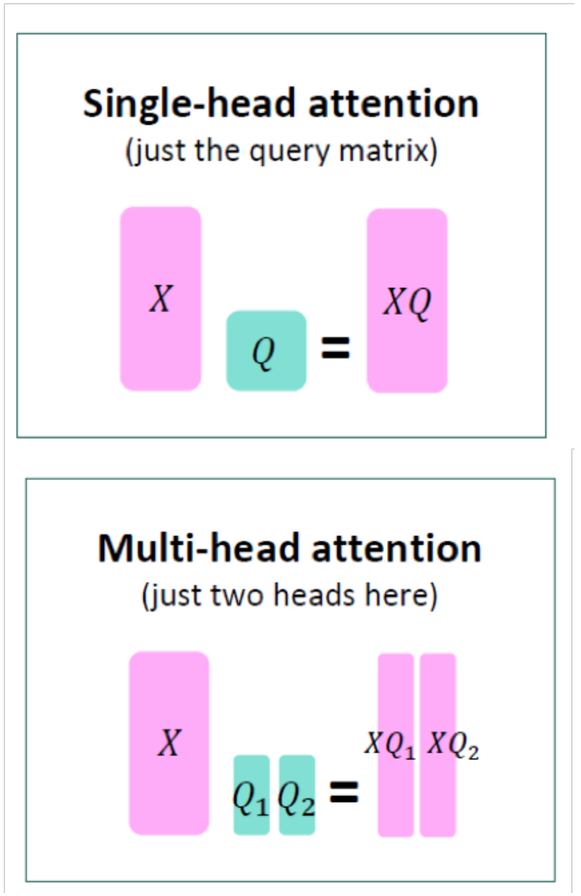


Multi-headed attention

- 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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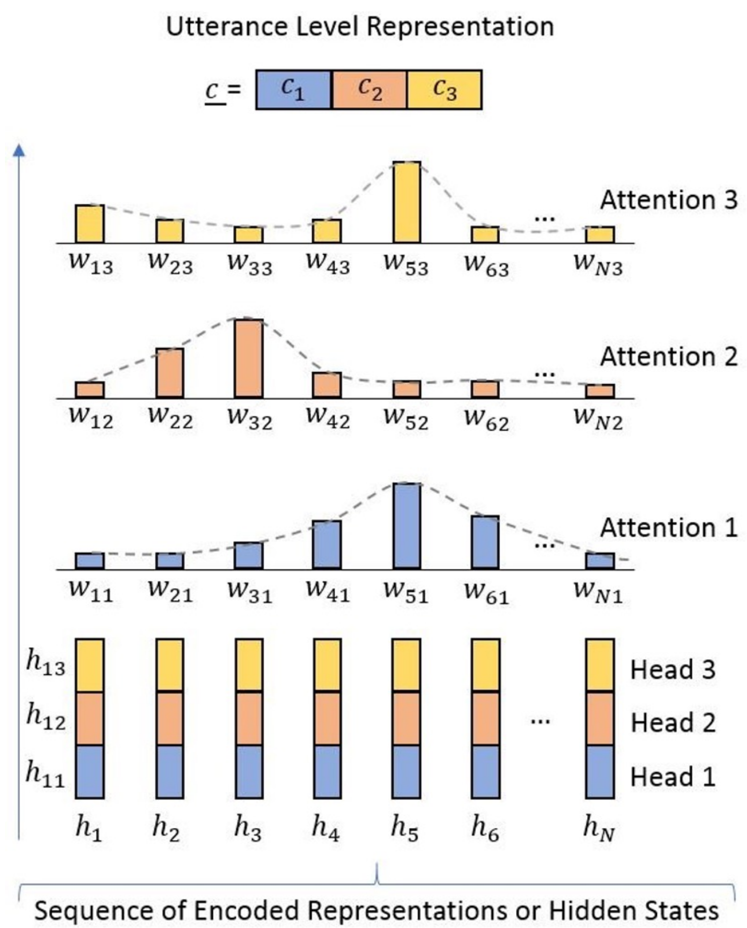
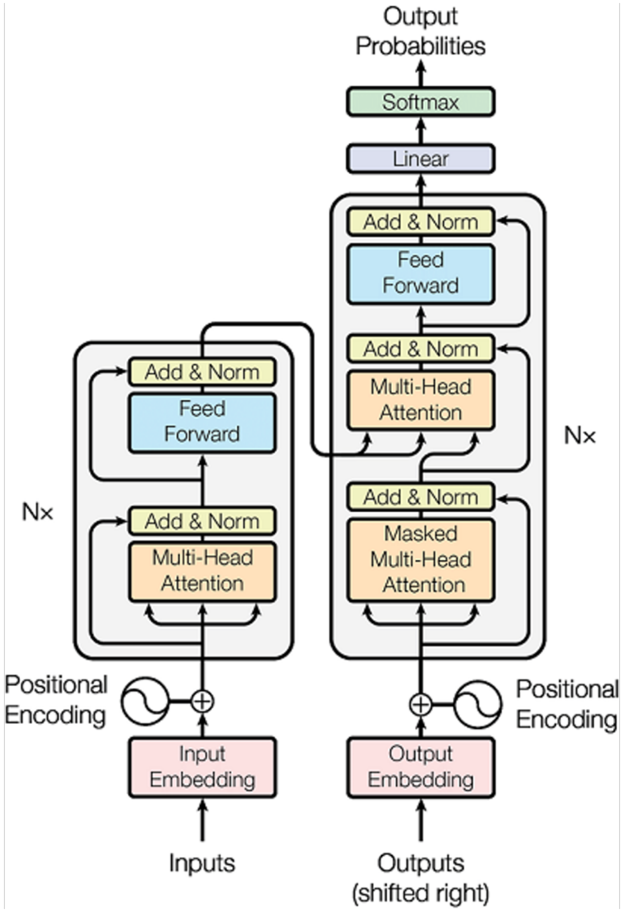


Transformer

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**	$2.3 \cdot 10^{19}$	

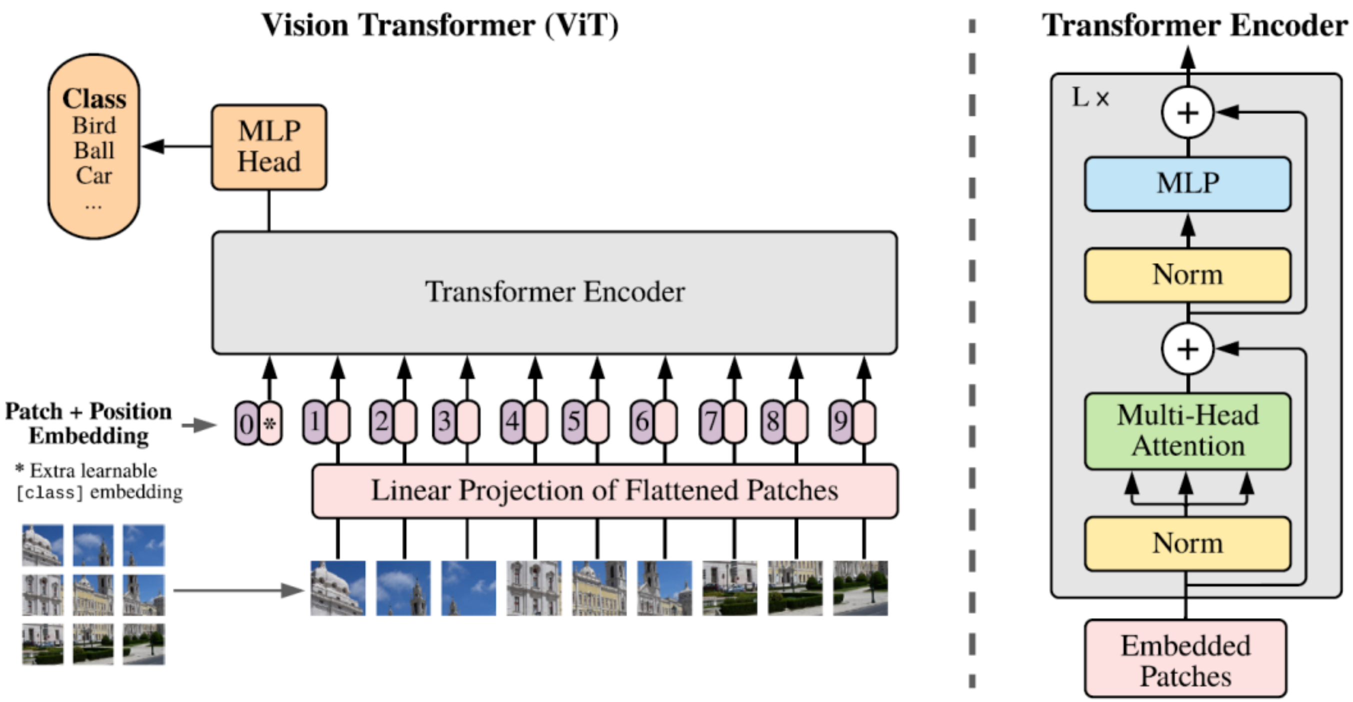
Transformer

- 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)

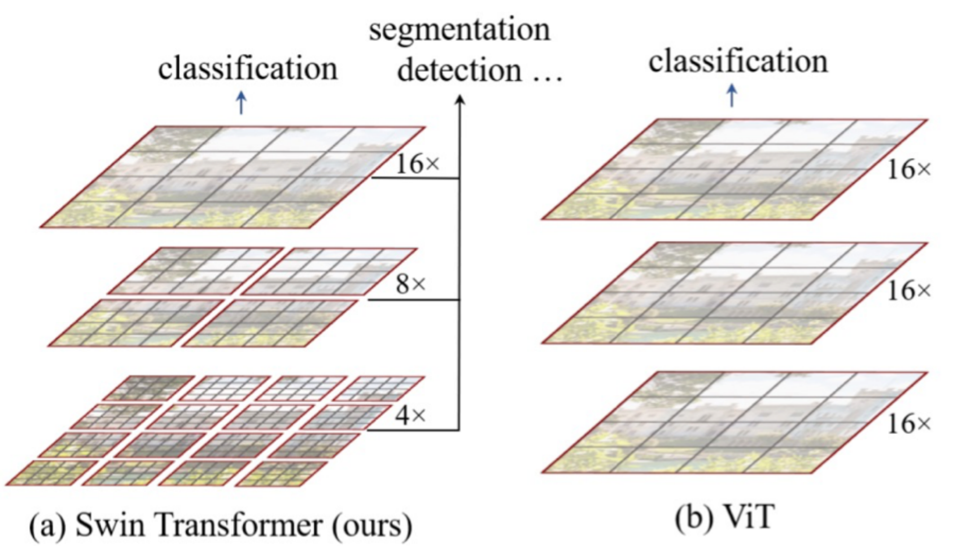
Transformer for Images

- 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



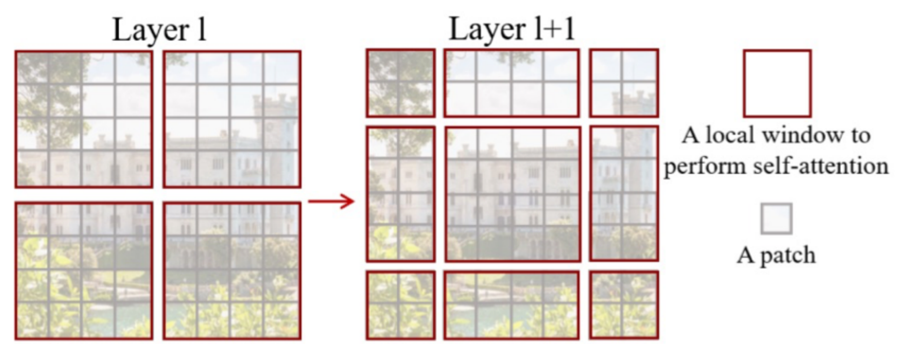
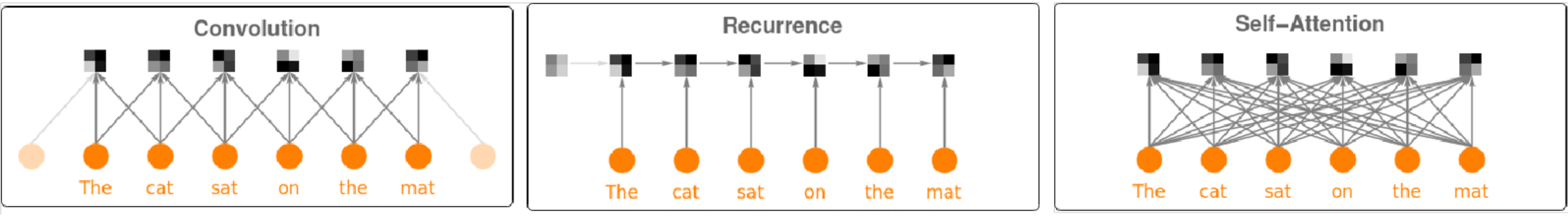


Figure 2. An illustration of the *shifted window* approach for com-

CNN vs. RNN vs. Attention



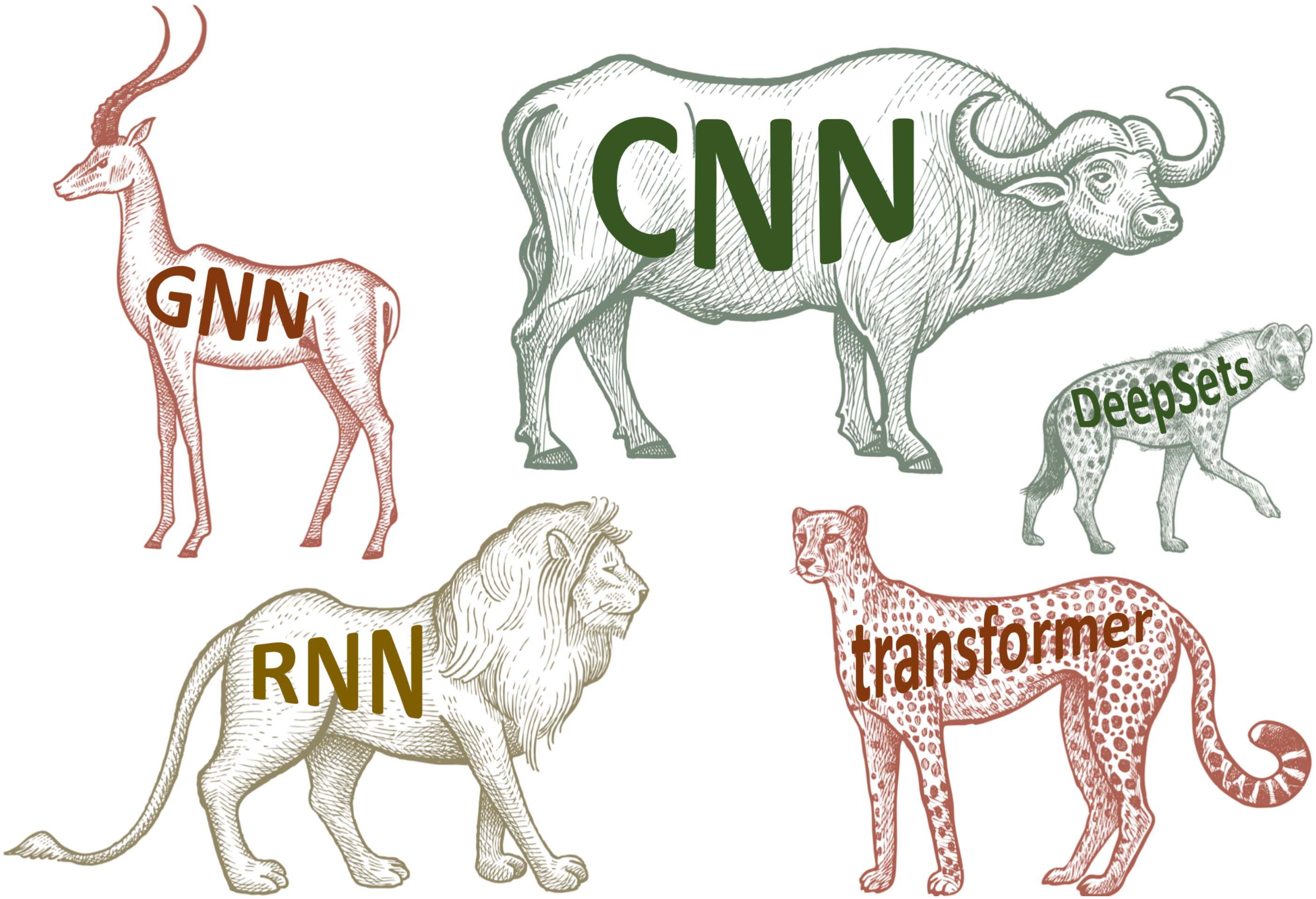
Summary

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

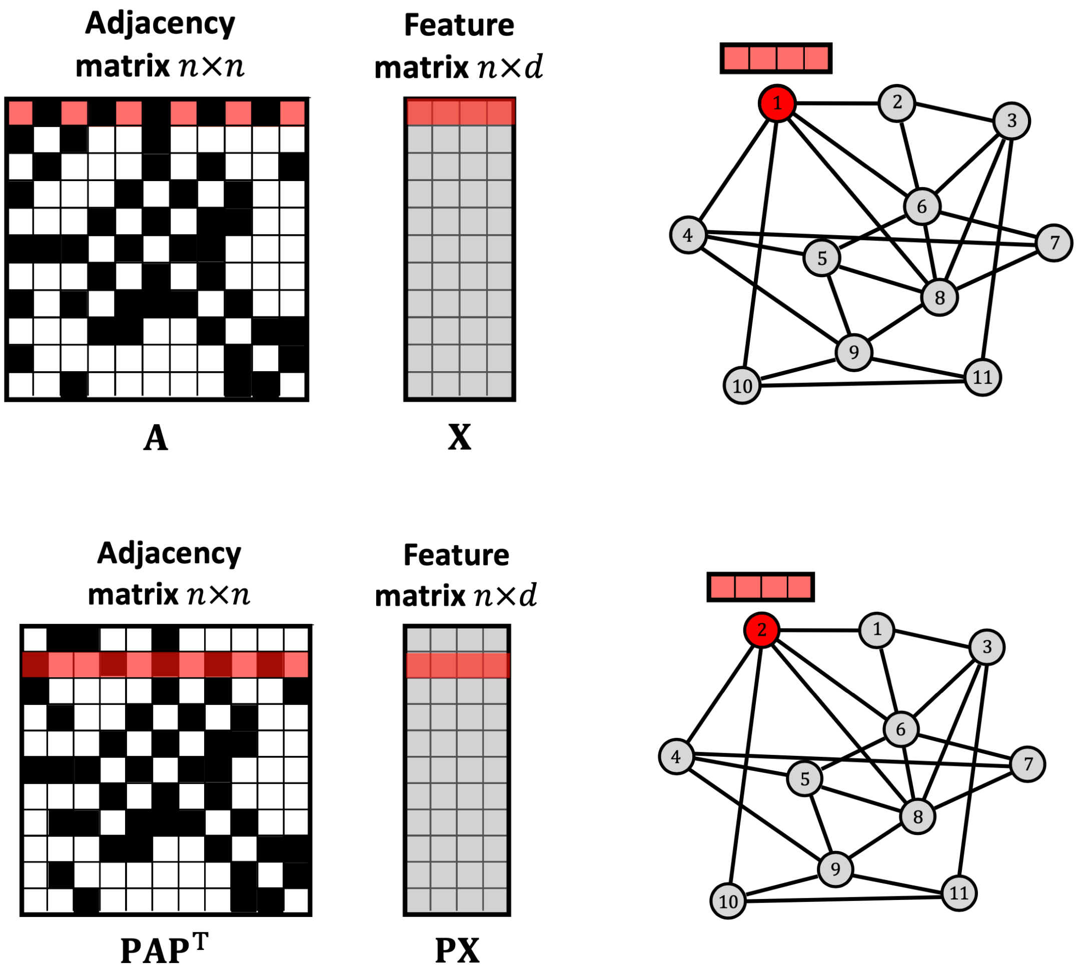
- Attention mechanism
  - So far the most successful idea for sequence data in deep learning
  - A scale/order-invariant representation
  - Transformer: a fully attention-based architecture for sequence data
  - Transformer + Pretraining: the core idea in today's NLP tasks

- LSTM is still useful in lightweight scenarios

Other architectures



Graph Neural Networks

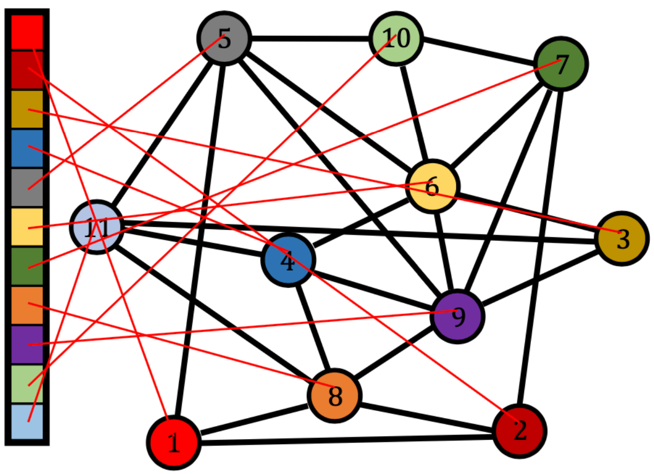


arbitrary ordering of nodes

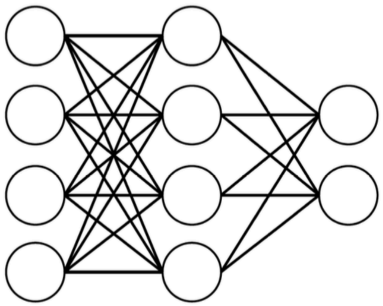
Graph Neural Networks

permutation-equivariant

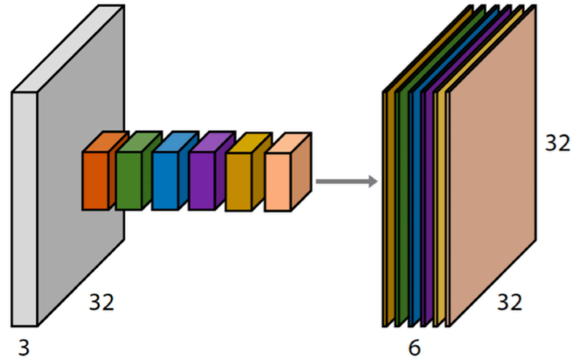
$$\mathbf{F}\left(\mathbf{PX}, \mathbf{PAP}^{\top}\right) = \mathbf{PF}(\mathbf{X}, \mathbf{A})$$



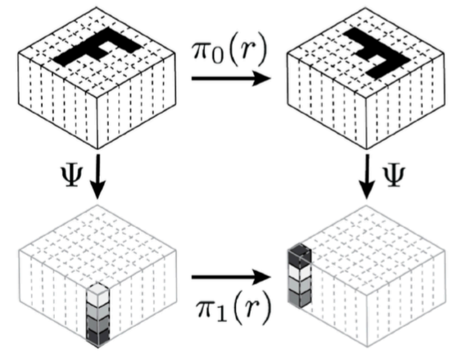
Geometric Deep Learning



Perceptrons
Function regularity

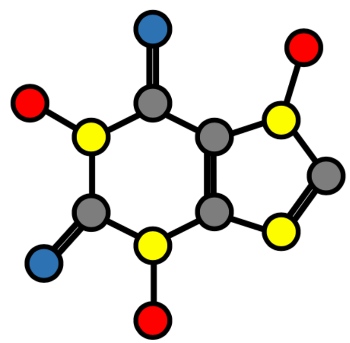


CNNs
Translation



Group-CNNs
Translation+Rotation

DeepSets / Transformers
Permutation

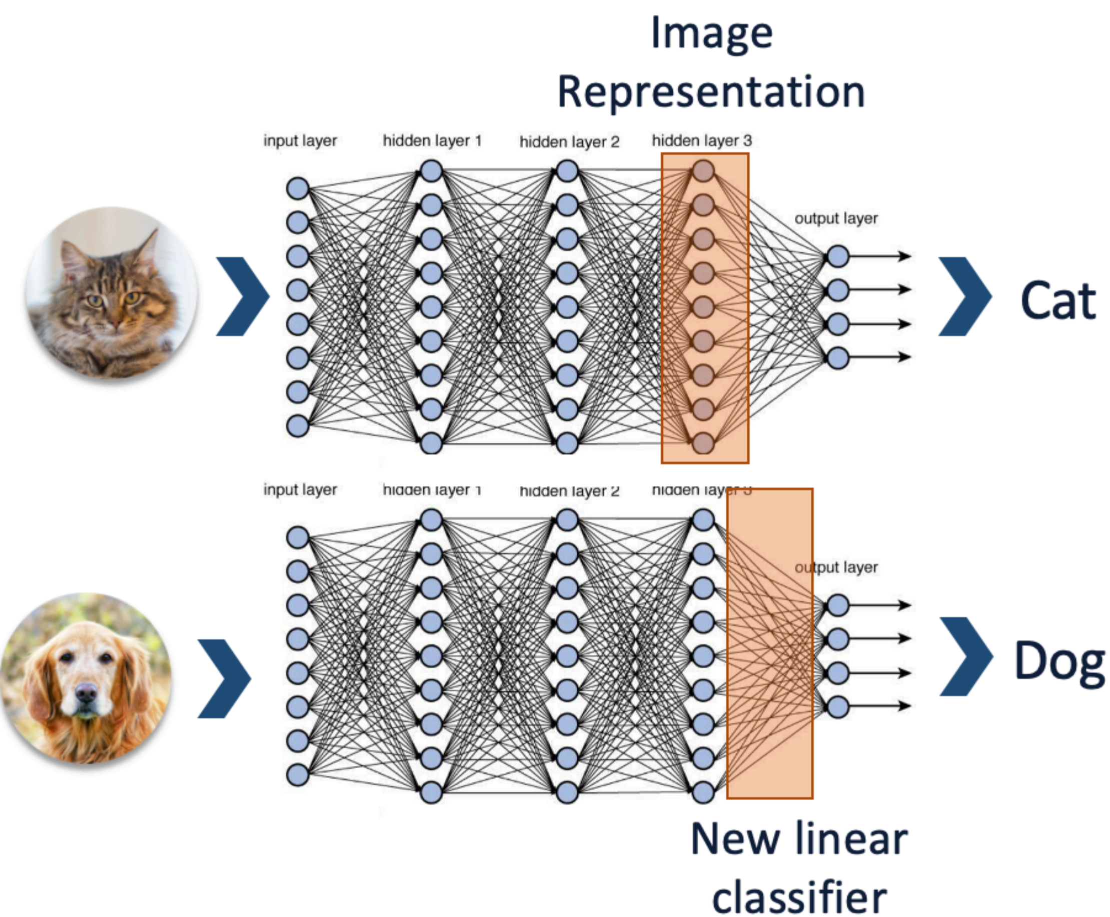


GNNs
Permutation

Intrinsic CNNs
Local frame choice

Representation Learning Pre-training

Example in image representation



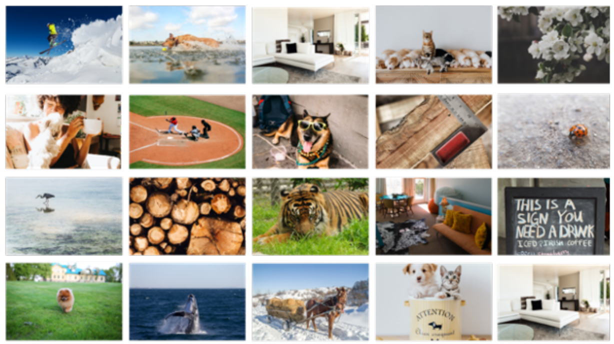
Train a neural network (ResNet) on ImageNet (1M data, 1000 classes)

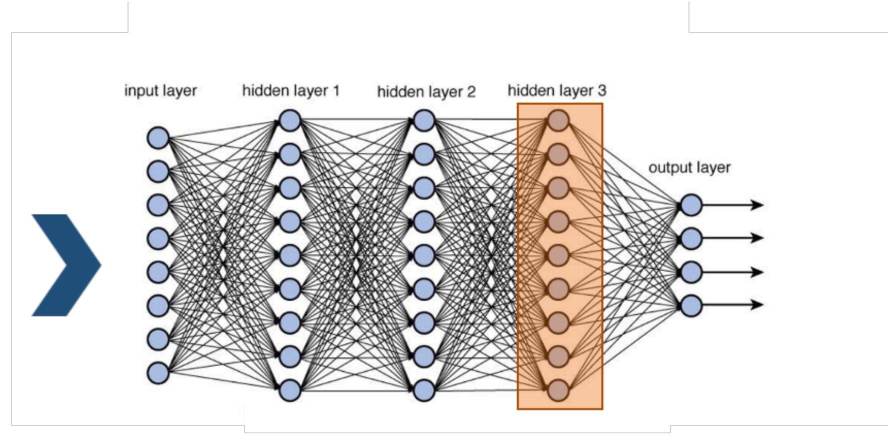
Representation (feature extractor): The mapping from image to the second-to-the-last layer.

Fix the representation, just re-train the last linear layer.

Example in image representation

Source tasks (for training representation): ImageNet



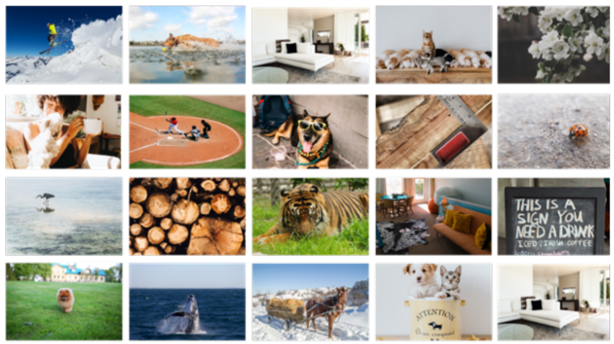


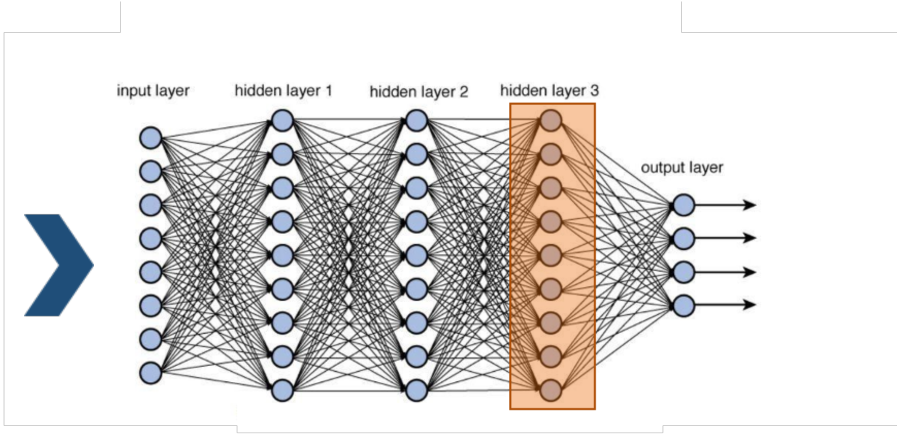
Target task: Few-shot Learning on VOC07 dataset (20 classes, 1-8 examples per class)

- Without representation learning: **5% - 10%** (random guess = **5%)**
- With representation learning: **50% - 80%**

Example in image representation

Source tasks (for training representation): ImageNet





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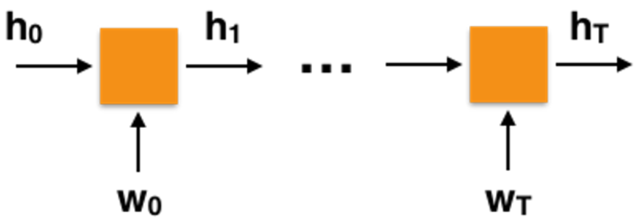
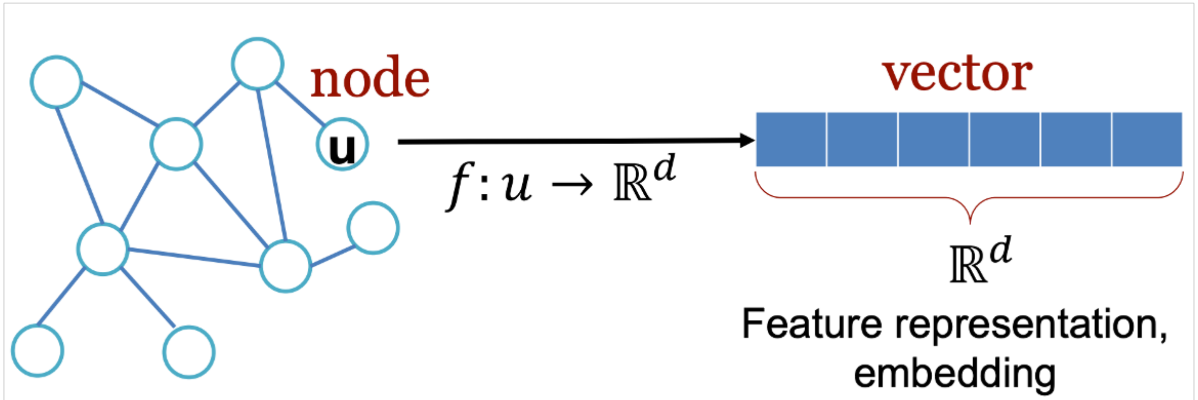
Examples

Natural Language Processing

Final hidden state: Sentence representation



Graph Representation Learning



Representation learning

- A function that maps the raw input to a compact representation (feature vector). Learn an **embedding / feature / representation** from **labeled/unlabeled data.**
- Supervised:
  - Multi-task learning
  - Meta-learning
  - Multi-modal learning
  - …
- Unsupervised:
  - PCA
  - ICA
  - Dictionary learning
  - Sparse coding
  - Boltzmann machine
  - Autoencoder
  - Contrastive learning
  - Self-supervised learning
  - …

Desiderata for representations

Many possible answers here.

- **Downstream usability:** the learned features are "useful" for downstream tasks:
  - Example: a linear (or simple) classifier applied on the learned features only requires a small number of labeled samples. A classifier on raw inputs requires a large mount of data.

- **Interpretability:** the learned features are semantically meaningful, interpretable by a human, can be easily evaluated.
  - Not well-defined mathematically.
  - **Sparsity** is an important subcase.

Desiderata for representations

From Bengio, Courville, Vincent ’14:

- **Hierarchy / compositionality:** video/image/text are expected to have hierarchial structure: need *deep* learning.

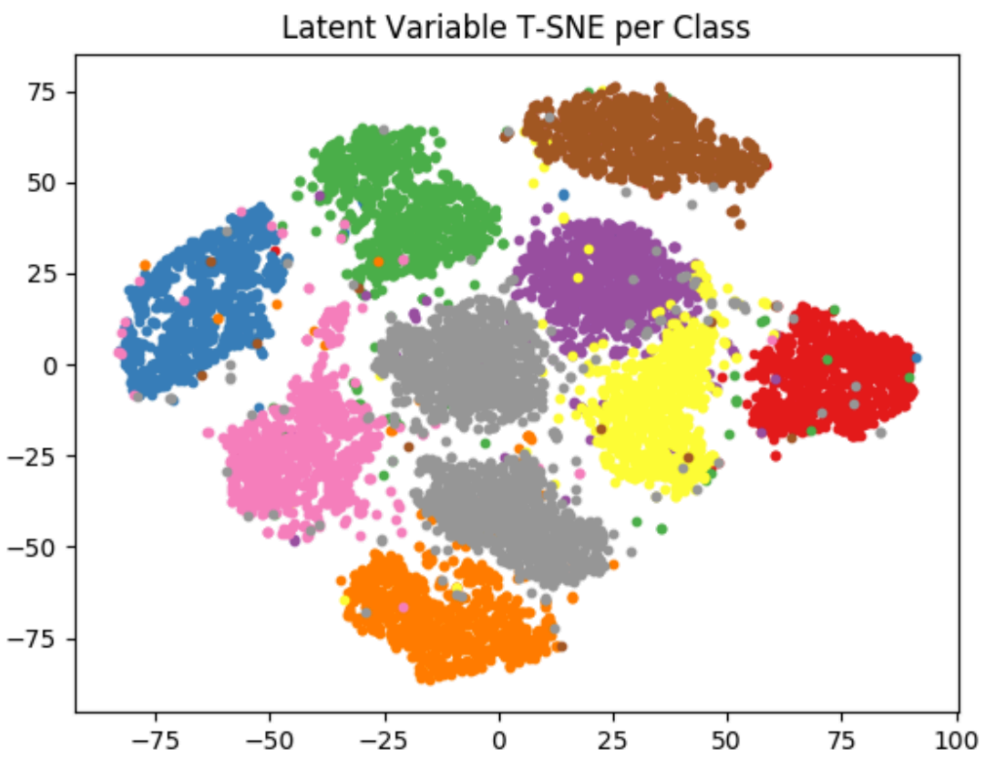
- **Semantic clusterability**: features of the same “semantic class” (e.g. images in the same class) are clustered together.

- **Linear interpolation**: in the representation space, linear interpolations produce meaningful data points (latent space is convex). Also called *manifold flattening.*

- **Disentanglement**: features capture “independent factors of variation” of data. A popular principle in modern unsupervised learning.

Semantic clustering

Semantic clusterability: features of the same “semantic class” (e.g. images in the same class) are clustered together.

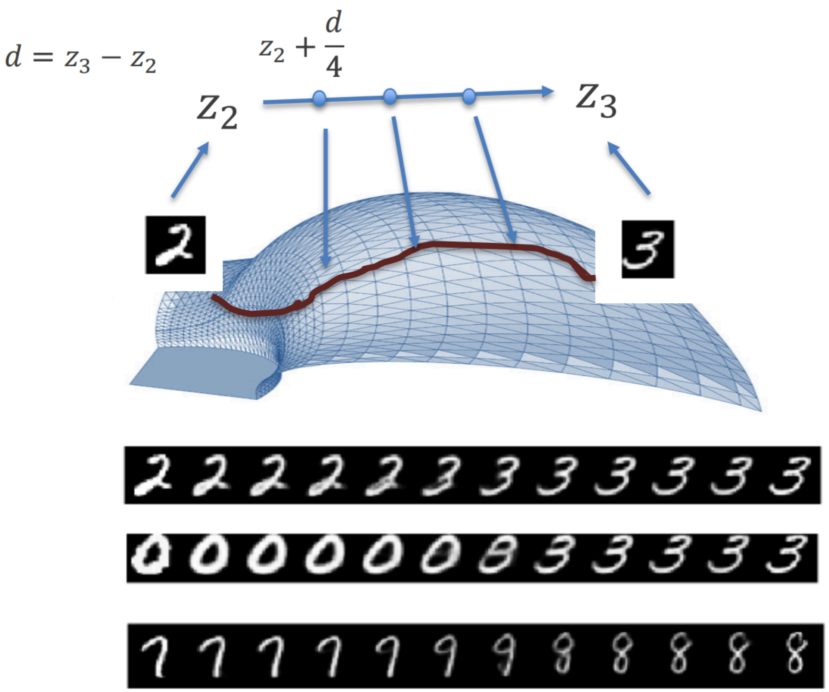


Intuition: If semantic classes are linearly separable, and labels on downstreams tasks depend linearly on semantic classes: we only need to learn a simple classifer.

t-SNE projection (a data visualization method) of VAE-learned features of 10 MNIST classes.

Linear interpolation

Linear interpolation: in the representation space, linear interpolations produce meaningful data points (latent space is convex).



Intuition: the data lies on a manifold which is complicated/ curved.

The latent variable manifold is a convex set: moving in straight lies is still on it.

Interpolations for a VAE trained feature on MNIST.

Linear interpolation

Linear interpolation: in the representation space, linear interpolations produce meaningful data points (latent space is convex).

Interpolations for a BigGAN image.

Disentanglement

Disentanglement: features capture "independent factors of variation" of data (Bengio, Courville, Vincent '14).

- Very popular in modern unsupervised learning.
- Strong connections with generative models: $p_\theta(z) = \Pi_i p_\theta(z_i)$.

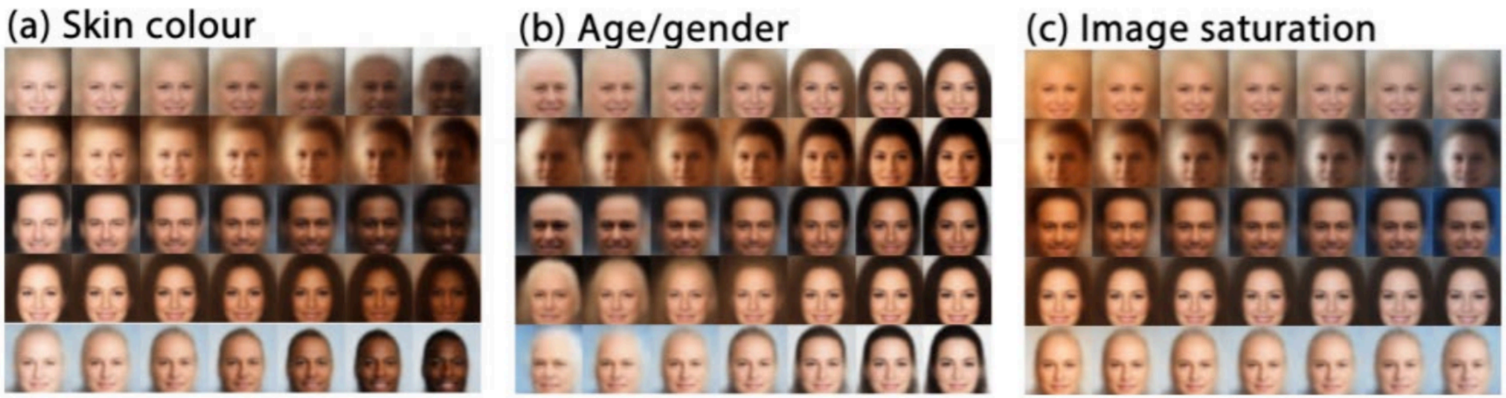


Figure 4: **Latent factors learnt by β-VAE on celebA:** traversal of individual latents demonstrates that β-VAE discovered in an unsupervised manner factors that encode skin colour, transition from an elderly male to younger female, and image saturation.