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)

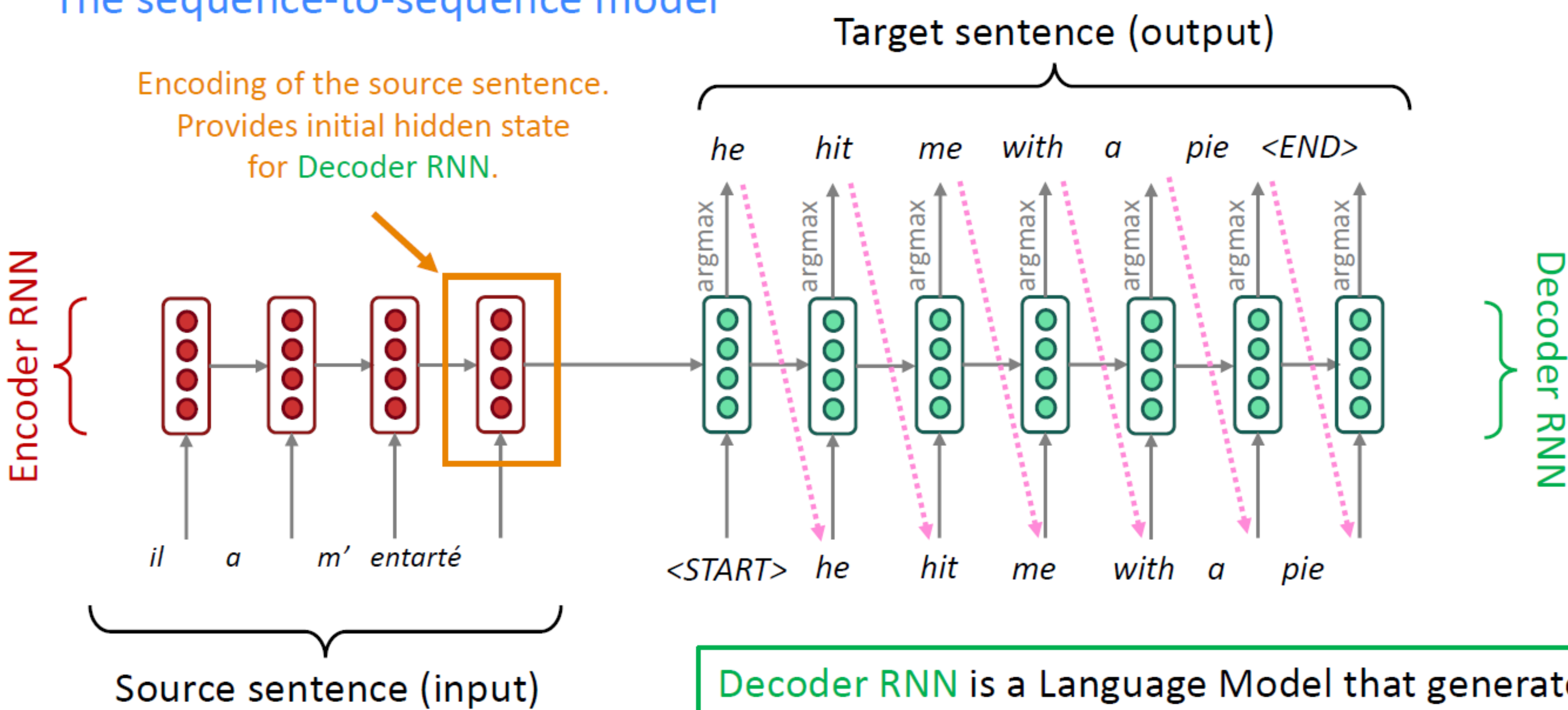
Sequence to Sequence Model

- 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

The sequence-to-sequence model



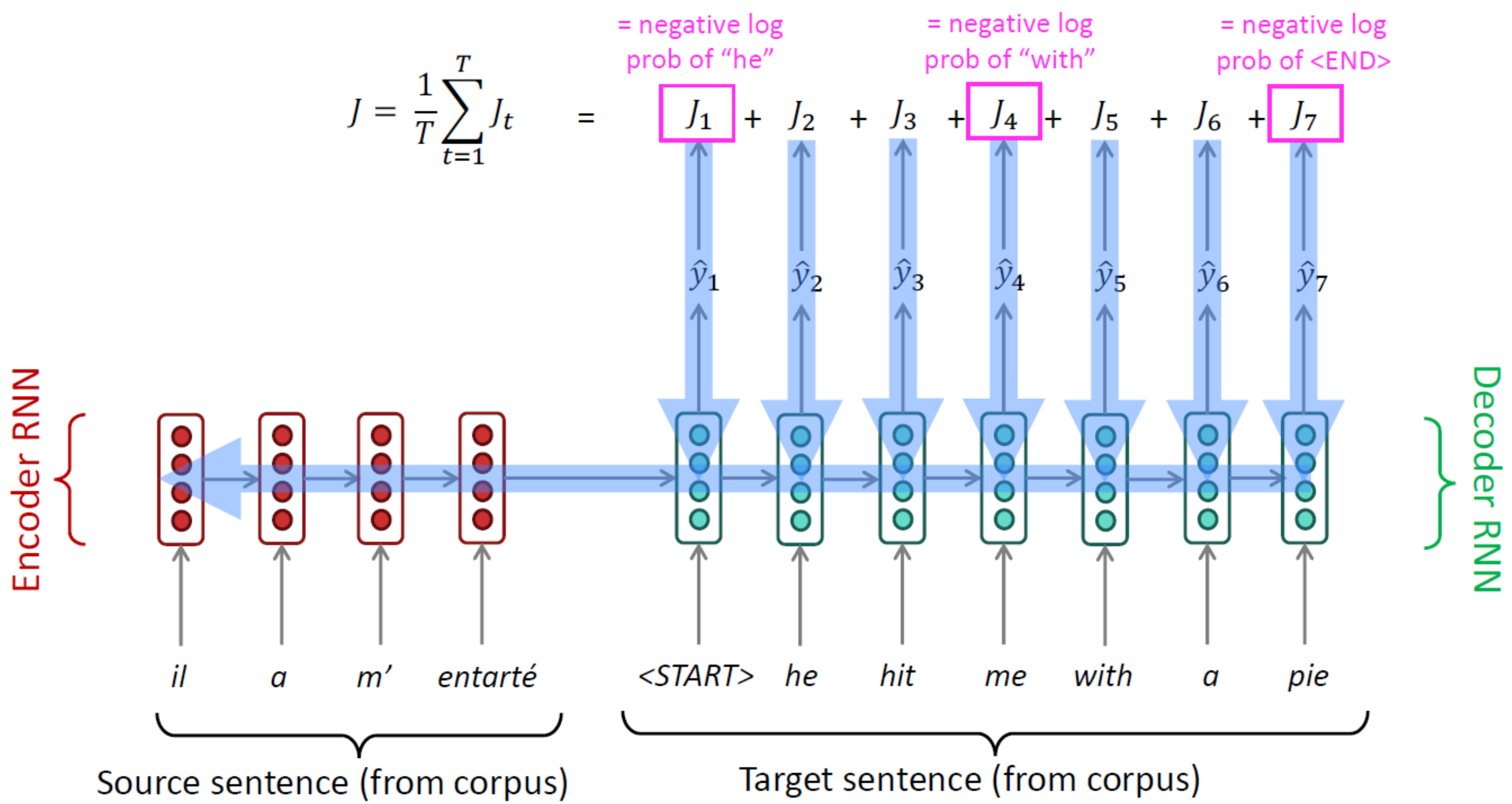
Encoder RNN produces an encoding of the source sentence.

Decoder RNN is a Language Model that generates target sentence, *conditioned on encoding*.

Note: This diagram shows **test time** behavior: decoder output is fed in as next step's input

Training Sequence to Sequence Model

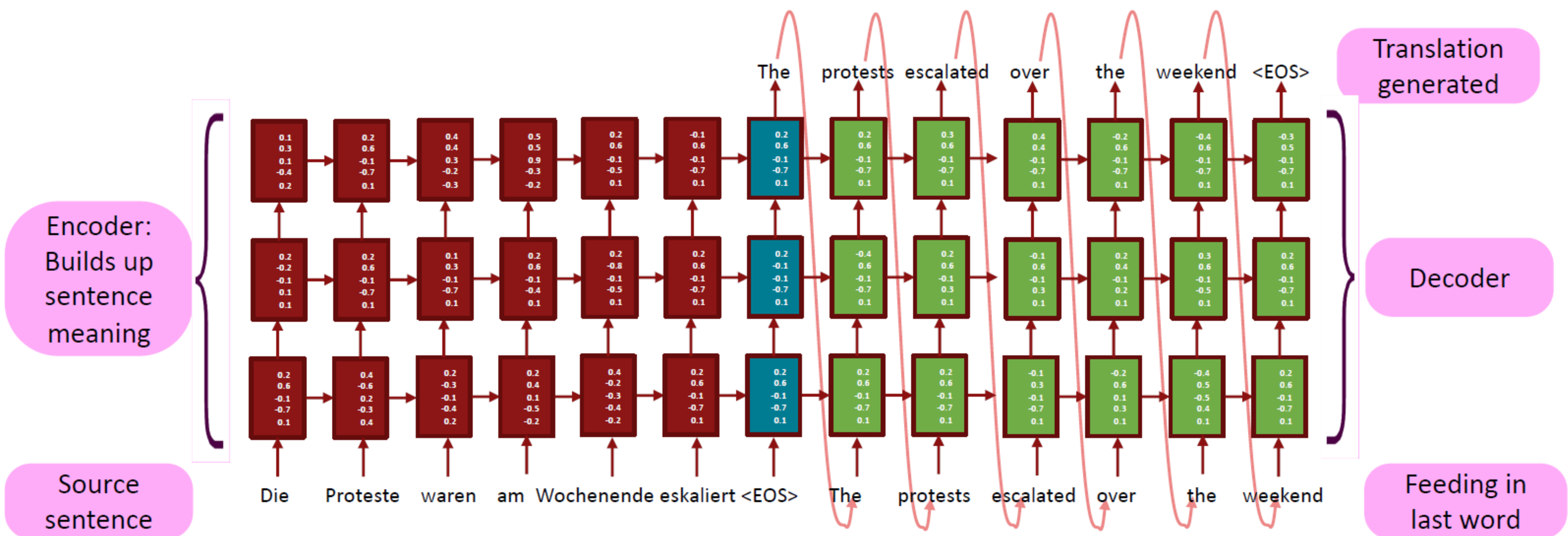
- Collect a huge paired dataset and train it end-to-end via BPTT
- Loss induced by MLE $P(Y|X) = P(Y|f_{enc}(X))$



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

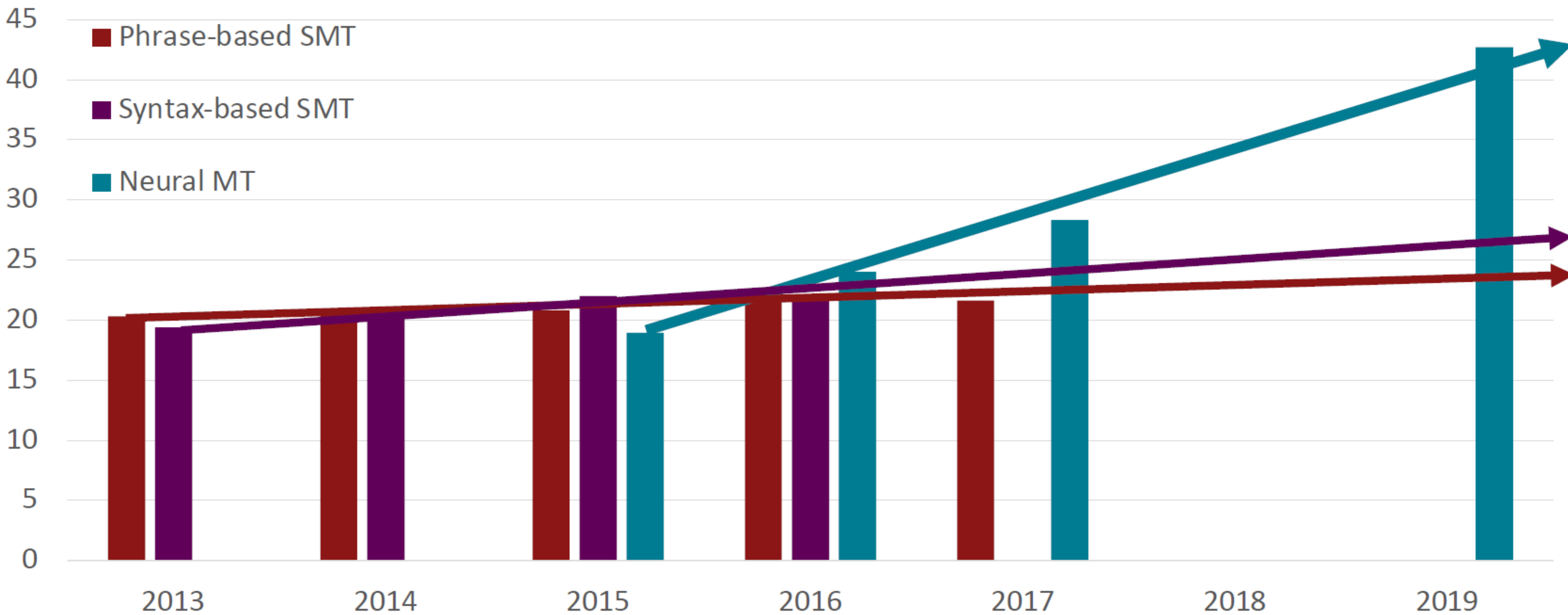
Deep Sequence to Sequence Model

- Stacked seq2seq model



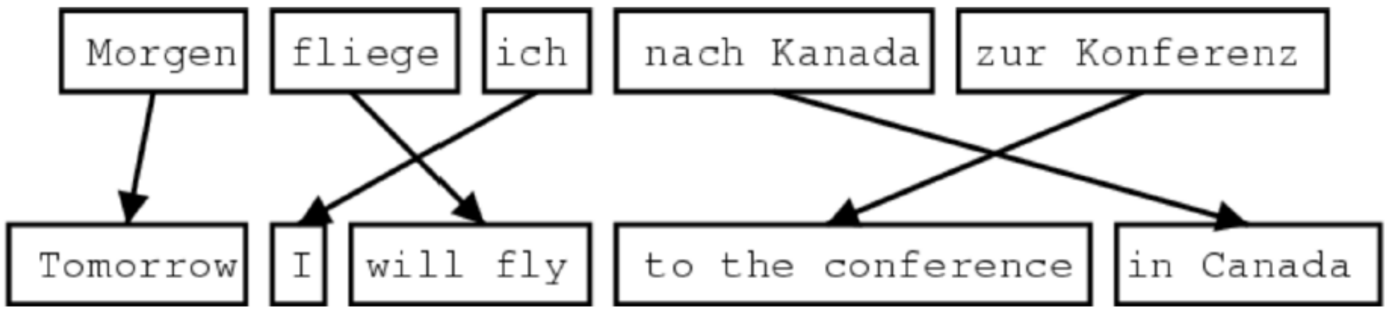
Machine Translation

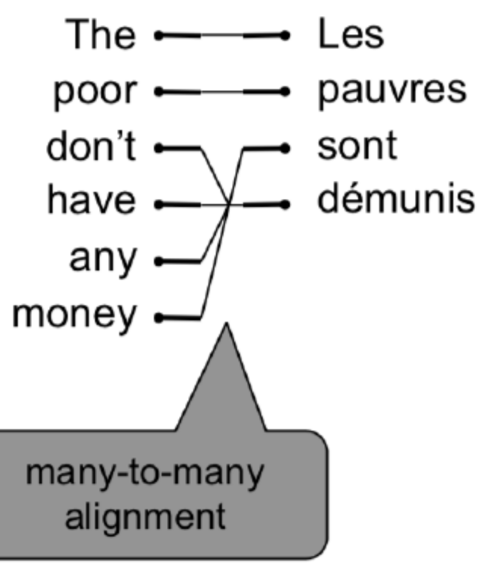
- 2016: Google switched Google Translate from SMT to NMT

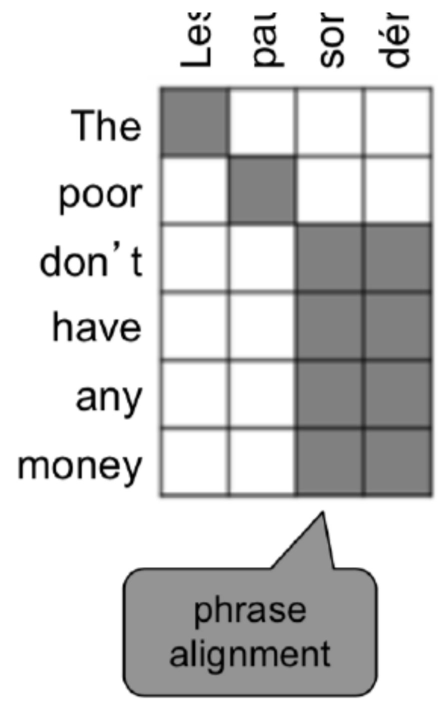


Alignment

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

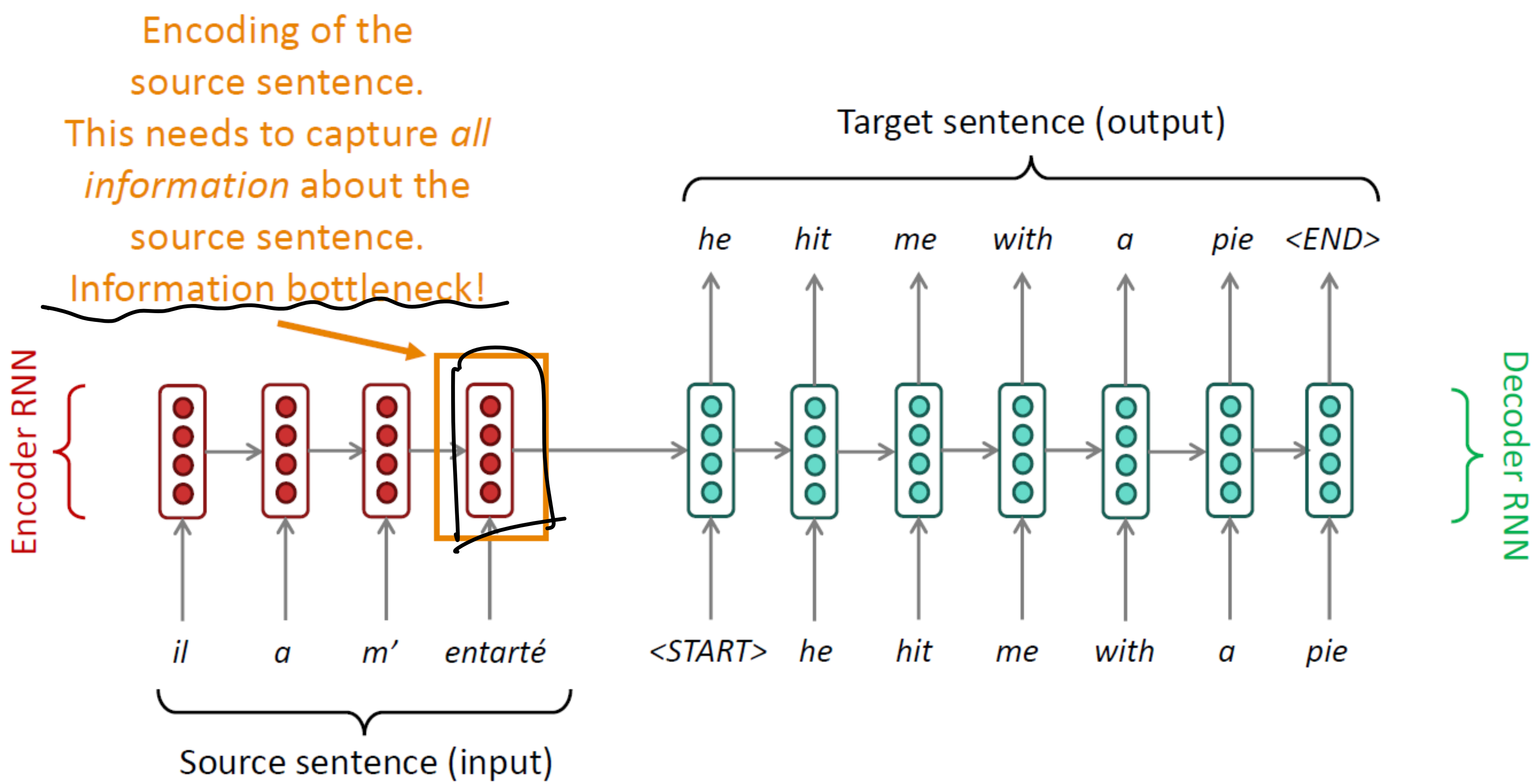






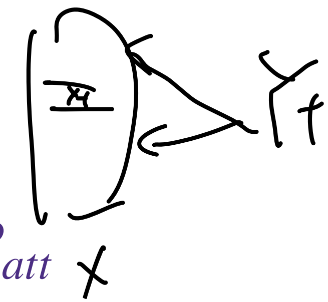
Issue in Seq2Seq

- 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

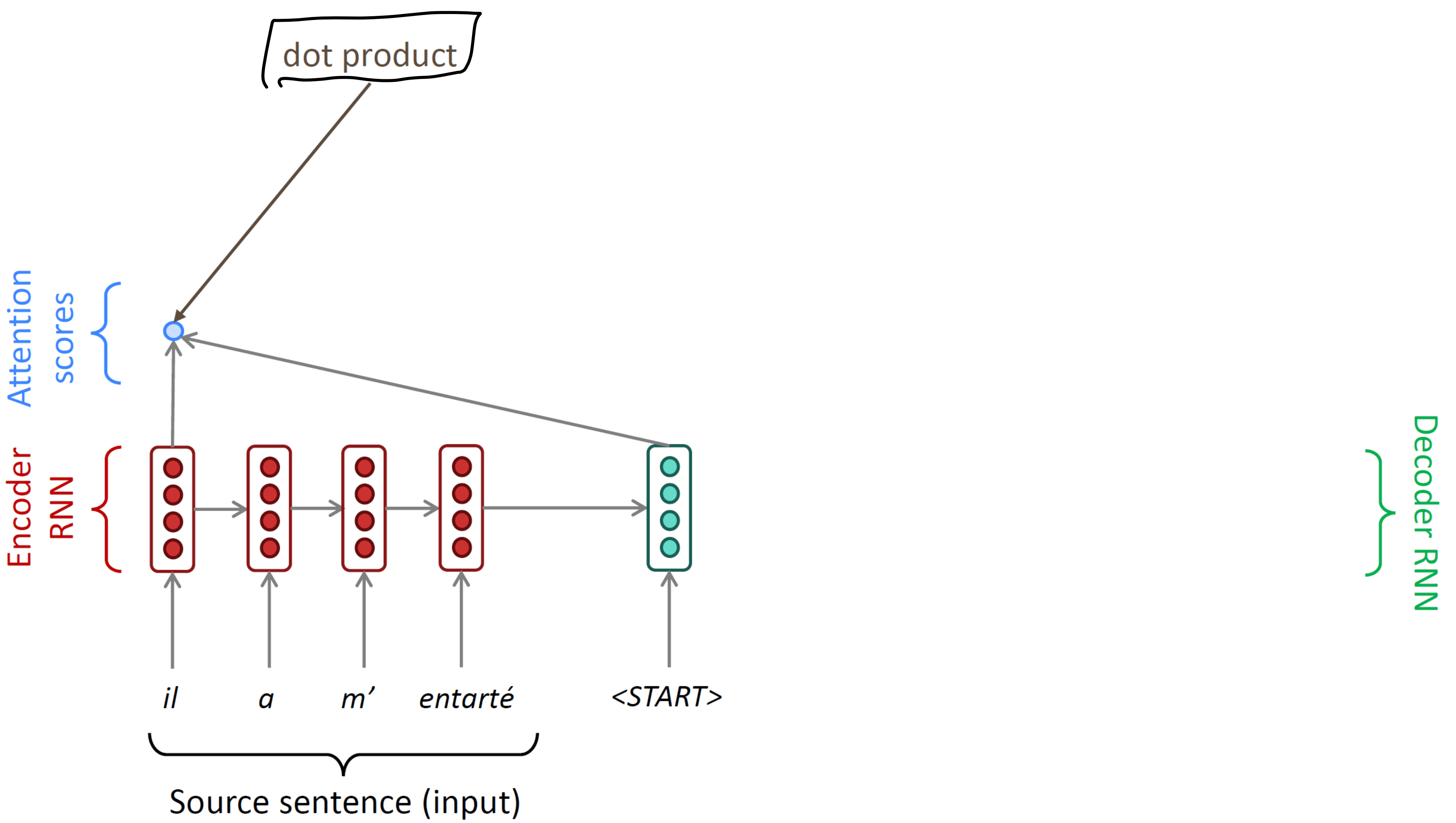


Seq2Seq with Attention

- 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



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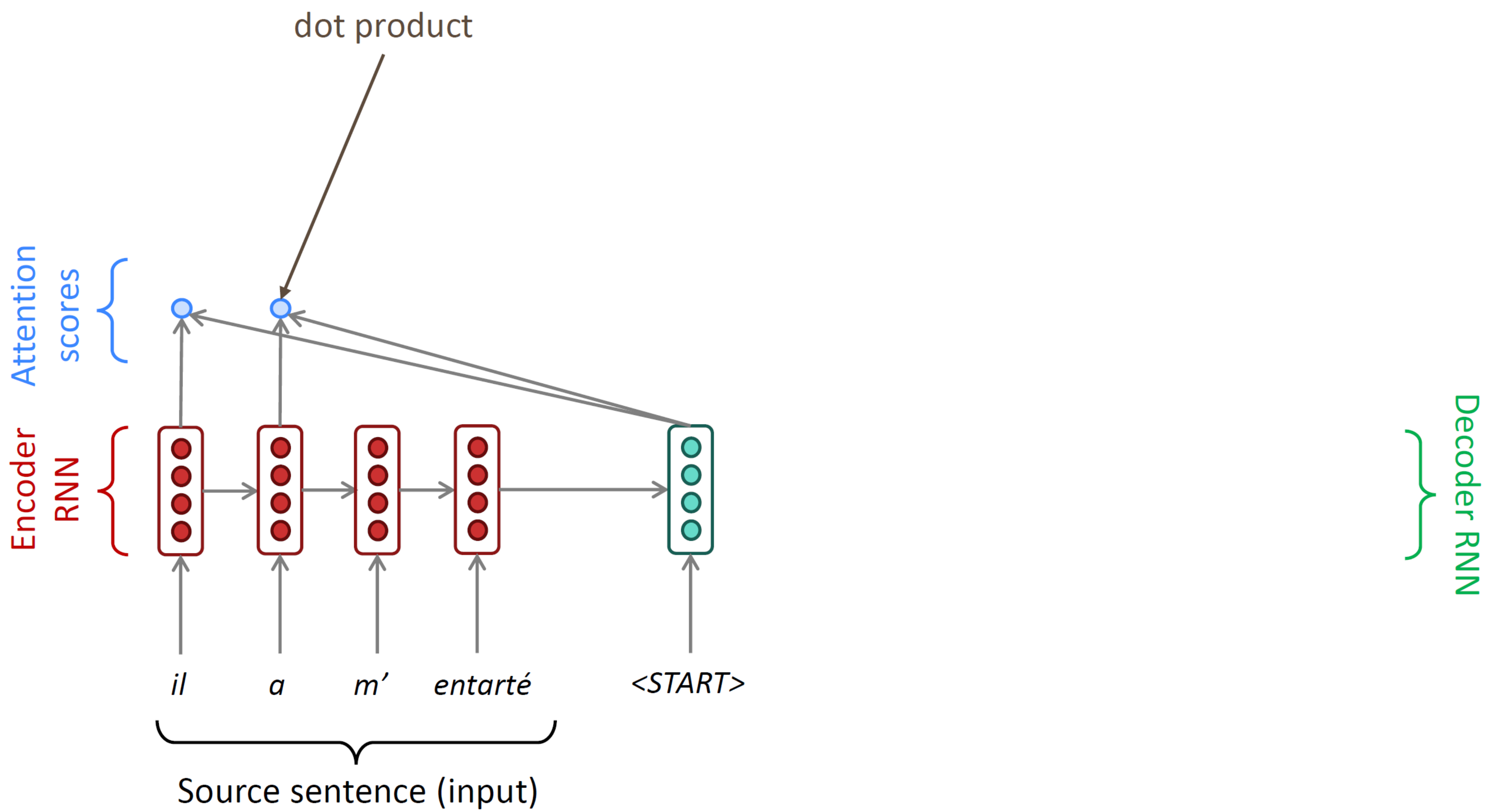
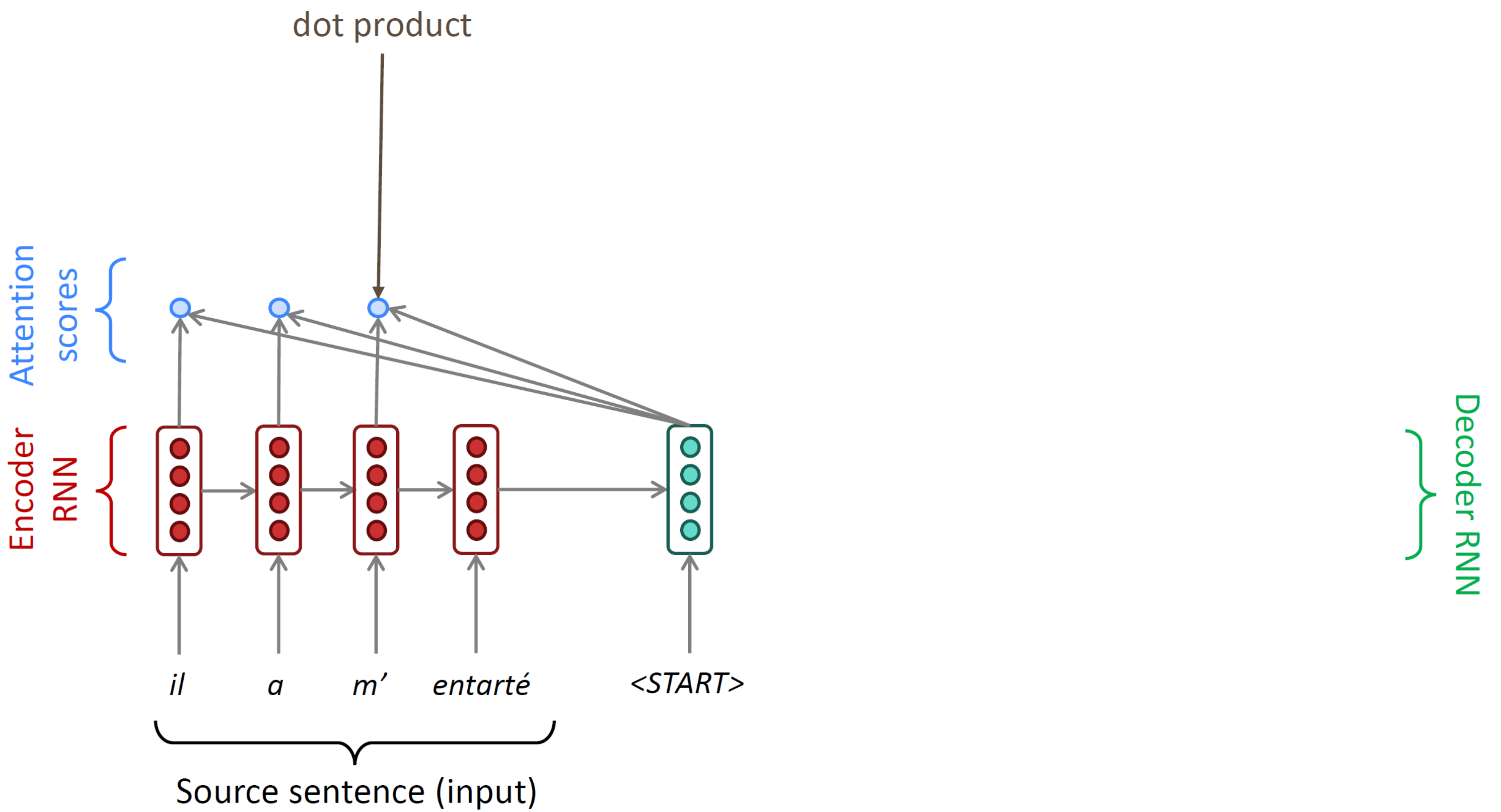
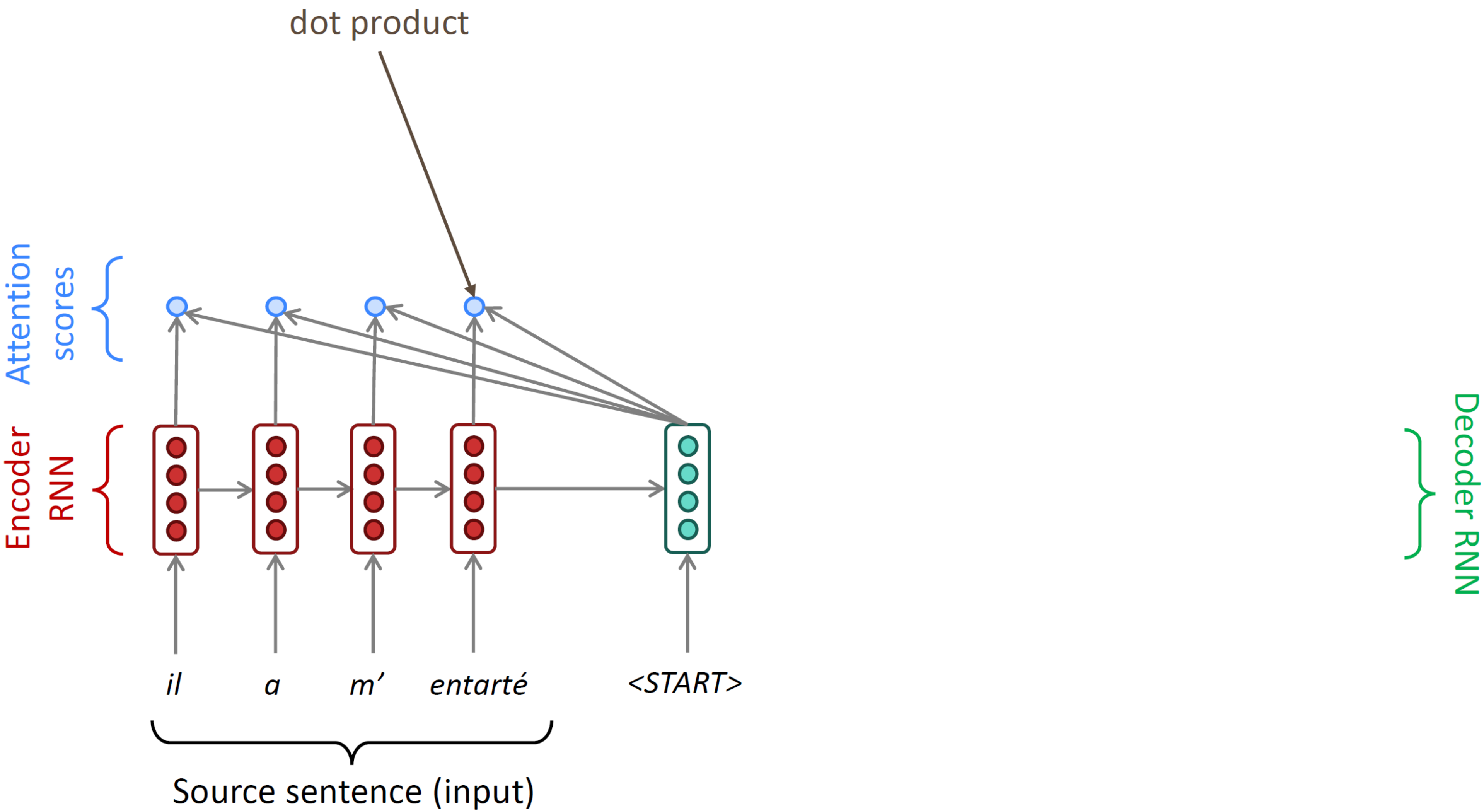


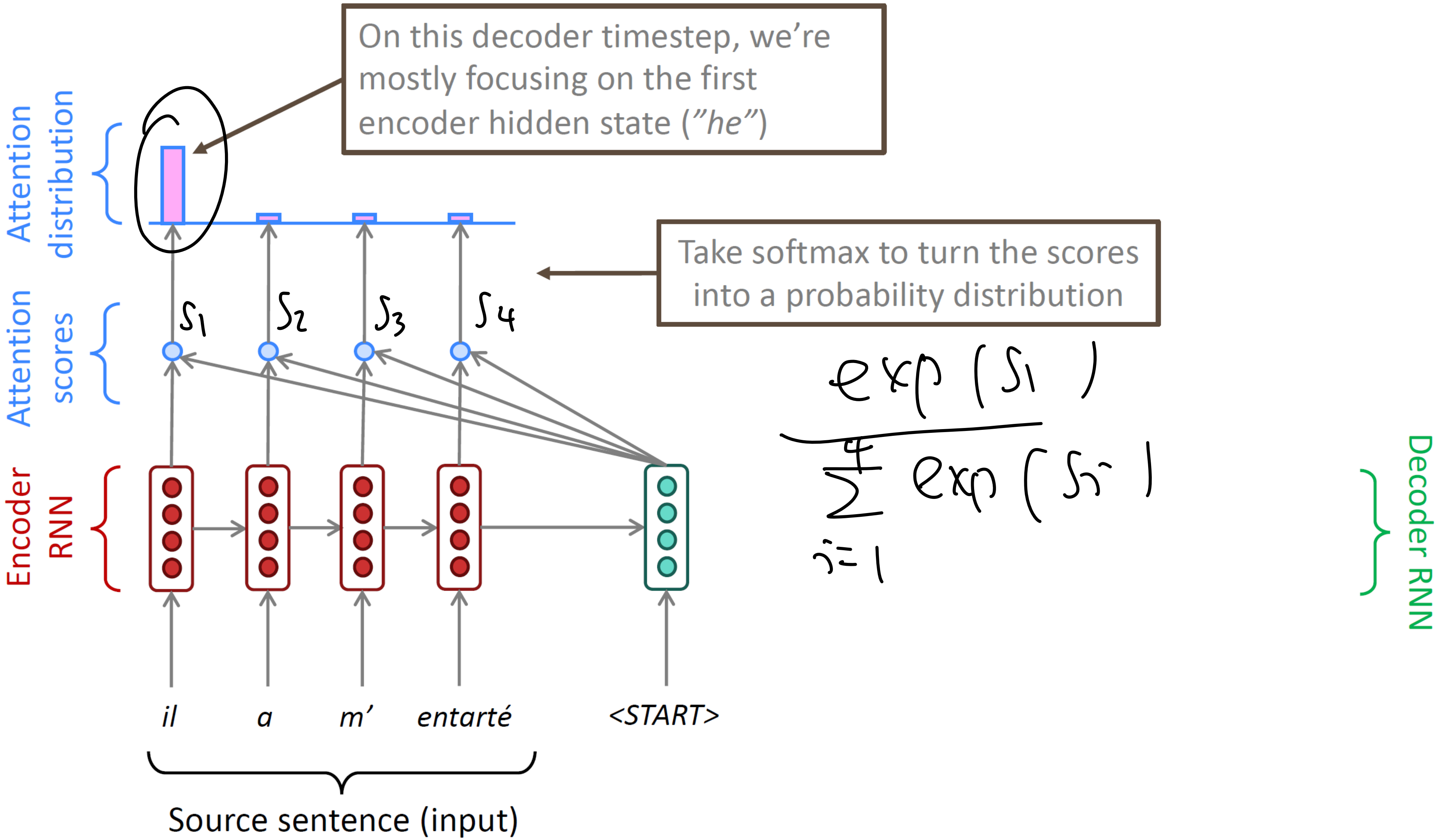
Seq2Seq with Attention



Seq2Seq with Attention

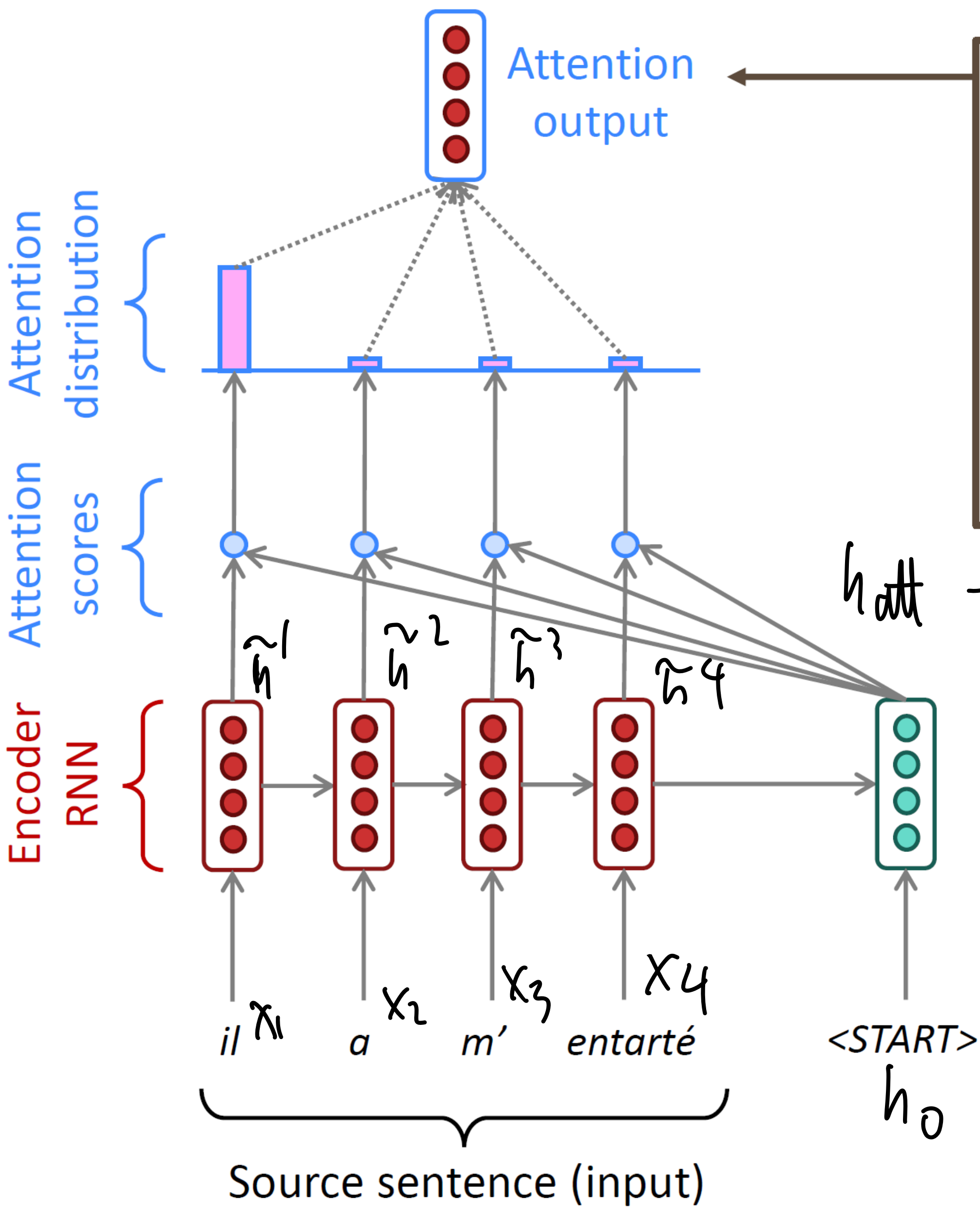


Seq2Seq with Attention



$$\frac{\exp(s_1)}{\sum_{j=1}^{4} \exp(s_j)}$$

Seq2Seq with Attention

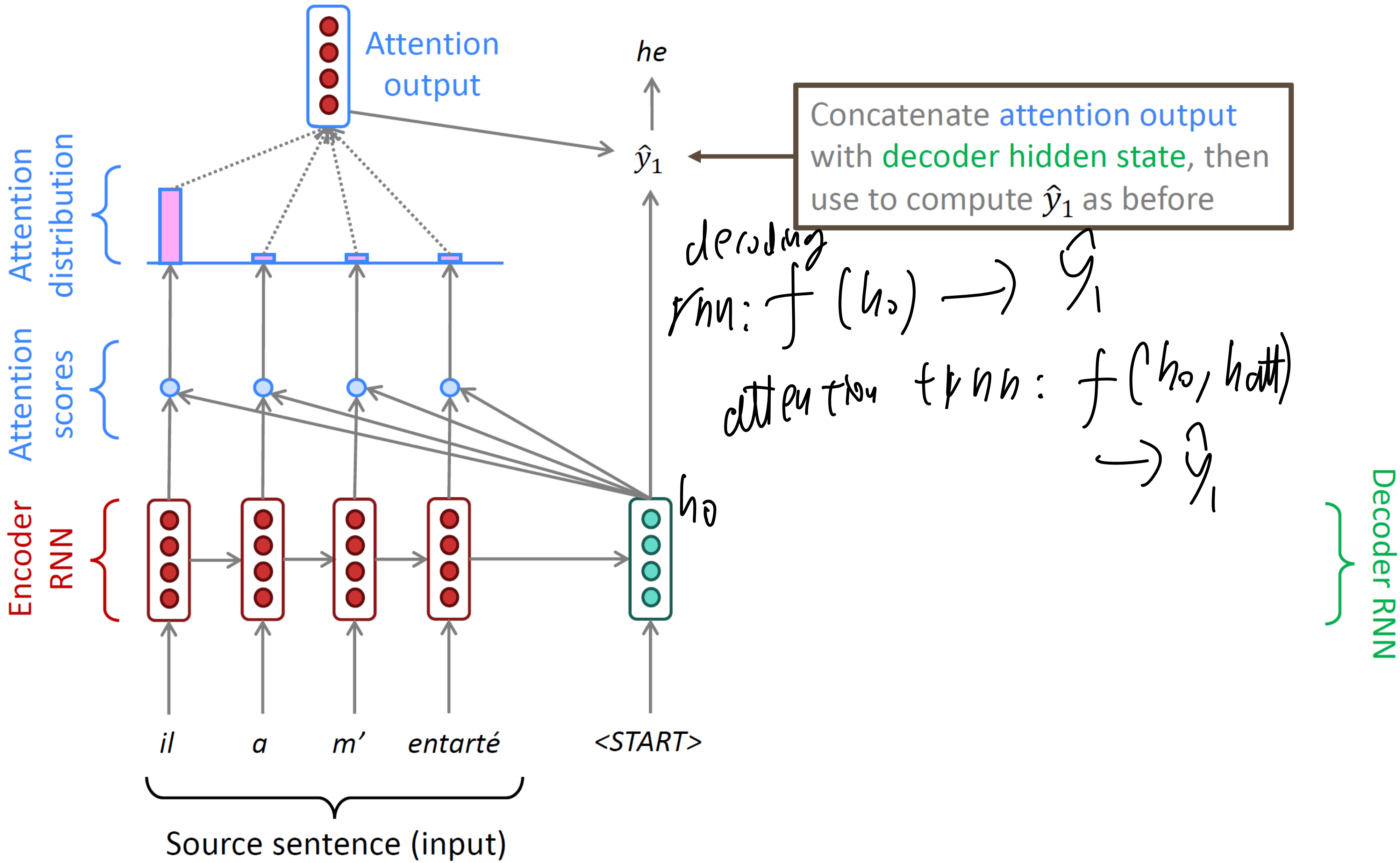


Use the attention distribution to take a **weighted sum** of the encoder hidden states.

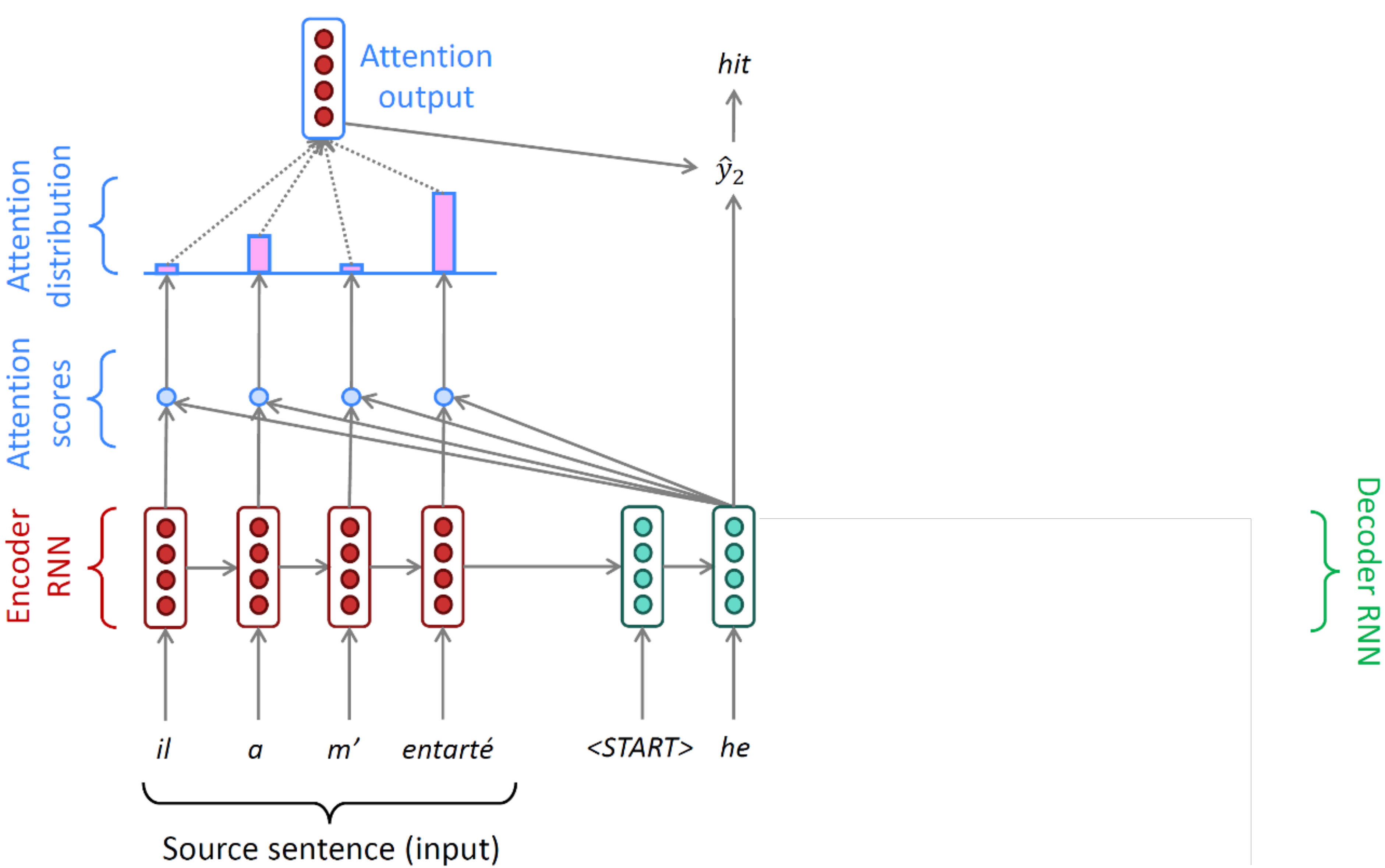
The attention output mostly contains information from the hidden states that received high attention.

$$h_{att} = \sum_{i=1}^{4} P_{att}(x_i \mid h_0) \cdot \tilde{h}_i$$

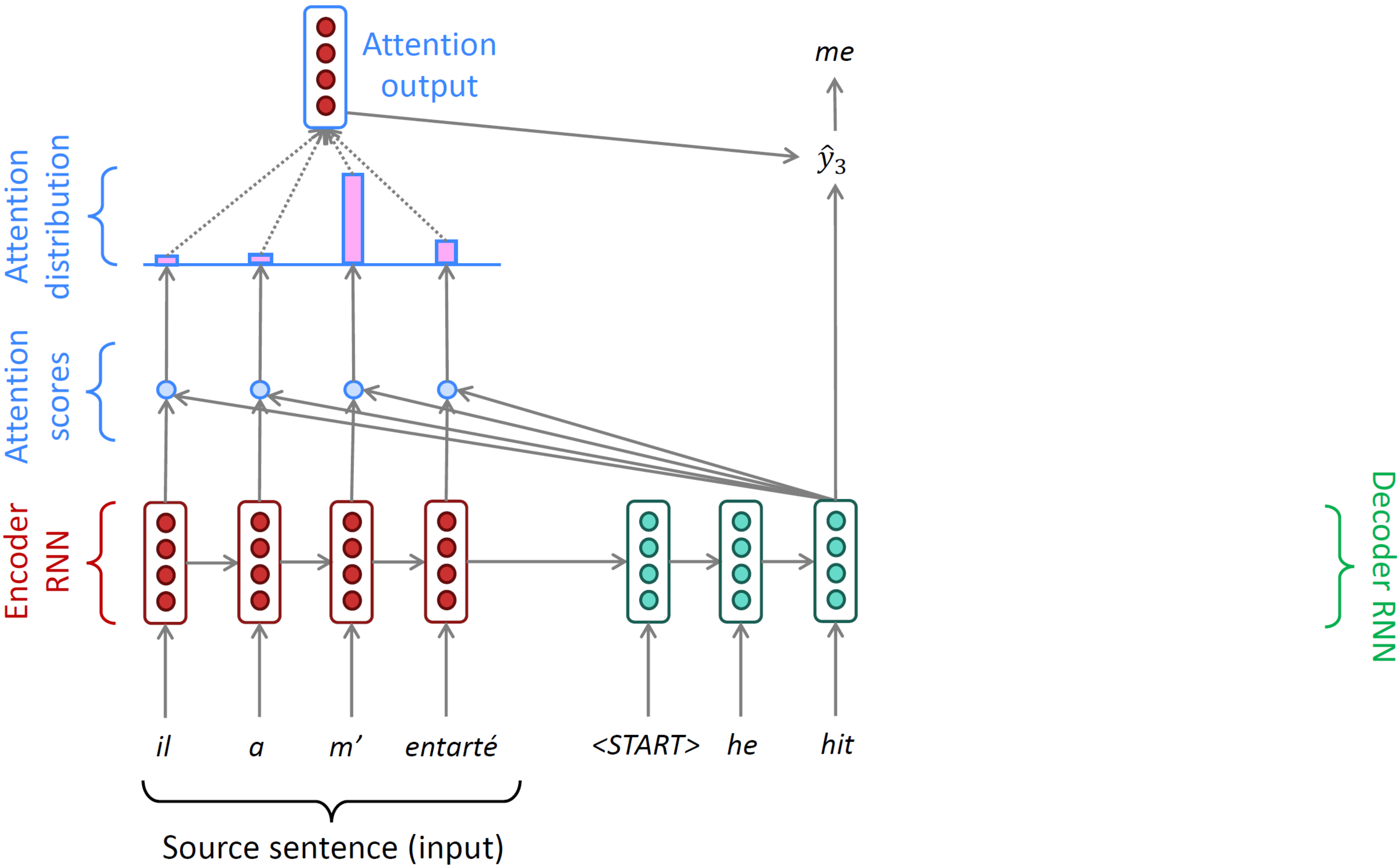
Seq2Seq with Attention



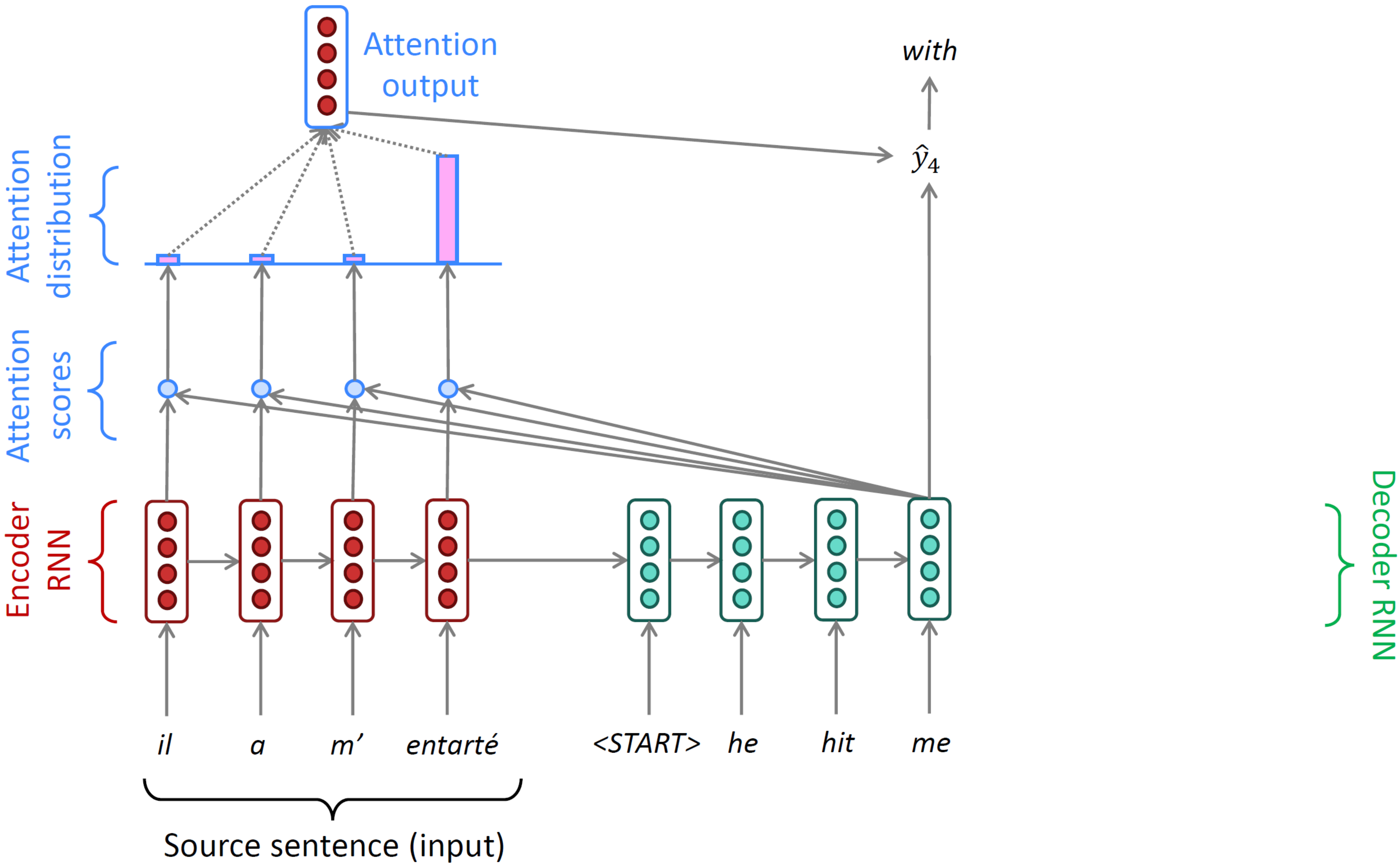
Seq2Seq with Attention



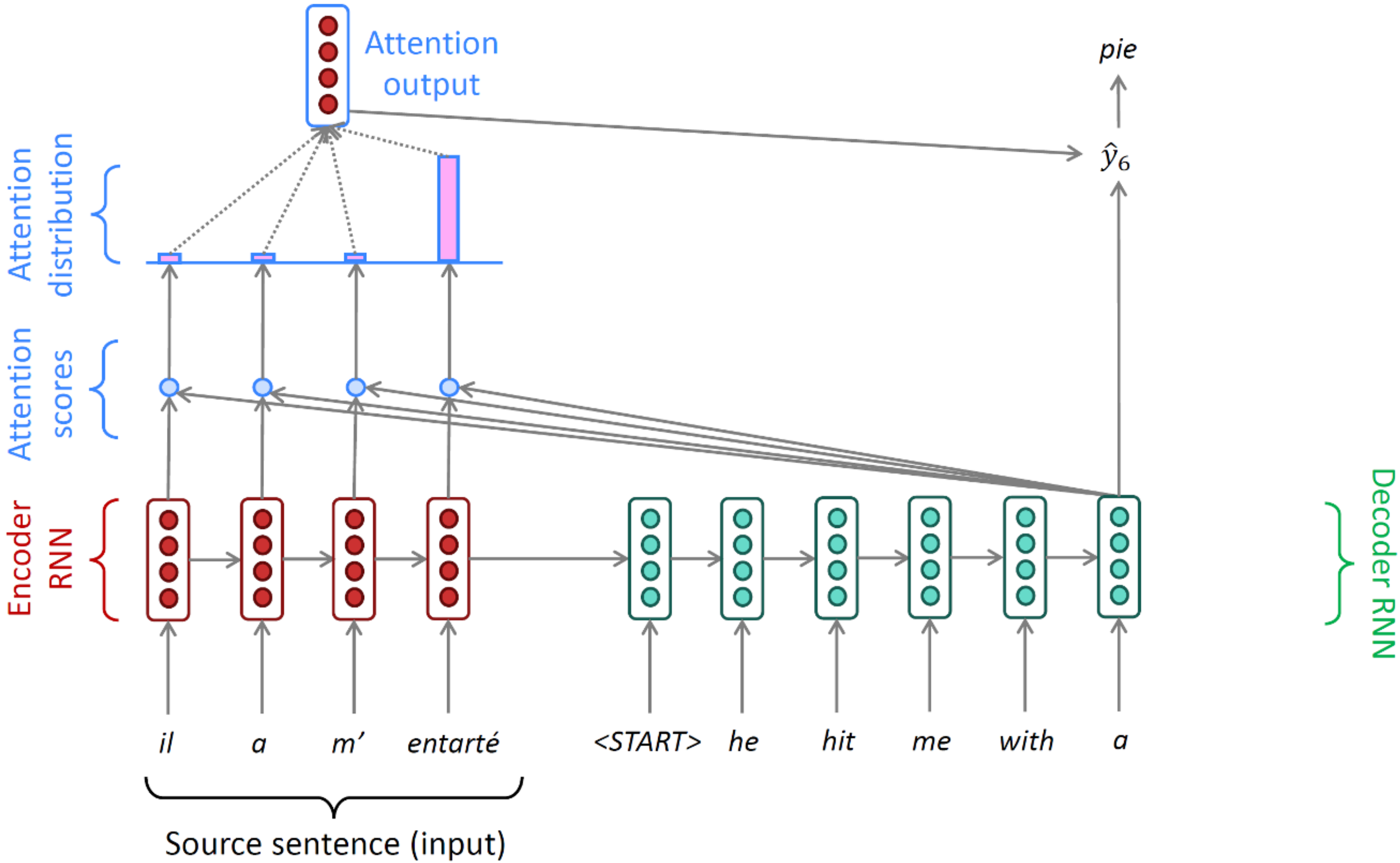
Seq2Seq with Attention



Seq2Seq with Attention



Seq2Seq with Attention



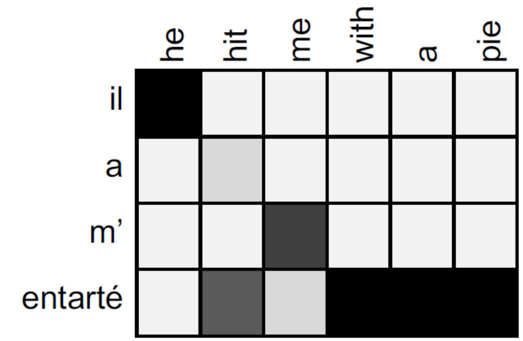
Seq2Seq with Attention

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:

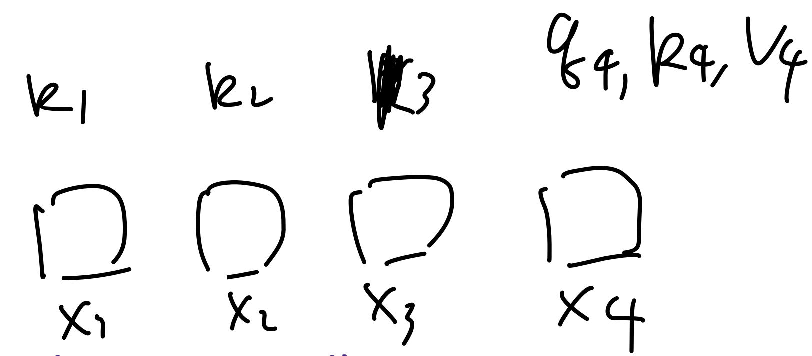
- Attention can be viewed as a module.
- In encoder and decoder (more on this later)
- A representation of a set of points
  - Pointer network (Vinyals, Forunato, Jaitly ’15)
  - Deep Sets (Zaheer et al., ’17)
- Convolutional neural networks
  - To include non-local information in CNN (Non-local network,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

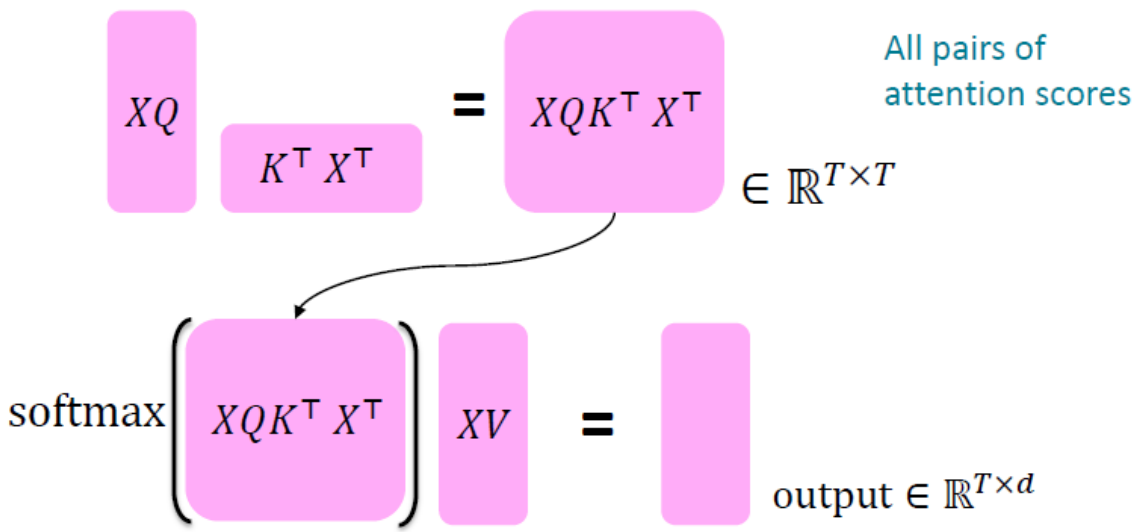
- Attent variant: $f(v_i, q)$
  - Multiplicative attention: $f(v_i, q) = q^\top W h_i$, W is a weight matrix
  - Additive attention: $f(v_i, q) = u^\top \tanh(W_1 v_i + W_2 q)$

Key-query-value attention



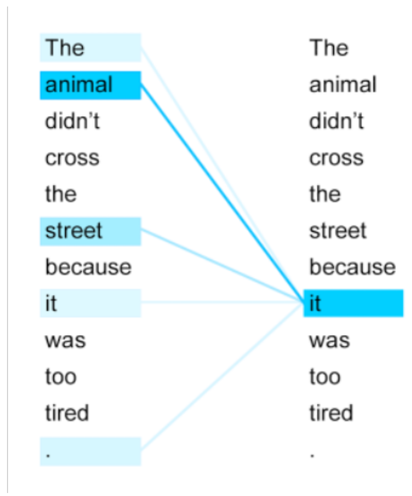
- Obtain q_t, v_t, k_t from X_t
- $q_t = W^q X_t$; $v_t = W^v X_t$; $k_t = W^k X_t$ (position encoding omitted)
  - W^q, W^v, W^k are learnable weight matrices
- $\alpha_{i,j} = \text{softmax}(q_i^\top k_j)$; $out_i = \sum_k \alpha_{i,j} v_j$
- Intuition: key, query, and value can focus on different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

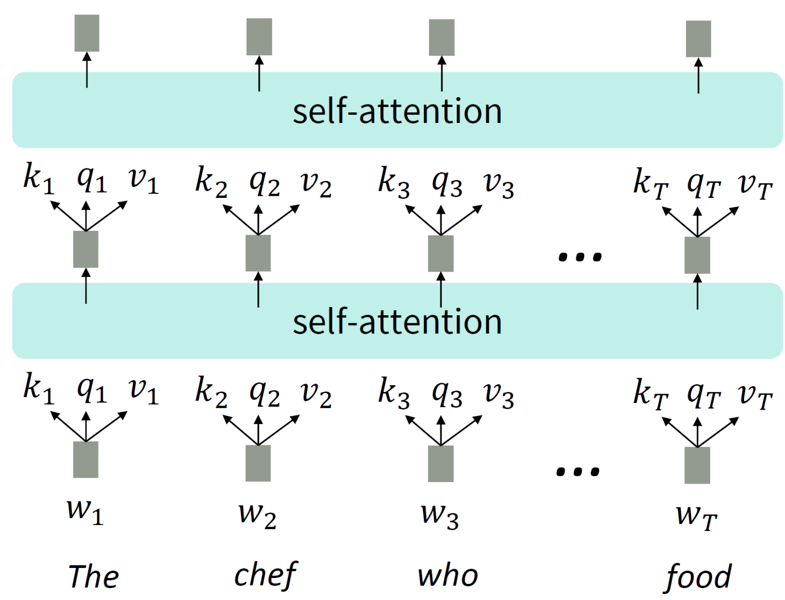
$\alpha_{4,1} = \text{softmax}(q_4^T k_1)$



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

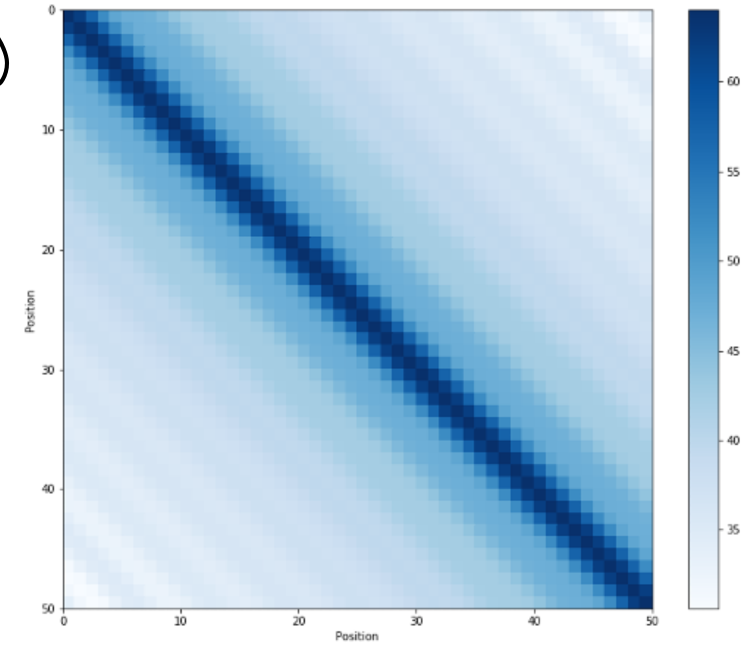
- Vanilla self-attention
  - $(k_t, v_t, q_t) = g_1(X_t; \theta)$
  - $\alpha_{t,j} = \text{softmax}(q_t^\top k_j)$
  - Attention output $out_t = \sum_j \alpha_{t,j} v_j$
- Idea: position encoding:
  - p_i: an embedding vector (feature) of position i
  - $(k_t, v_t, q_t) = g_1([X_t, p_t]; \theta)$ $p_t = i$
- 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

$i, j = 1, \ldots 50$

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

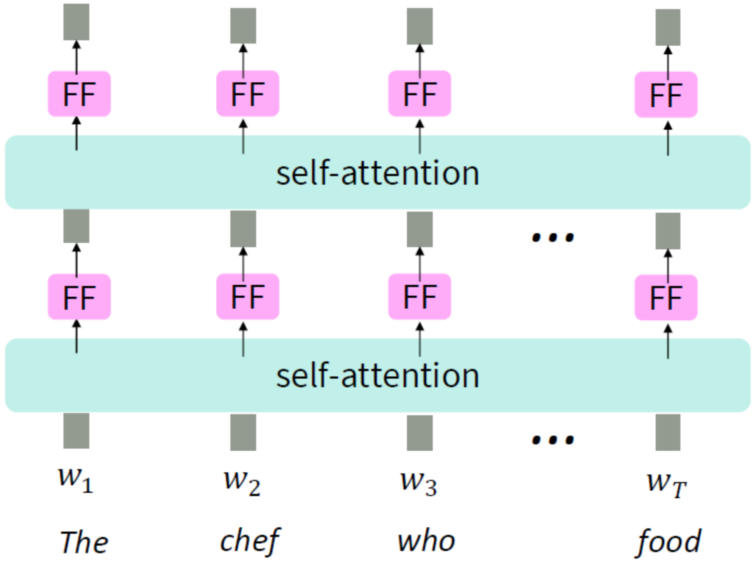
p_t design 2: **Learned representation**

- 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

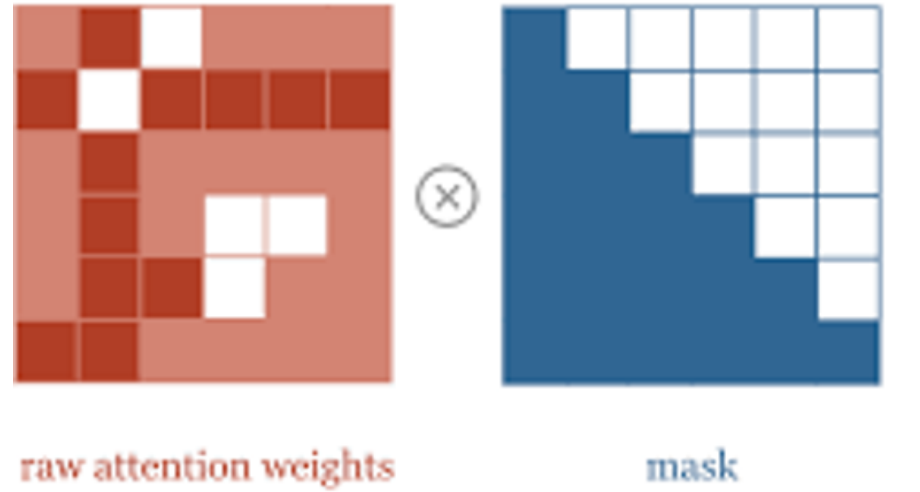
- Fix:
  - Add an MLP to process out_i
  - $m_i = MLP(out_i) = W_2\text{ReLU}(W_1 out_i + b_1) + b_2$
  - Usually do not put activation layer before softmaax

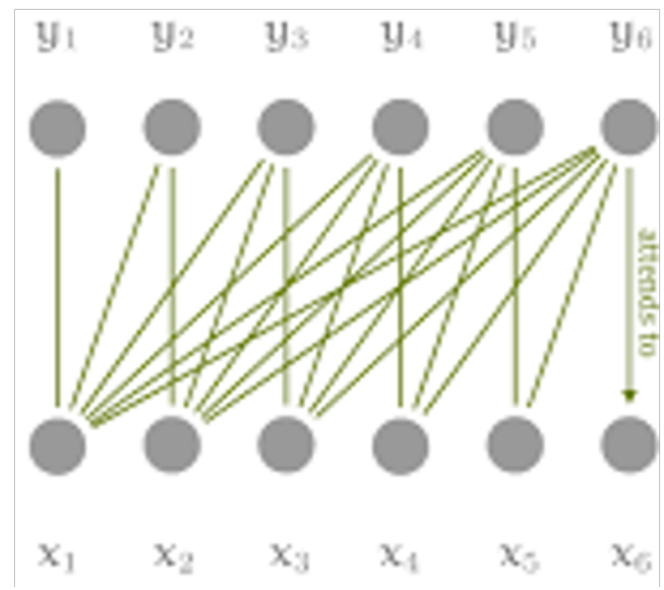


Masked Attention

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

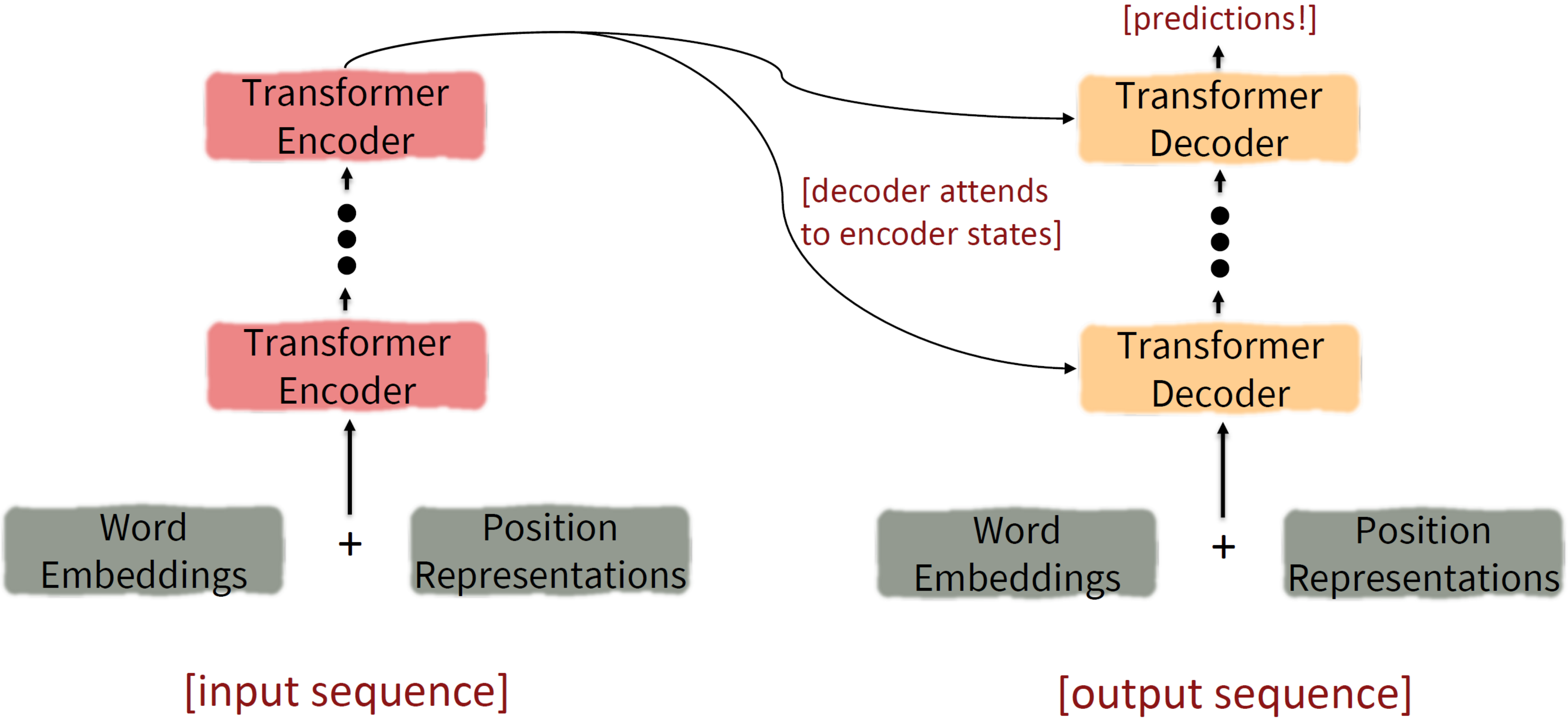
- Masked attention
  - Compute $e_{i,j} = q_i^\top k_j$ as usuall
  - Mask out $e_{i>j}$ by setting $e_{i>j} = -\infty$
    - $e \odot (1 - M) \leftarrow -\infty$
    - M is a fixed 0/1 mask matrix
  - Then compute $\alpha_i = \text{softmax}(e_i)$
  - Remarks:
    - $M = 1$ for full self-attention
 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





Transformer

Transformer-based sequence-to-sequence modeling



Key-query-value attention

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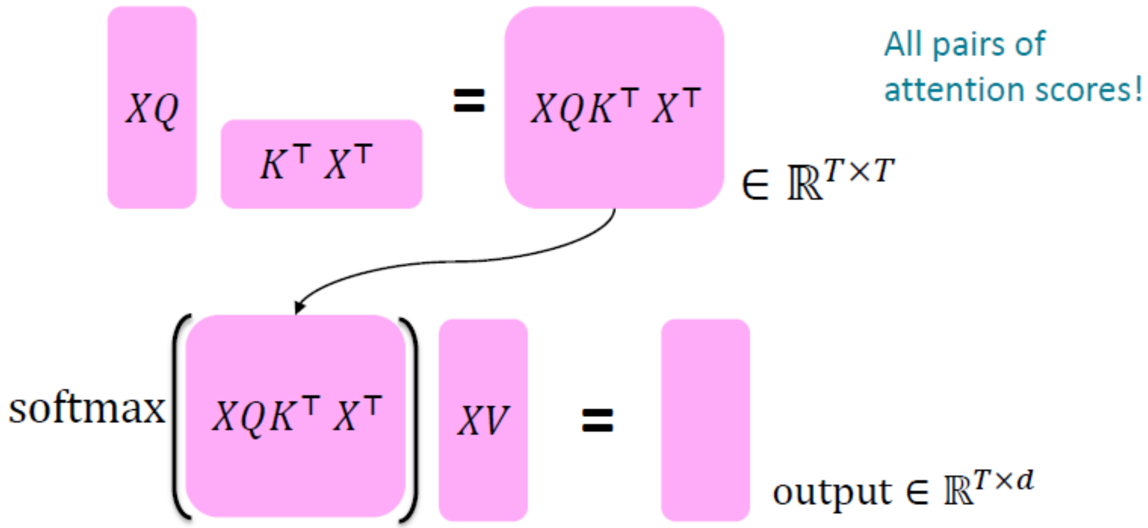


Multi-headed attention

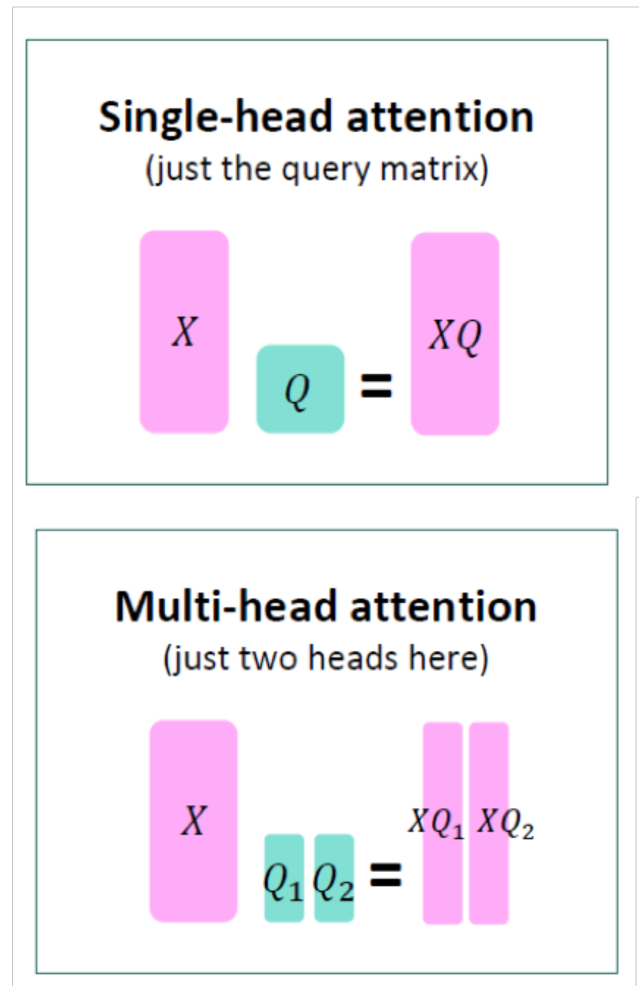
- Standard attention: single-headed attention
  - $X_t \in \mathbb{R}^d, Q, K, V \in \mathbb{R}^{d \times d}$
  - We only look at a single position j with high $\alpha_{i,j}$
  - What if we want to look at different j for different reasons?
- Idea: define h separate attention heads
  - h different attention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

$X_t \to \{q_t^\ell\}_{\ell=1}^h, \{k_t^\ell\}, \{v_t^\ell\}$

$\{out_t^\ell\}_{\ell=1}^h$

$[out_t^1, out_t^2, \ldots, out_t^h]$

#Params Unchanged!



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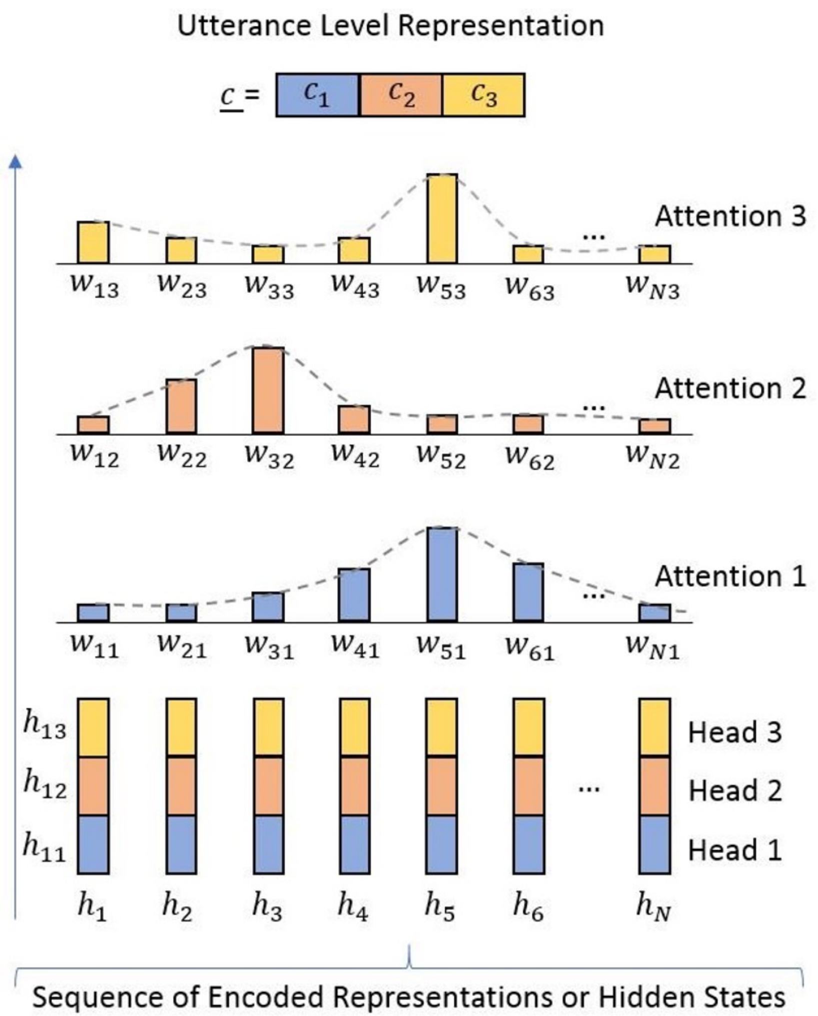
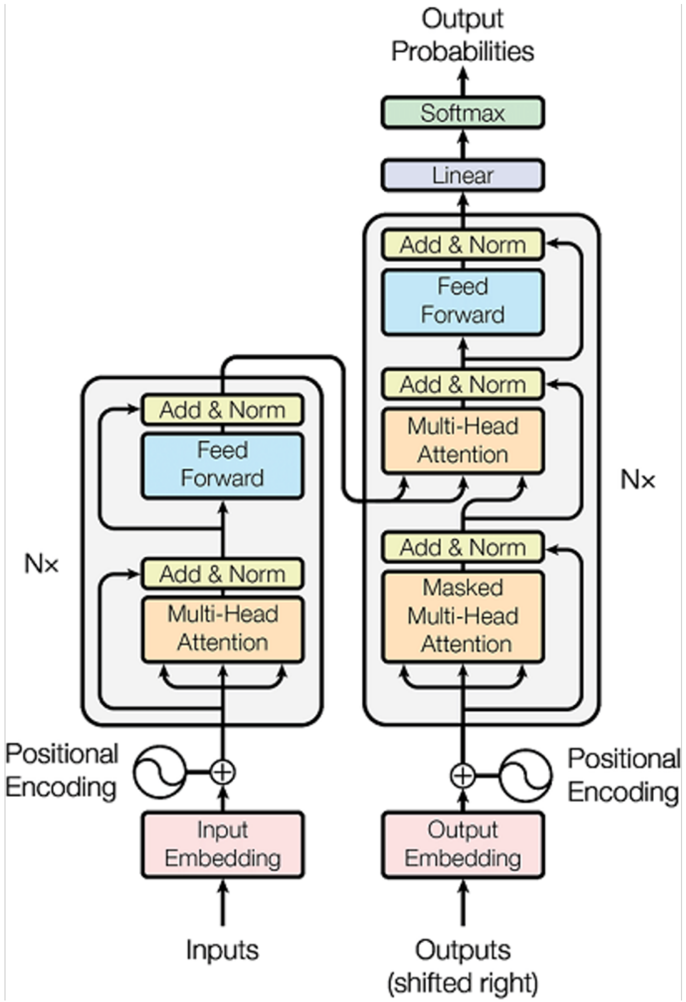


Transformer

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

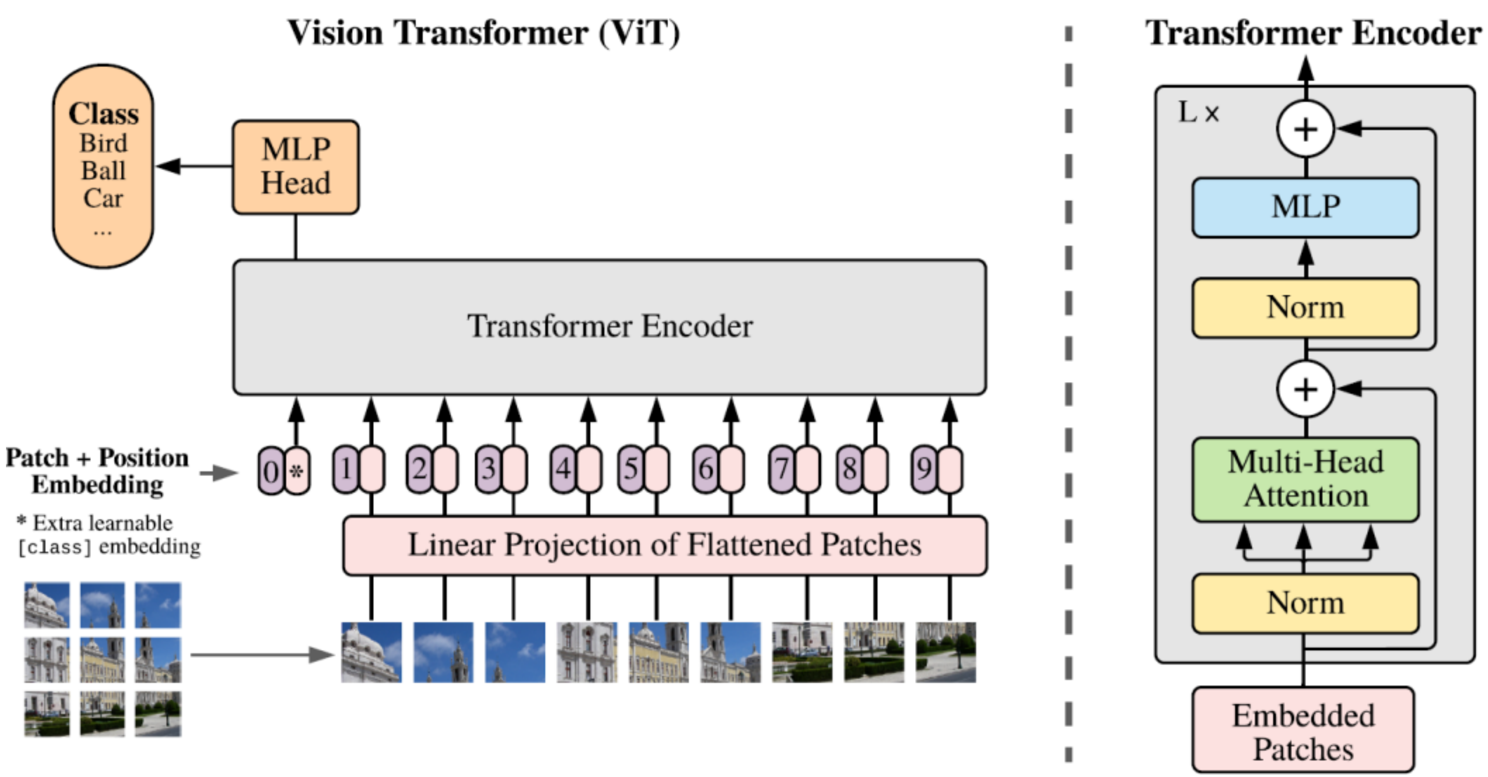
Transformer

- 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)

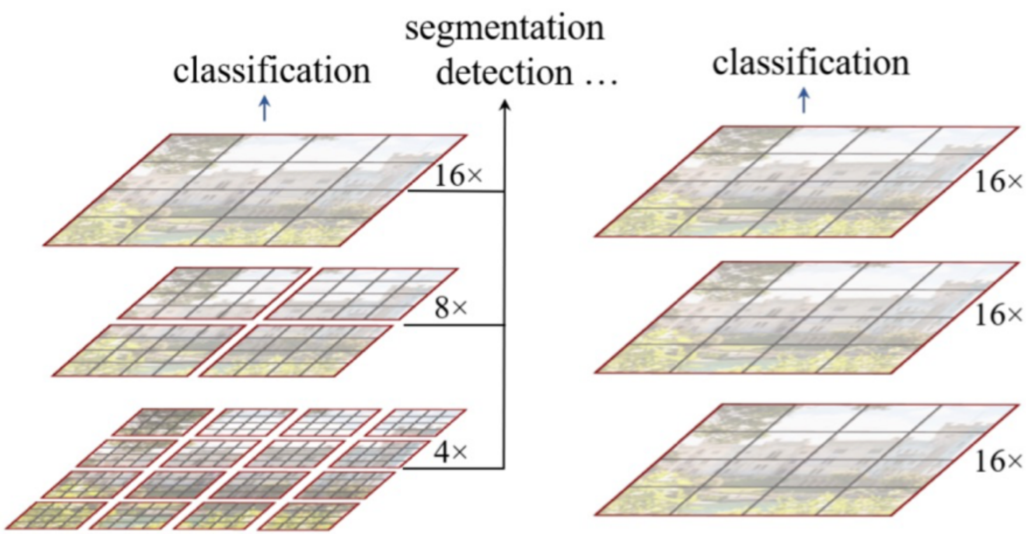
Transformer for Images

- 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

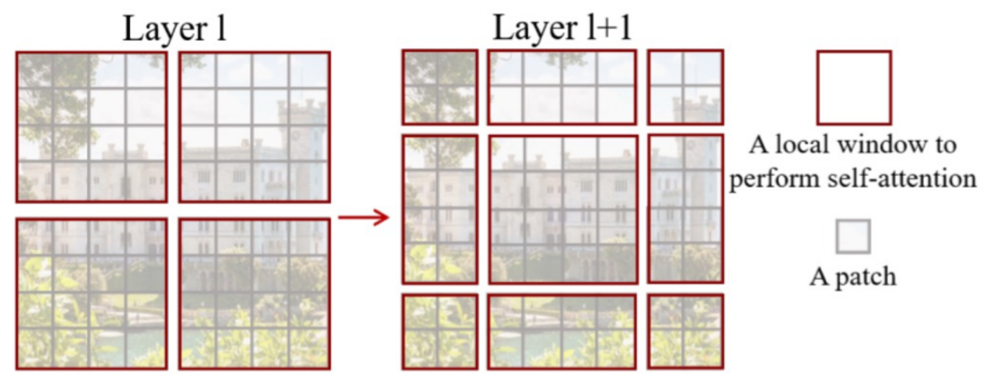
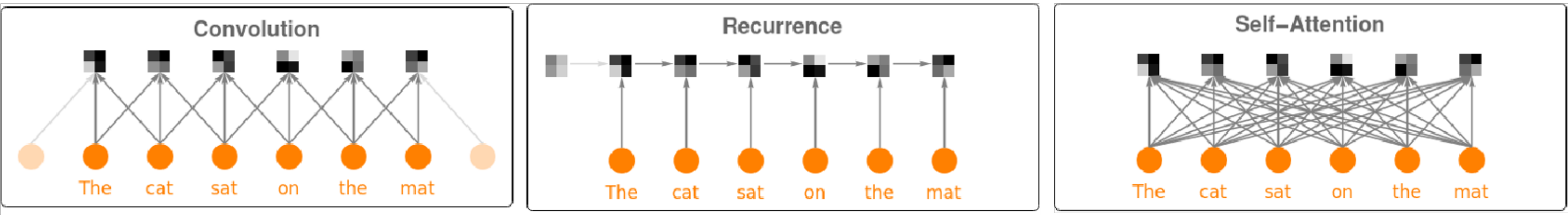


Figure 2. An illustration of the *shifted window* approach for com-

CNN vs. RNN vs. Attention



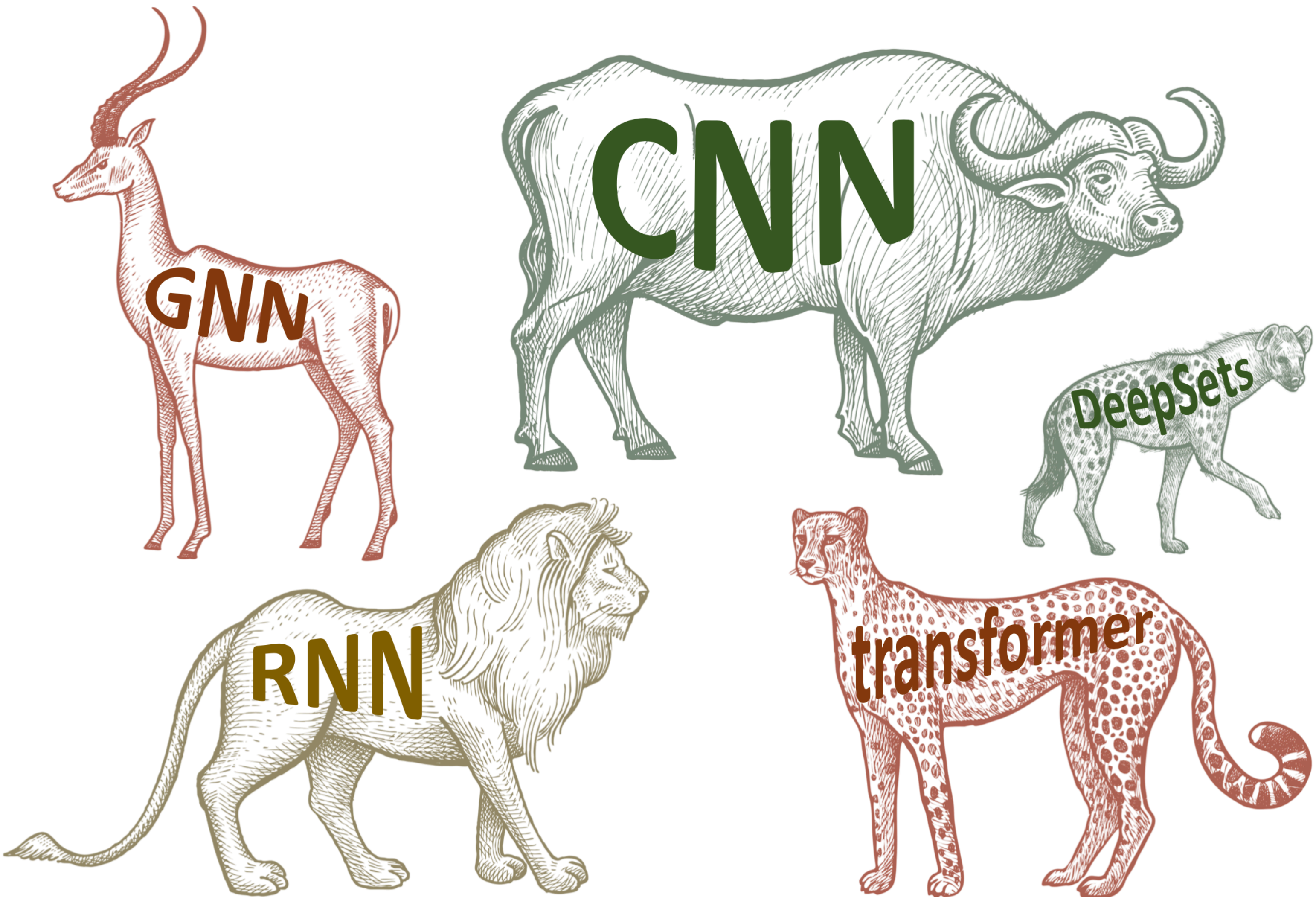
Summary

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

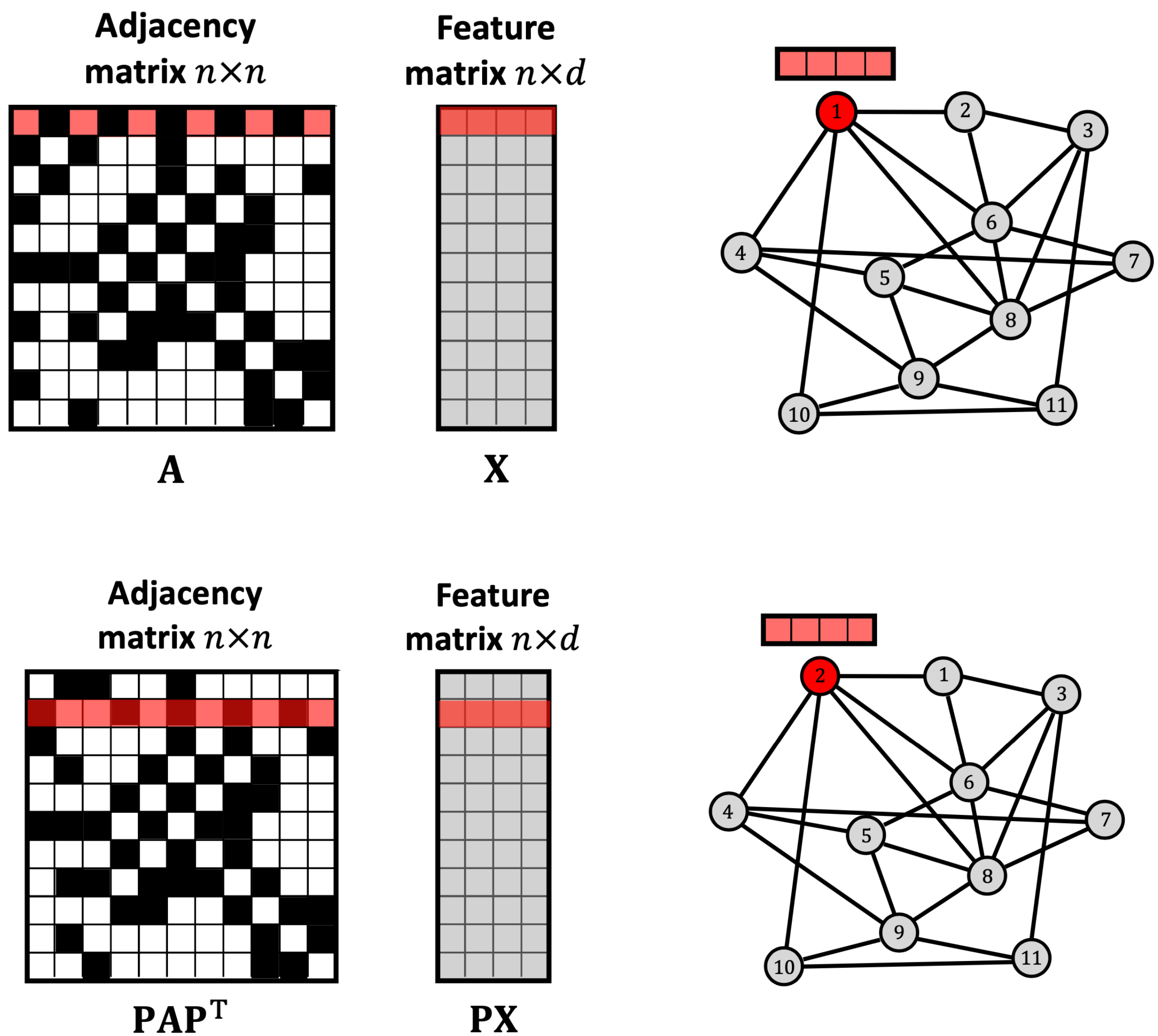
- Attention mechanism
  - So far the most successful idea for sequence data in deep learning
  - A scale/order-invariant representation
  - Transformer: a fully attention-based architecture for sequence data
  - Transformer + Pretraining: the core idea in today's NLP tasks

- LSTM is still useful in lightweight scenarios

Other architectures



Graph Neural Networks



arbitrary ordering of nodes

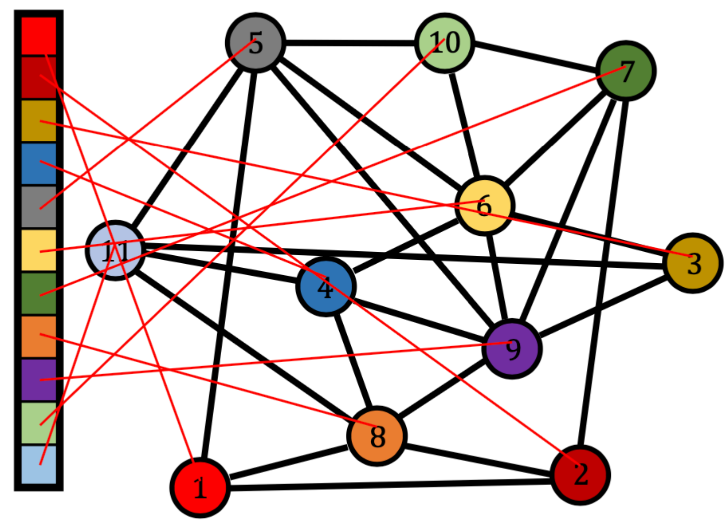
Graph Neural Networks

$F: \mathbb{R}^{n \times d} \to \mathbb{R}^{n \times d}$

GCN

permutation-equivariant

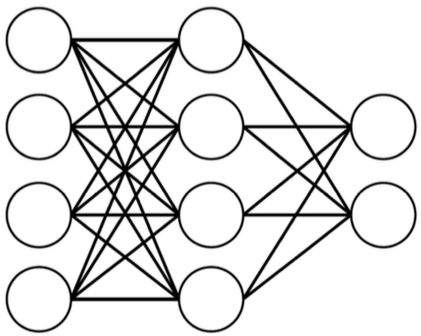
$$\mathbf{F}(\mathbf{PX}, \mathbf{PAP}^{\top}) = \mathbf{PF}(\mathbf{X}, \mathbf{A})$$



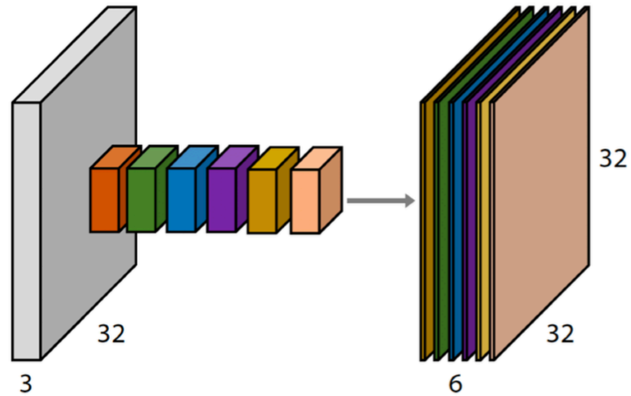
X , A

P , PAP^T

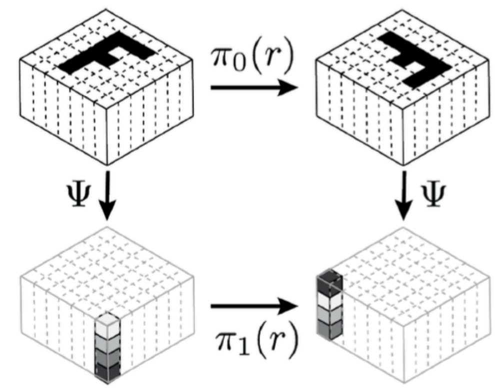
Geometric Deep Learning



Perceptrons
Function regularity

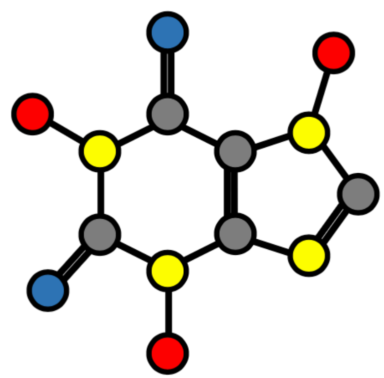


CNNs
Translation



Group-CNNs
Translation+Rotation

DeepSets / Transformers
Permutation

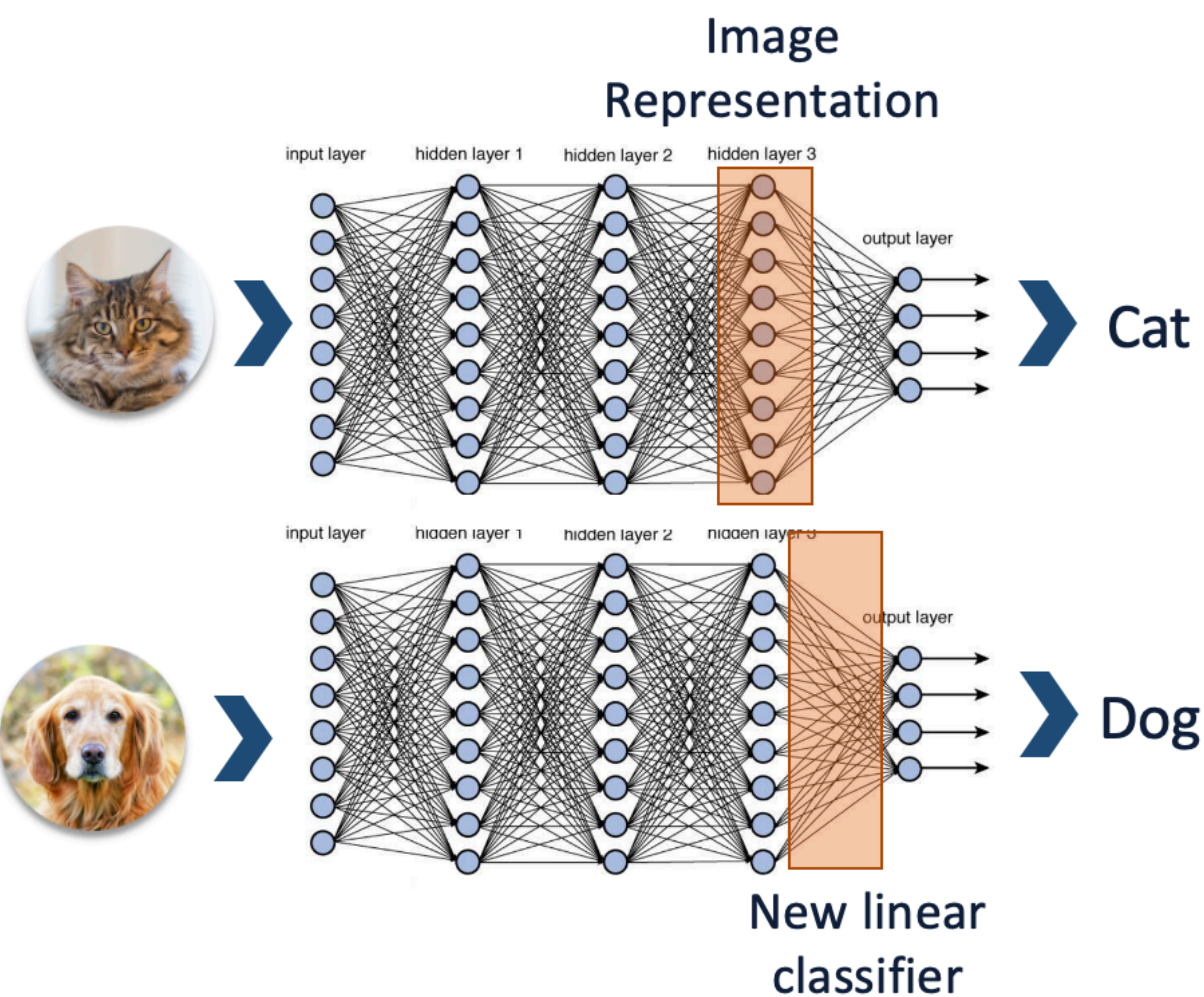


GNNs
Permutation

Intrinsic CNNs
Local frame choice

Representation Learning
Pre-training

Example in image representation



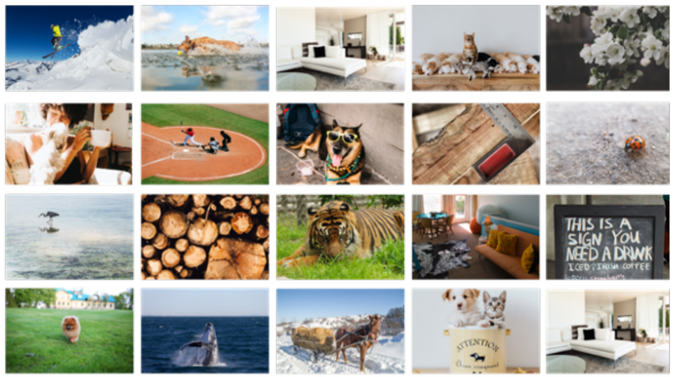
Train a neural network (ResNet) on ImageNet (1M data, 1000 classes)

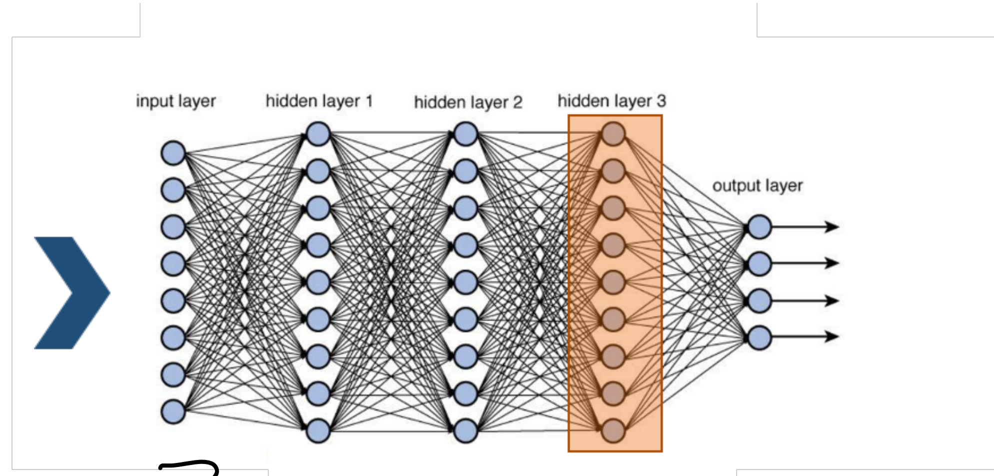
Representation (feature extractor): The mapping from image to the second-to-the-last layer.

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

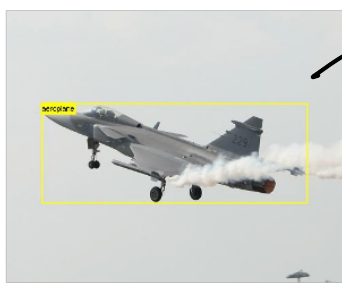
Example in image representation

Source tasks
(for training representation):
ImageNet





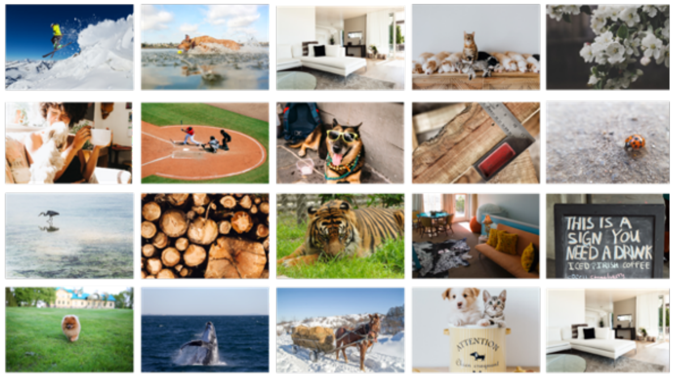
Target task:
Few-shot Learning on VOC07 dataset (20 classes, 1-8 examples per class)

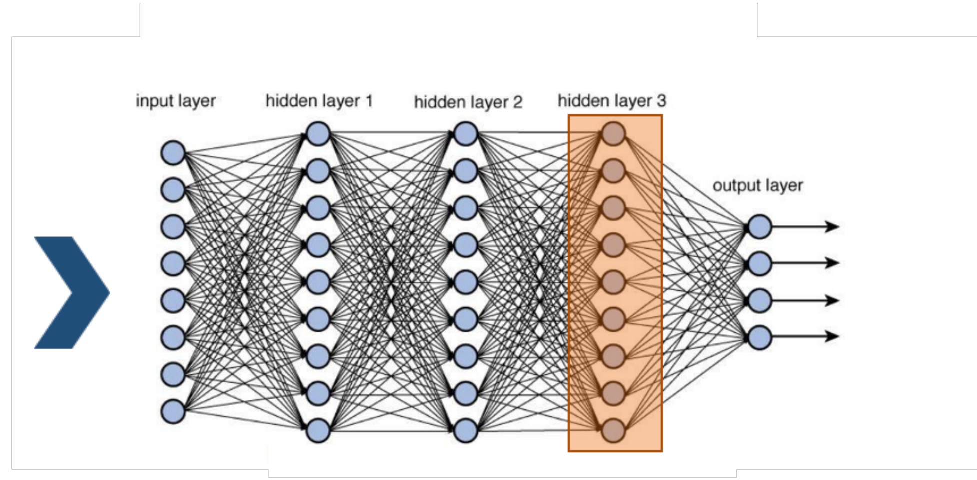


- Without representation learning: **5% - 10%** (random guess = **5%**)
- With representation learning: **50% - 80%**

Example in image representation

Source tasks (for training representation): ImageNet





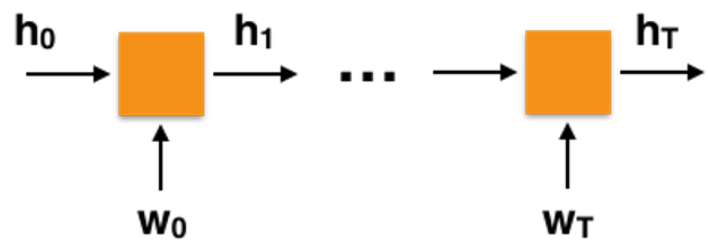
Target task: Few-shot Learning on VOC07 dataset (20 classes, 1-8 examples per class)

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

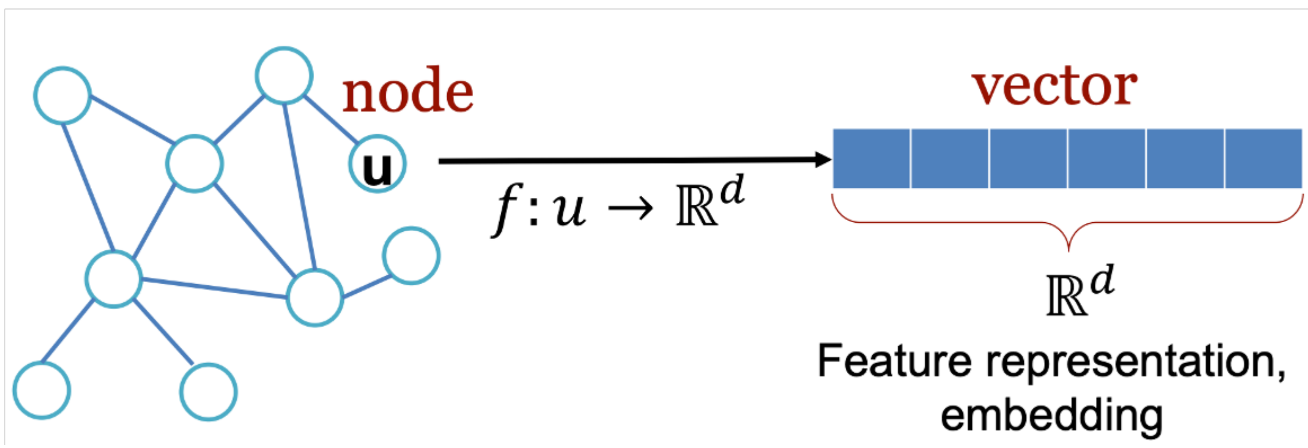
Examples

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.

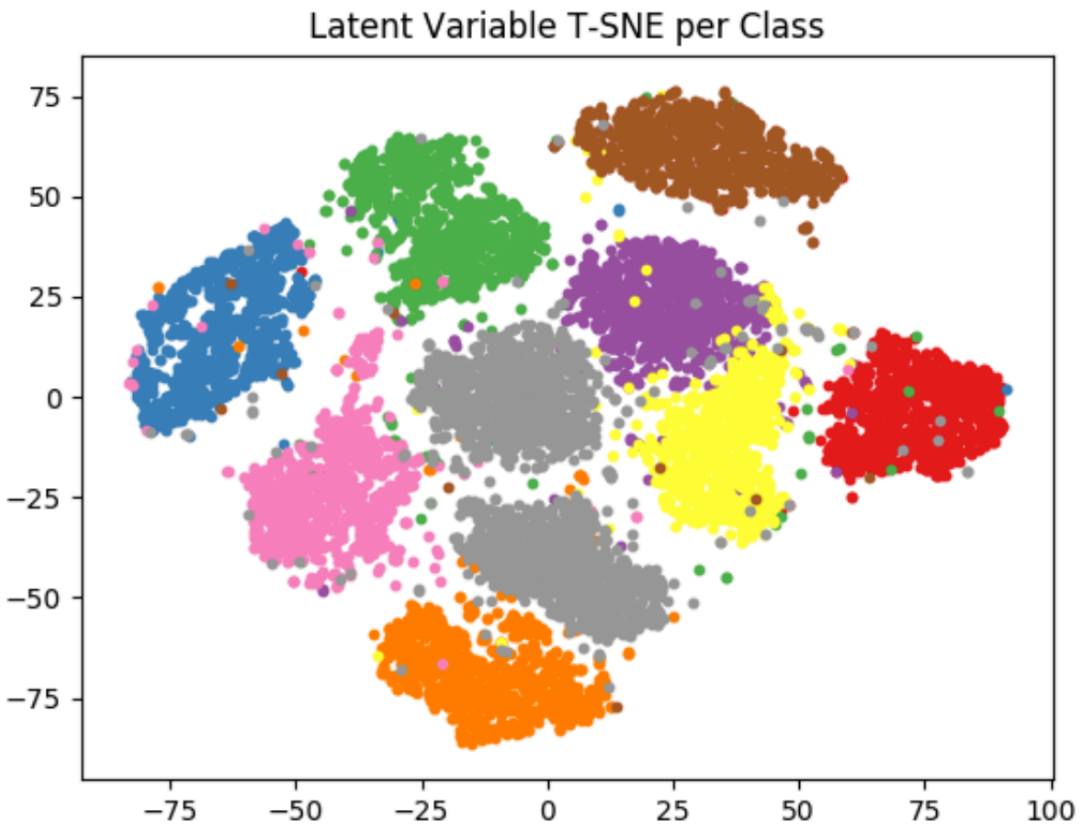
- **Semantic clusterability**: features of the same "semantic class" (e.g. images in the same class) are clustered together.

- **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.

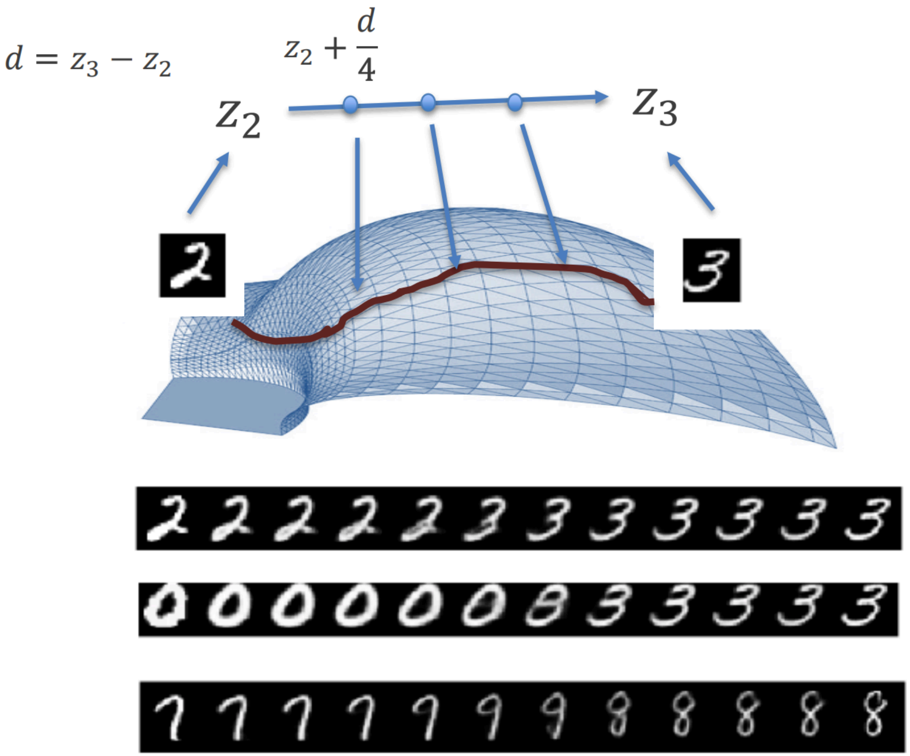


Intuition: If semantic classes are linearly separable, and labels on downstreams tasks depend linearly on semantic classes: we only need to learn a simple classifer.

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: $p_\theta(z) = \Pi_i p_\theta(z_i)$.

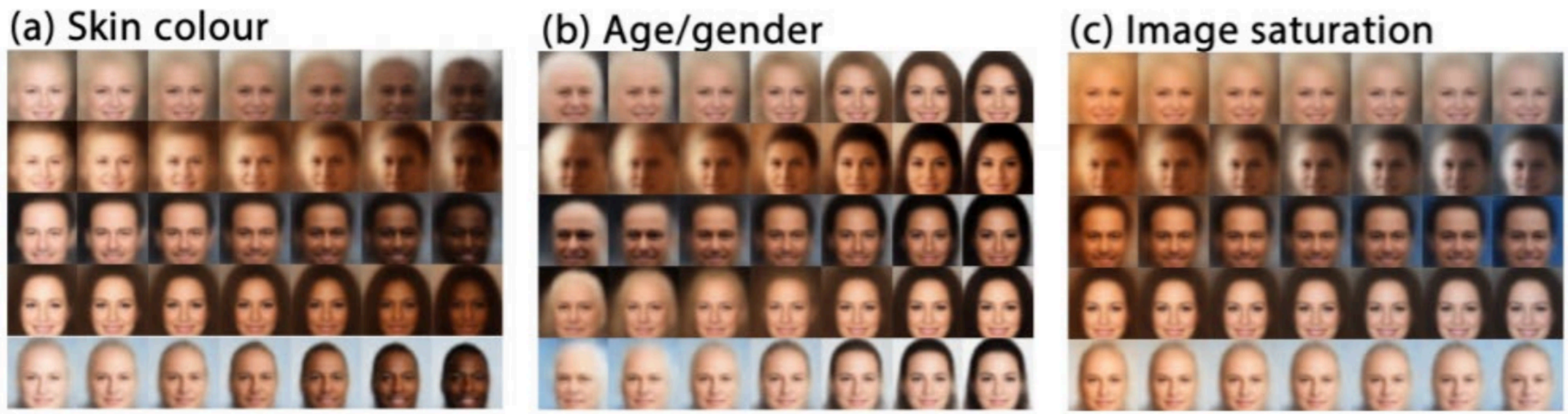


Figure 4: **Latent factors learnt by β-VAE on celebA:** traversal of individual latents demonstrates that β-VAE discovered in an unsupervised manner factors that encode skin colour, transition from an elderly male to younger female, and image saturation.