

# Attention Mechanism

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# Machine Translation

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- 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)

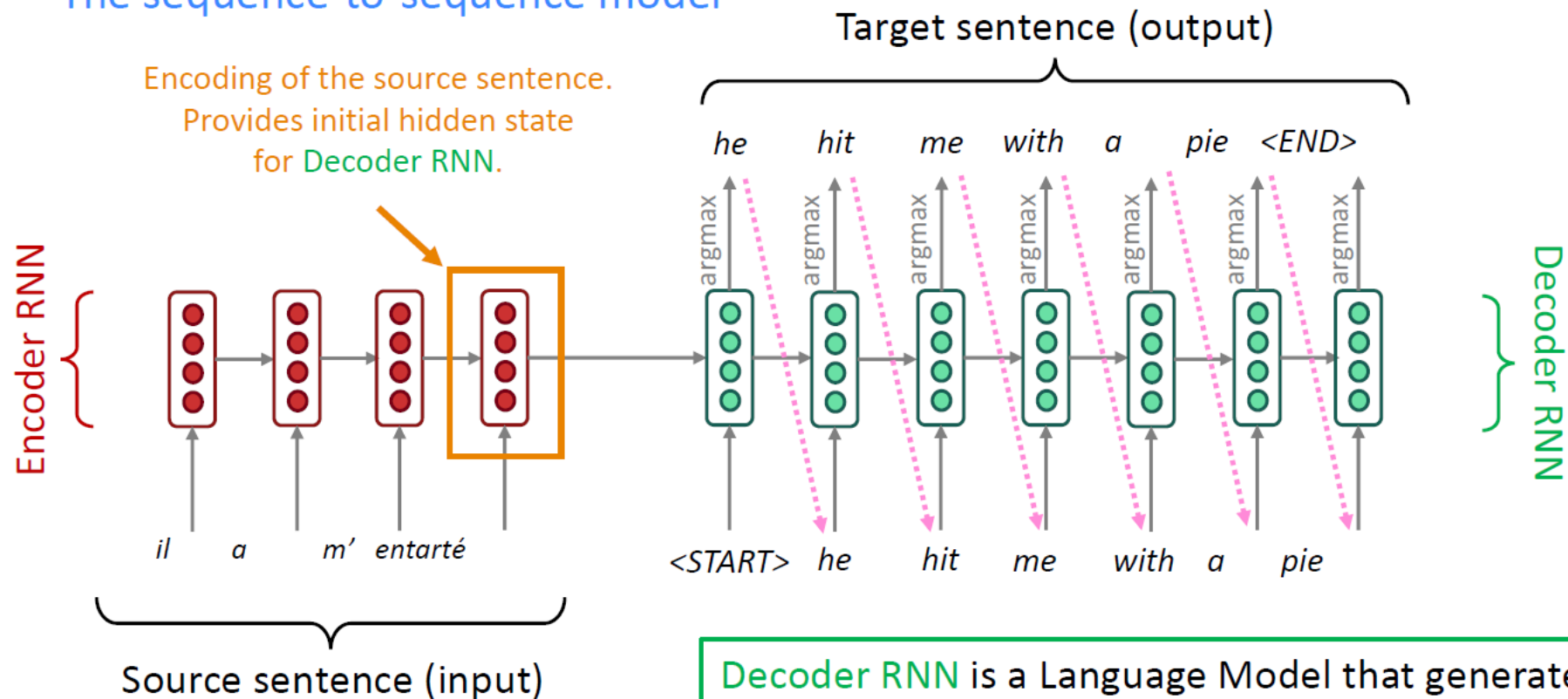
# Sequence to Sequence Model

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- 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.

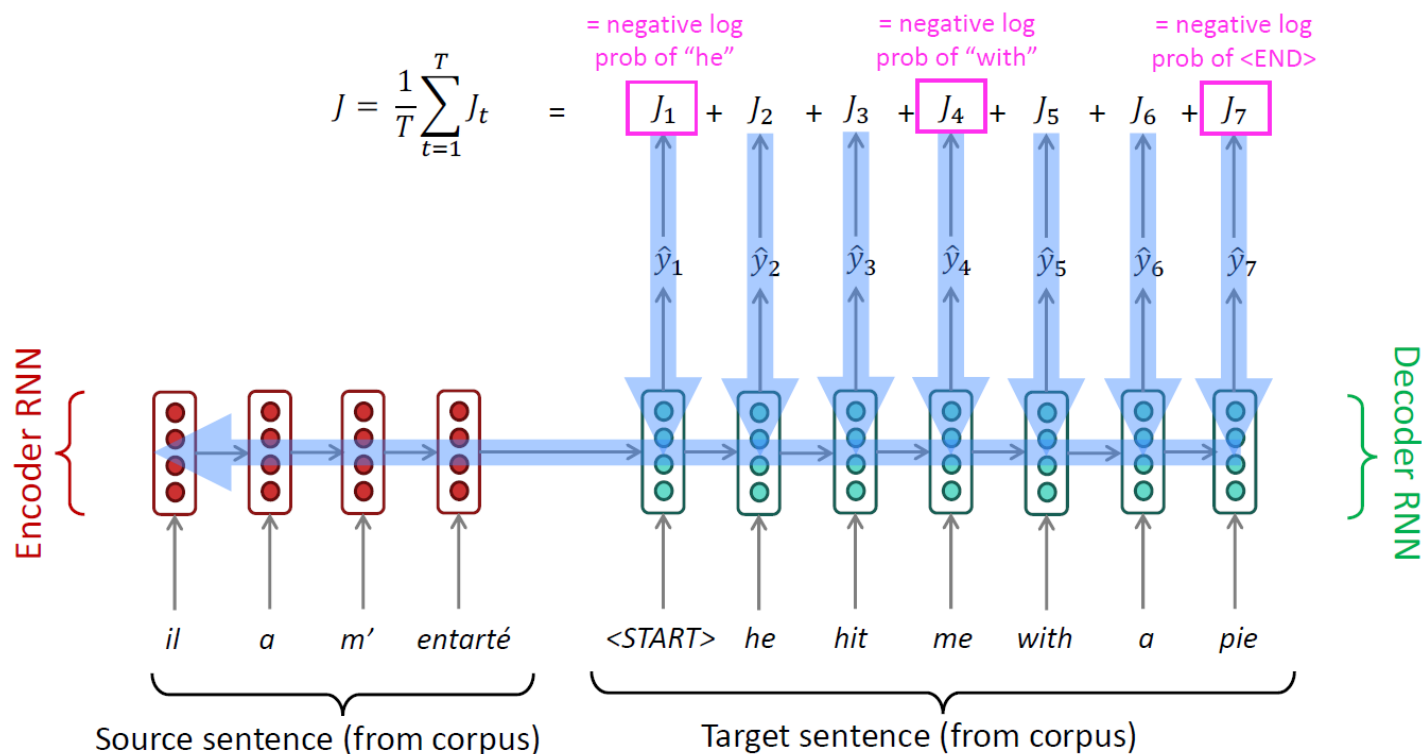
Decoder RNN is a Language Model that generates target sentence, *conditioned on encoding*.

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



# Training Sequence to Sequence Model

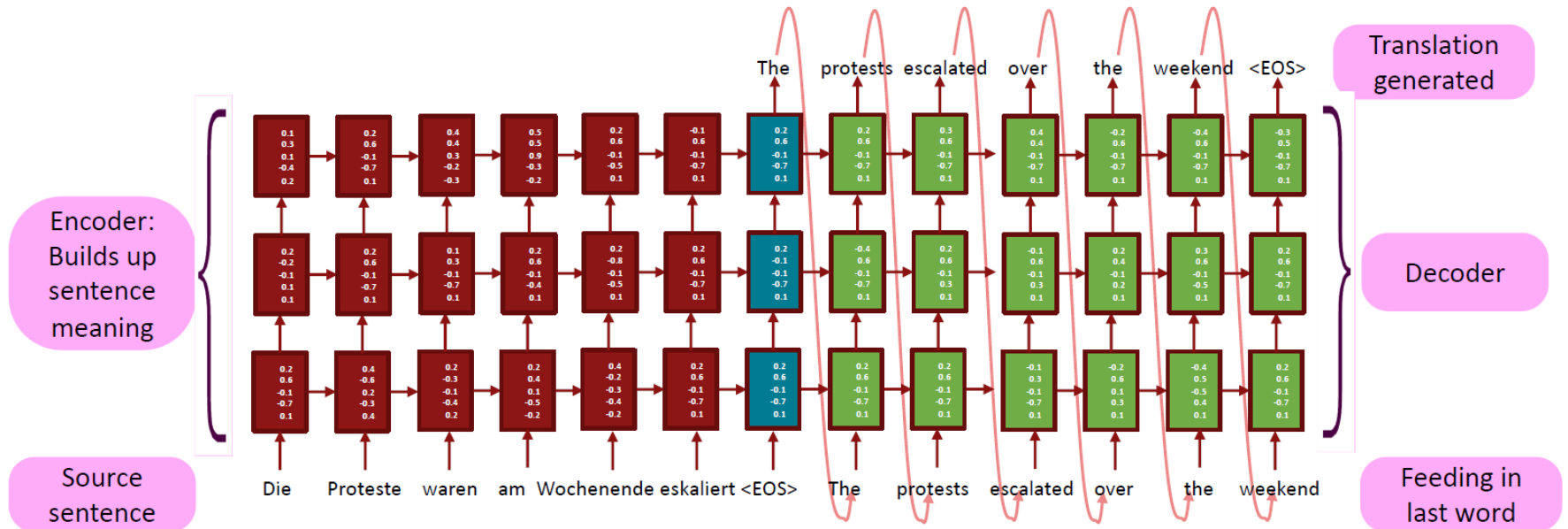
- Collect a huge paired dataset and train it end-to-end via BPTT
- Loss induced by MLE  $P(Y|X) = P(Y|f_{enc}(X))$



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

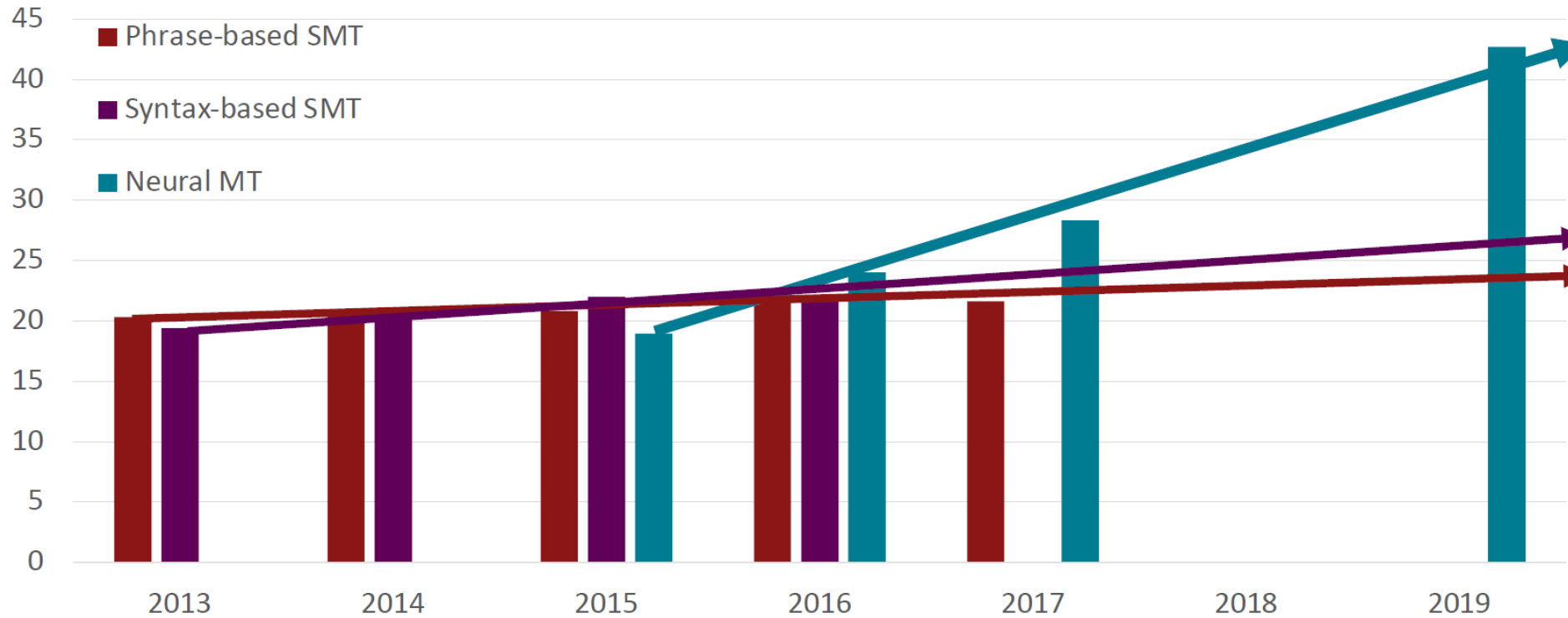
# Deep Sequence to Sequence Model

- Stacked seq2seq model



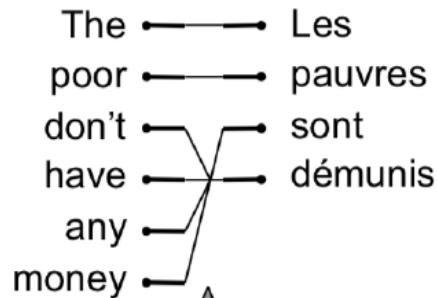
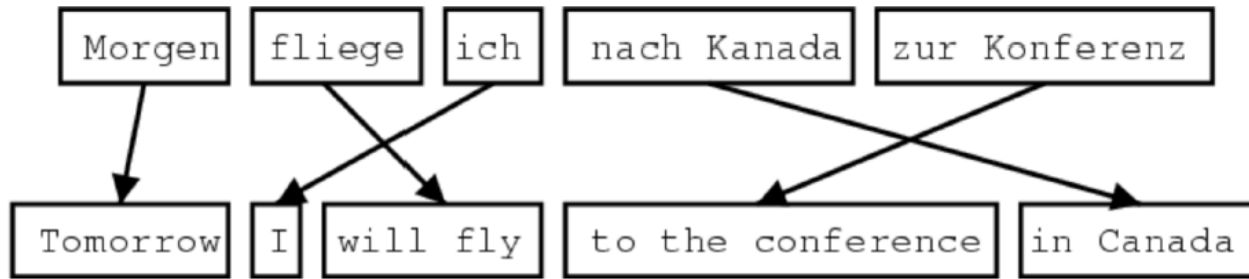
# Machine Translation

- 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



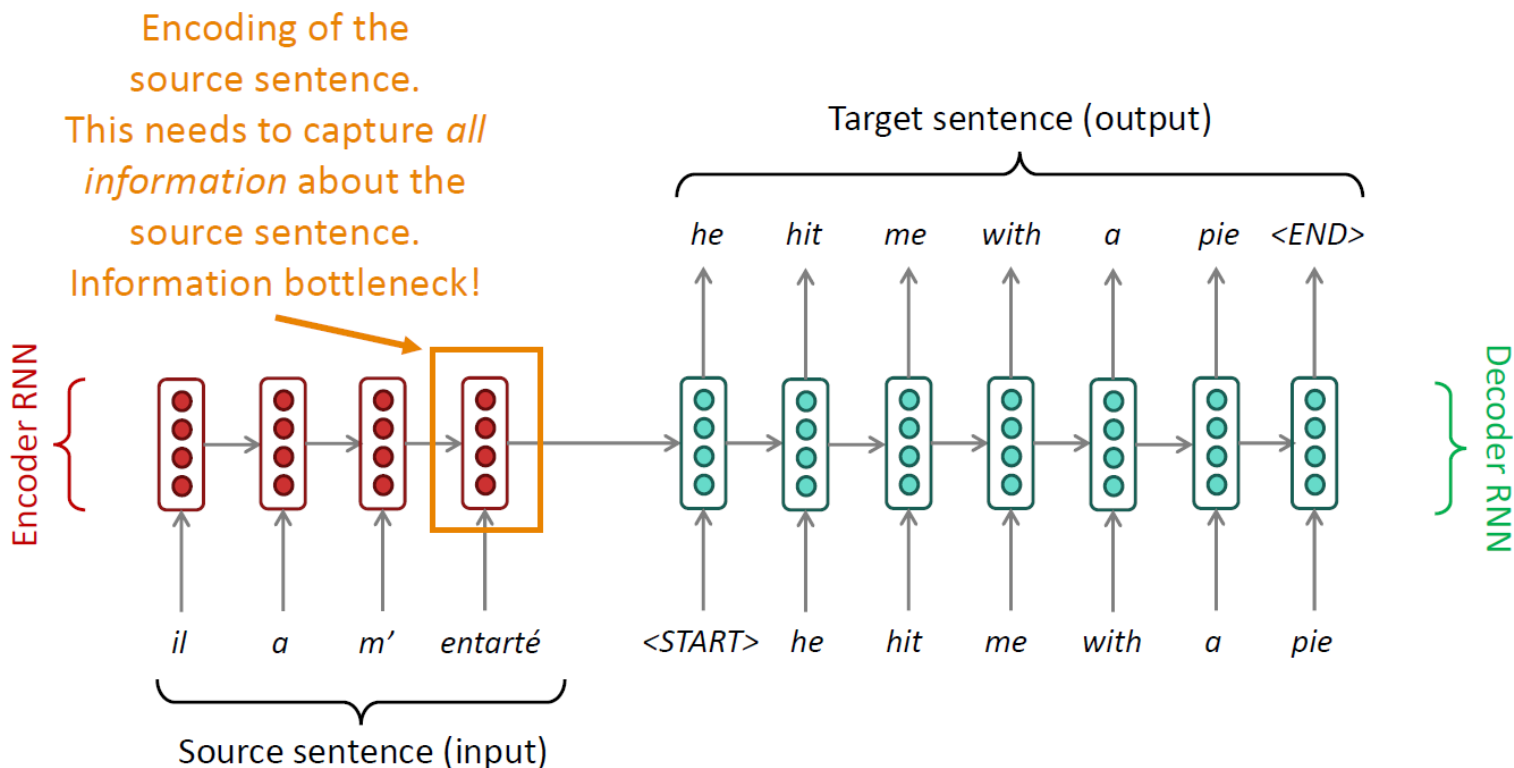
many-to-many  
alignment

	Les	pai	sor	dér
The				
poor				
don't				
have				
any				
money				

phrase  
alignment

# Issue in Seq2Seq

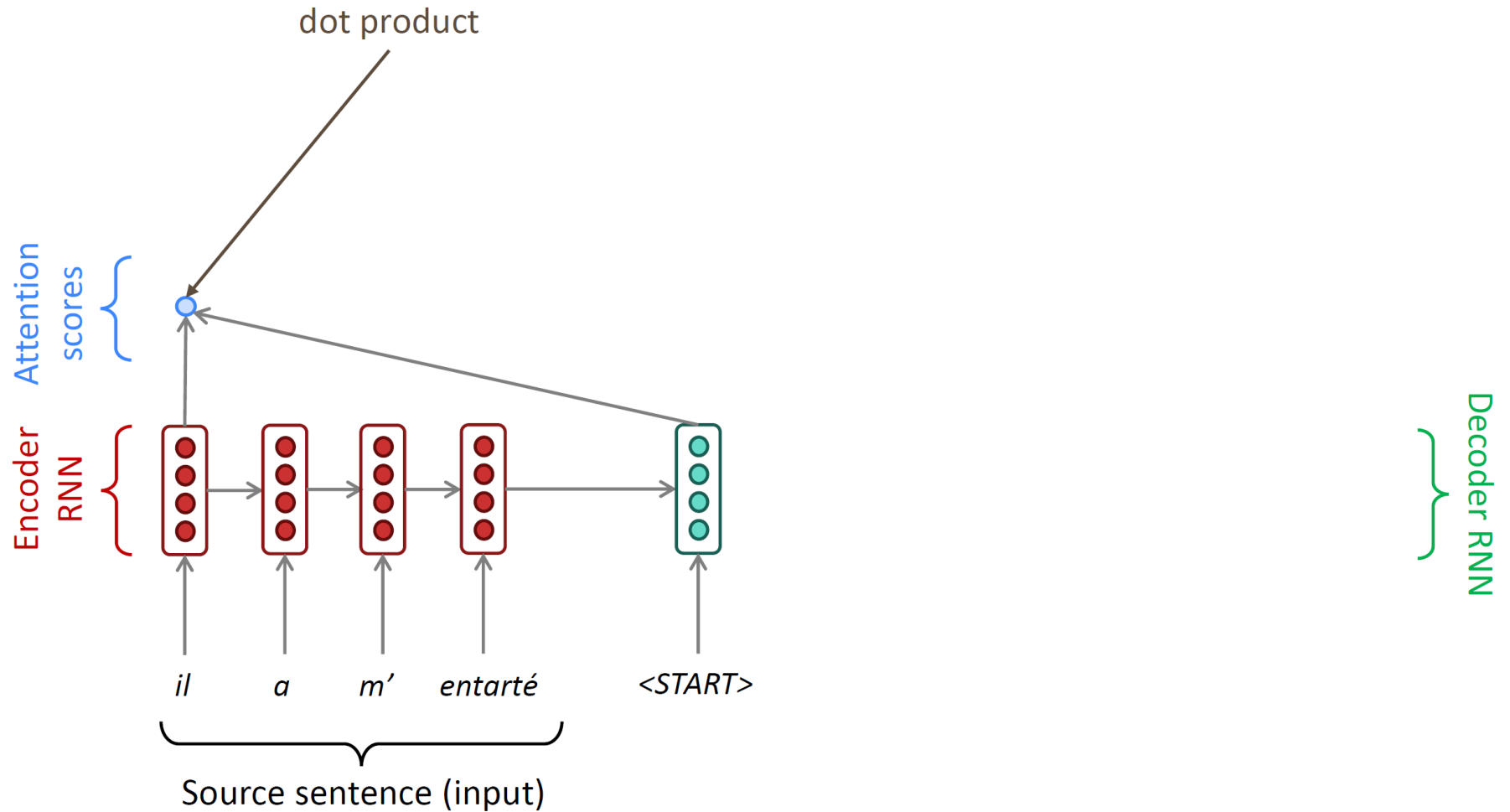
- Alignment: the word-level correspondence between  $X$  and  $Y$ 
  - The information bottleneck due to the hidden state  $h$
  - We want each  $Y_t$  to also focus on some  $X_i$  that it is aligned with



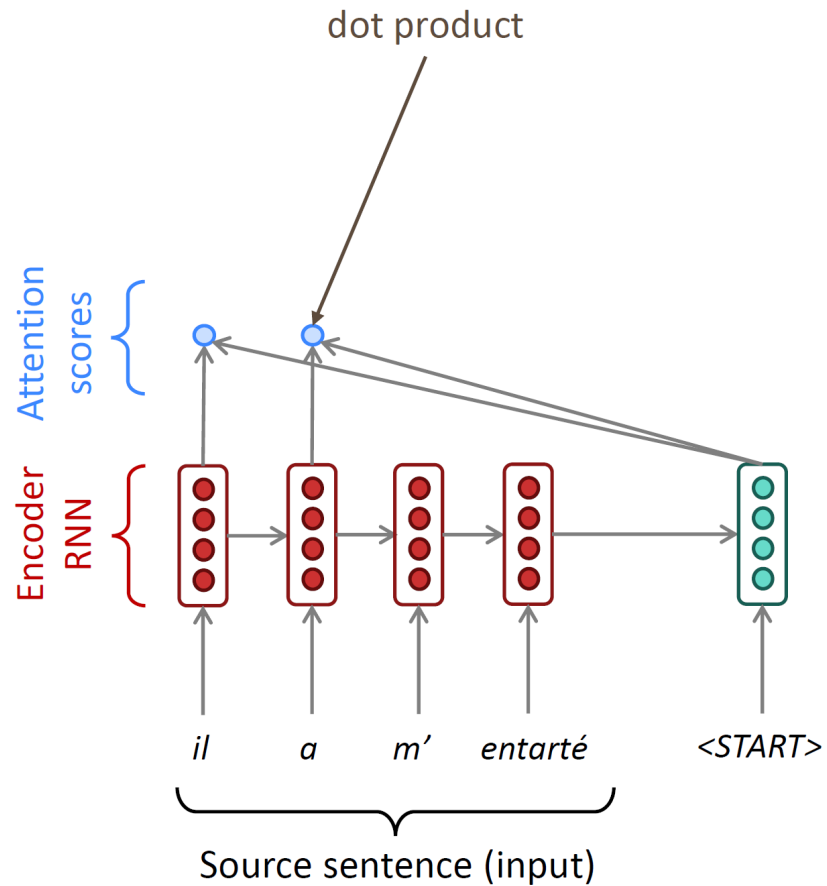
# Seq2Seq with Attention

- 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  $P_{att}$
    - $P_{att}(X_i | h_t)$ : how much attention to put on word  $X_i$
    - Attention output  $h_{att} = \sum_i f_{enc}(X_i | X_{j < i}) \cdot P_{att}(X_i | h_{t-1})$
    - Use  $h_{t-1}$  and  $h_{att}$  to compute  $Y_t$

# Seq2Seq with Attention

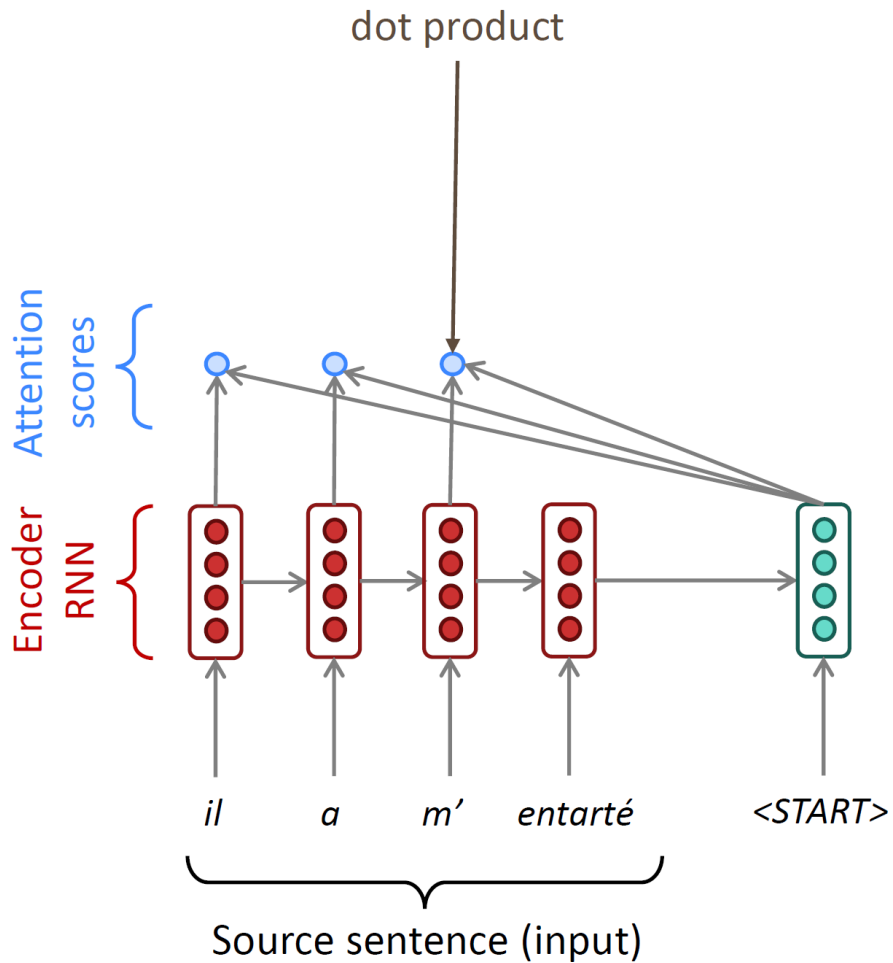


# Seq2Seq with Attention

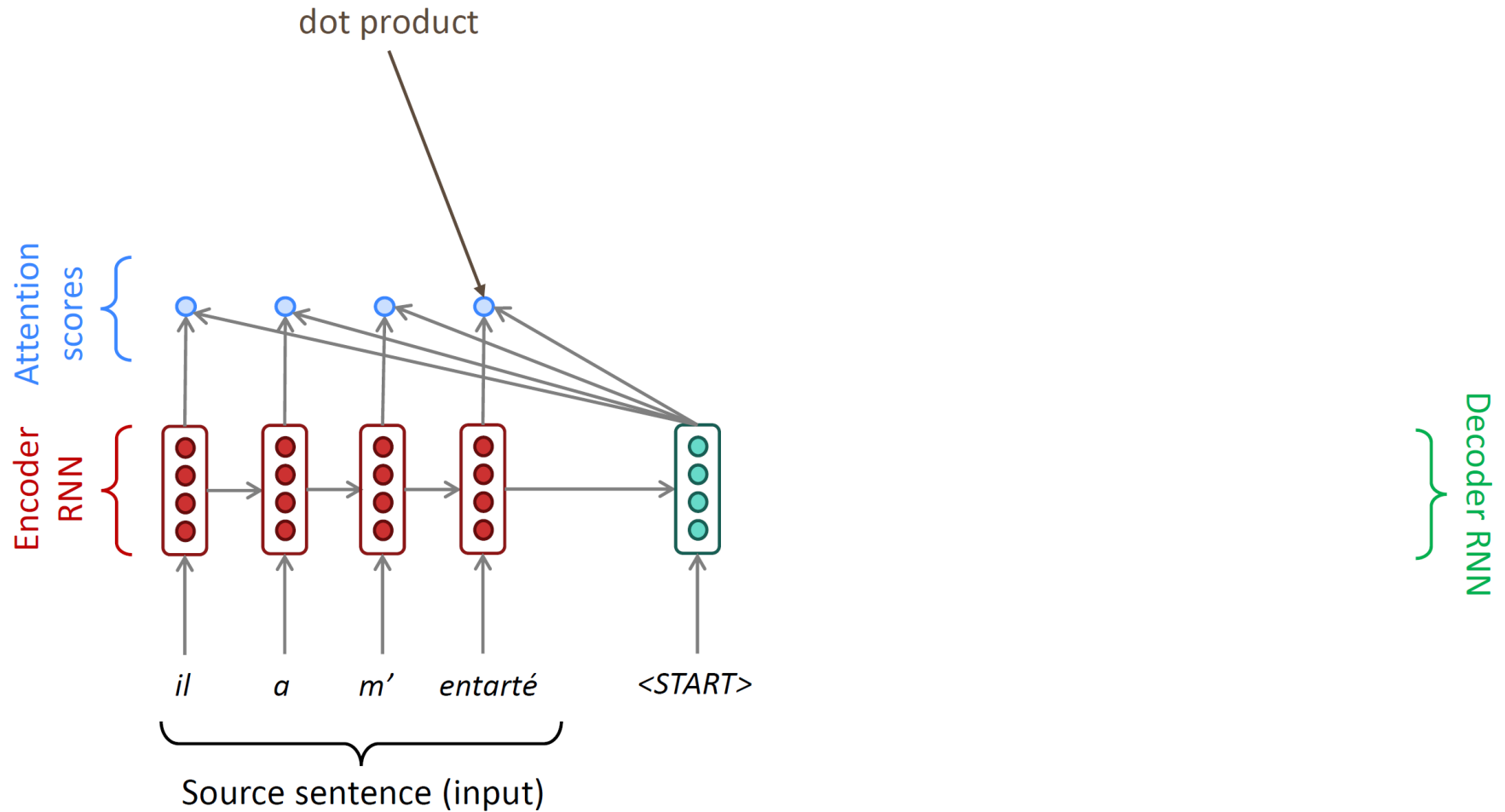




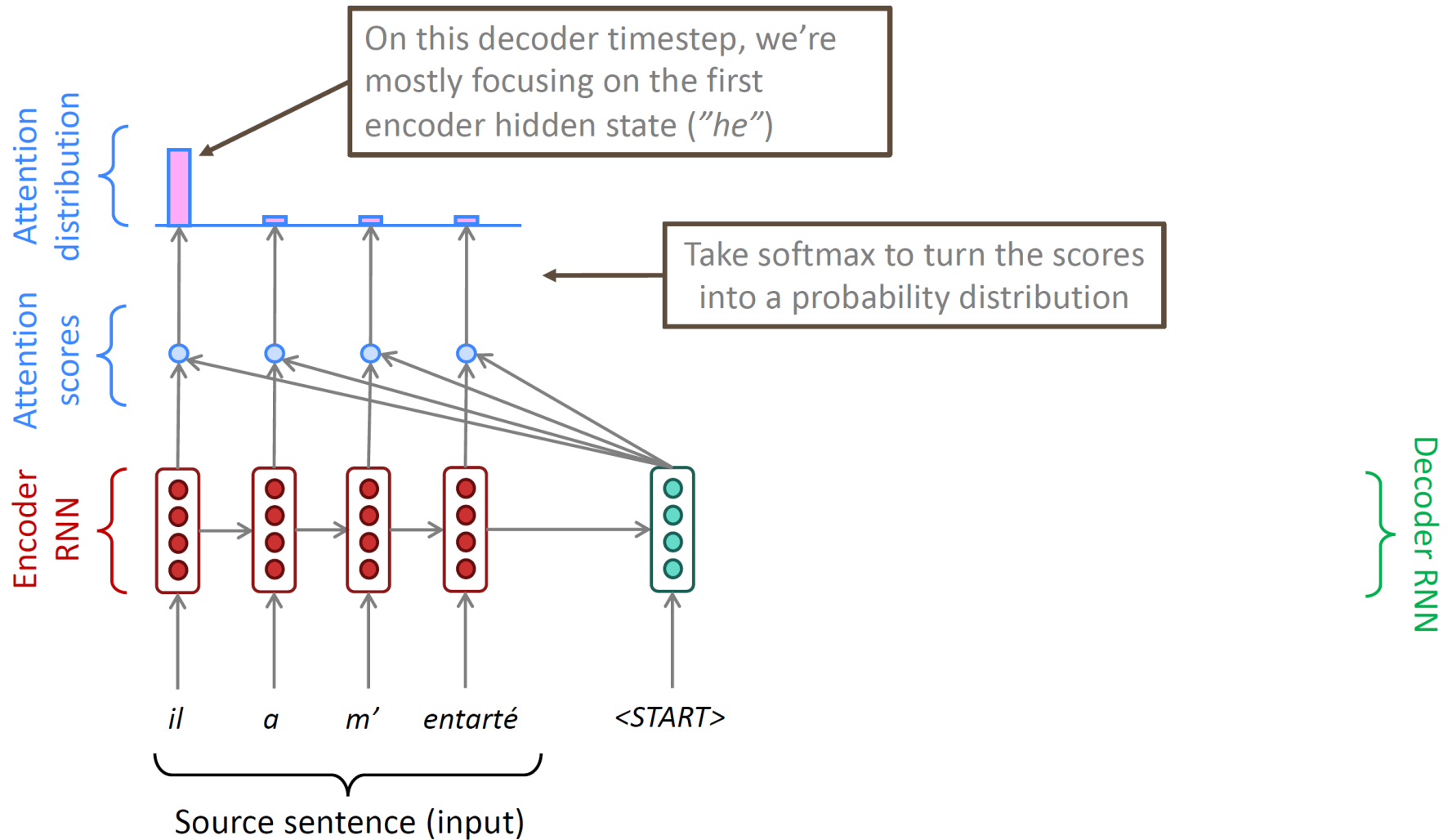
# Seq2Seq with Attention



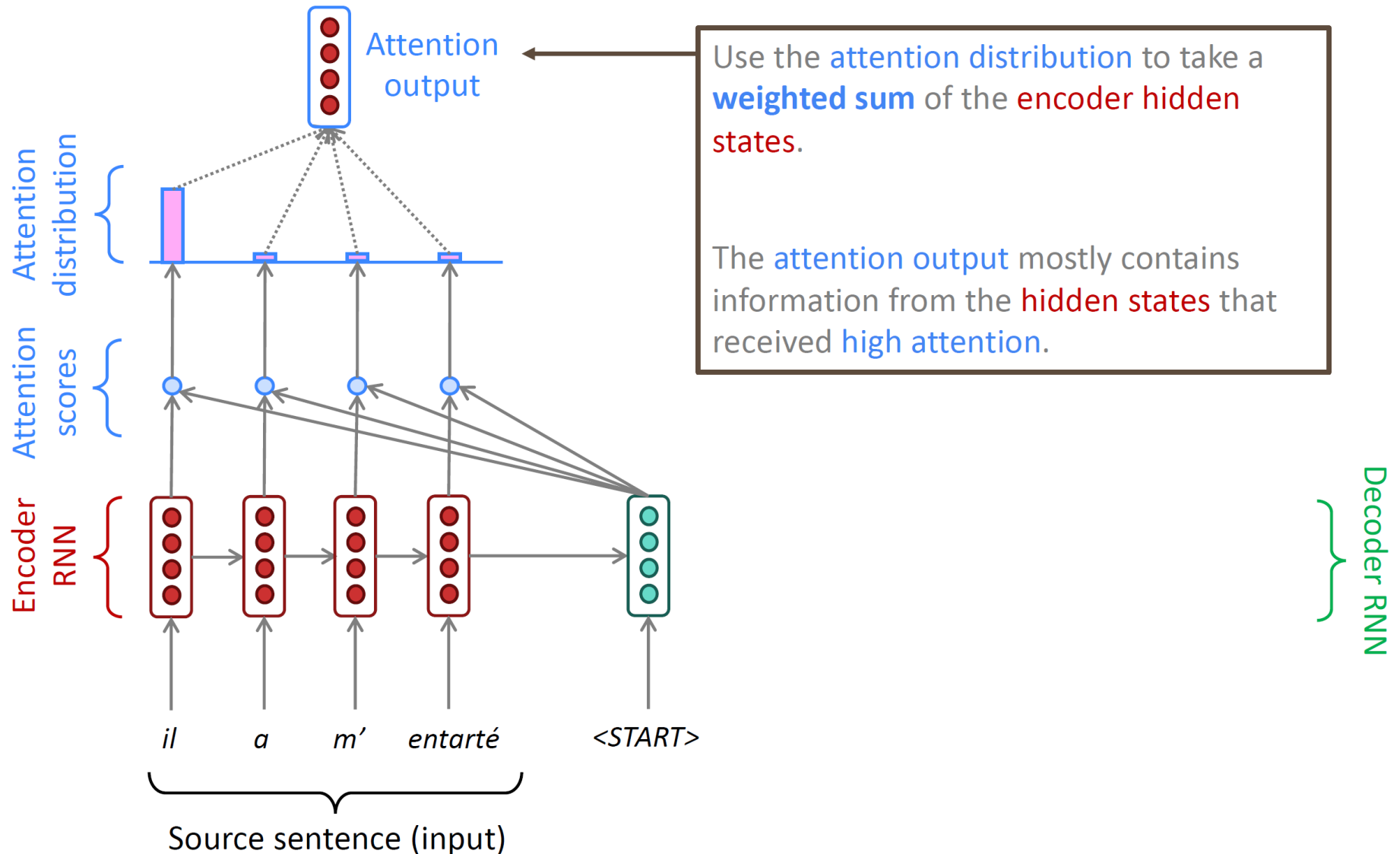
# Seq2Seq with Attention



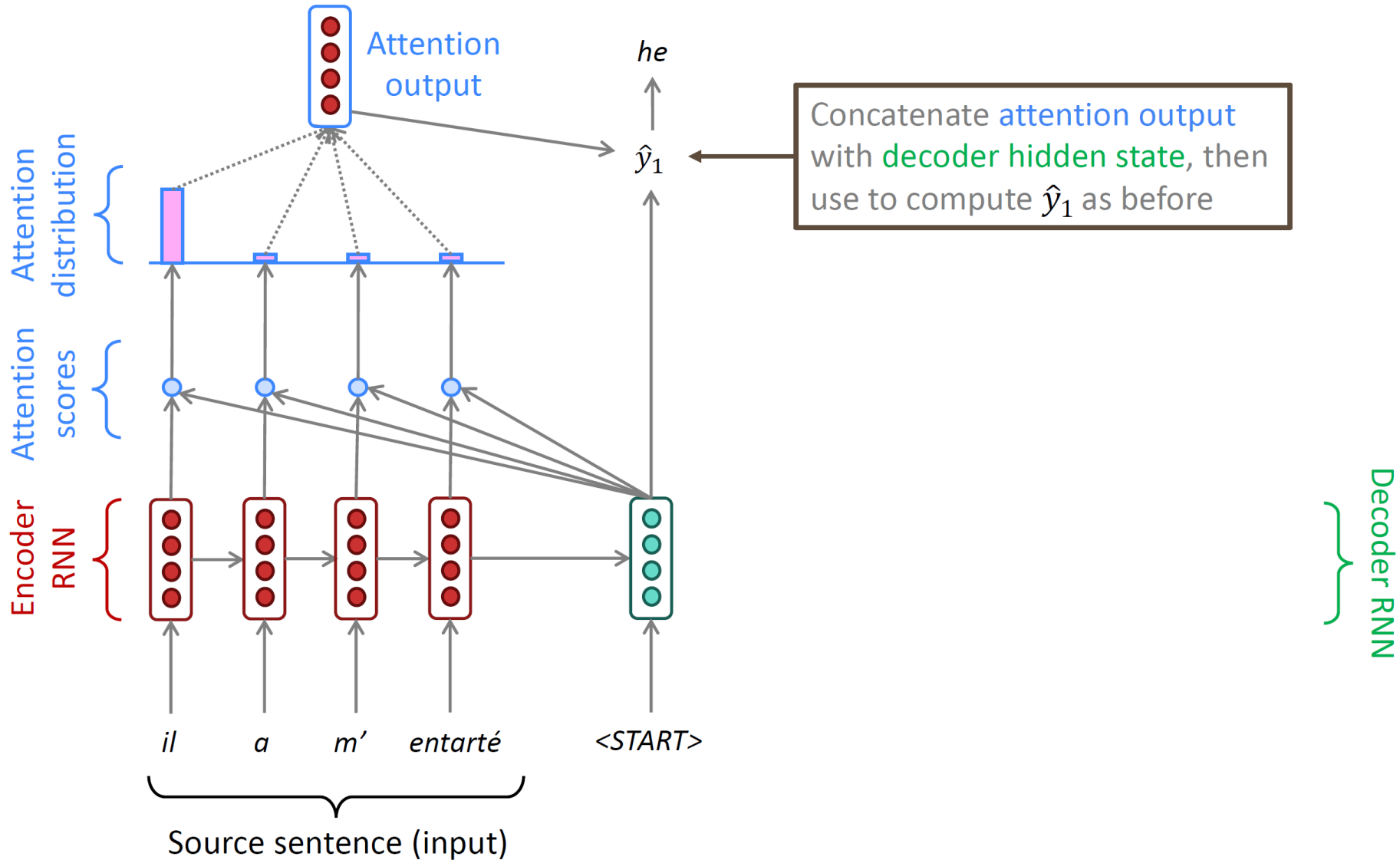
# Seq2Seq with Attention



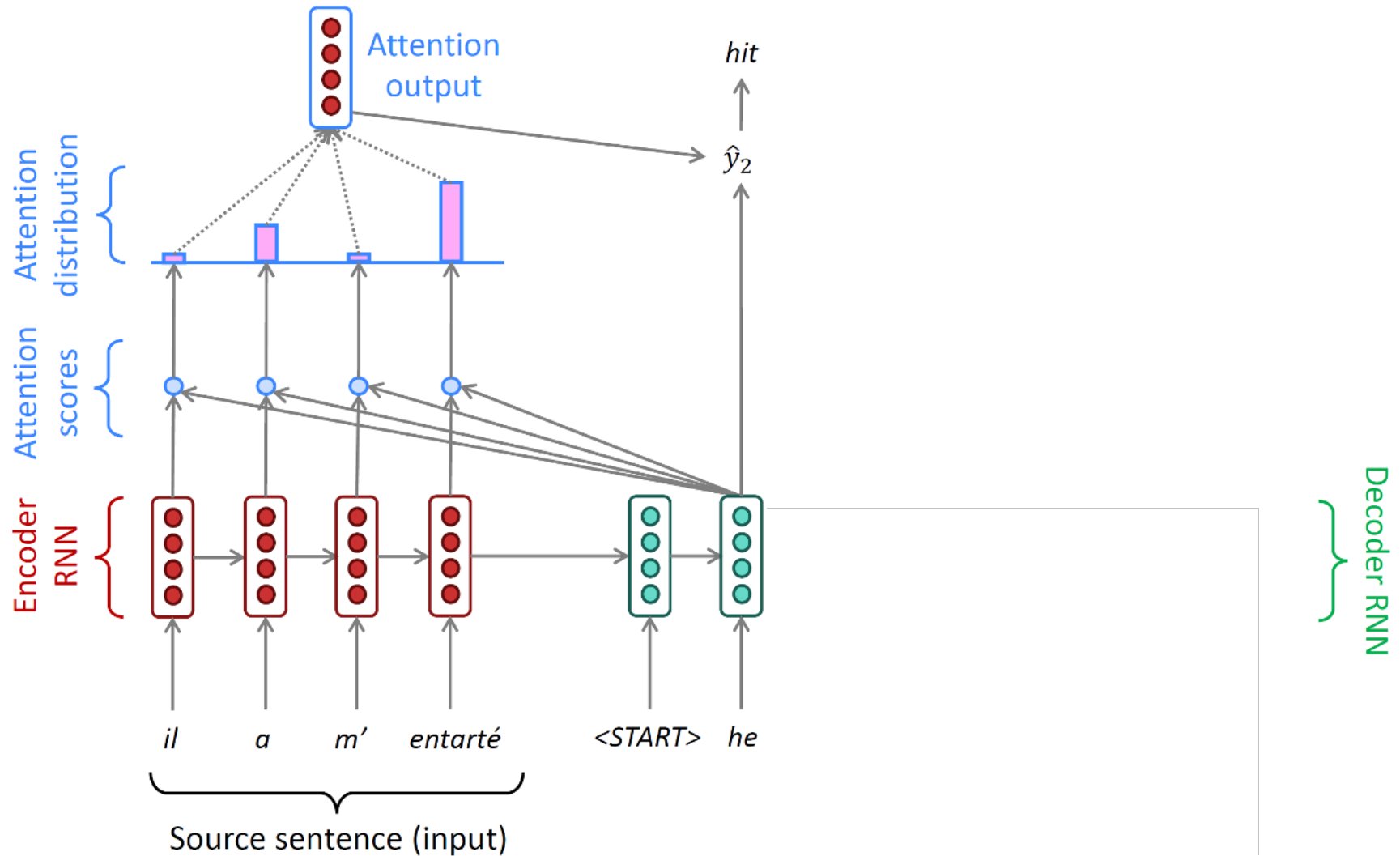
# Seq2Seq with Attention



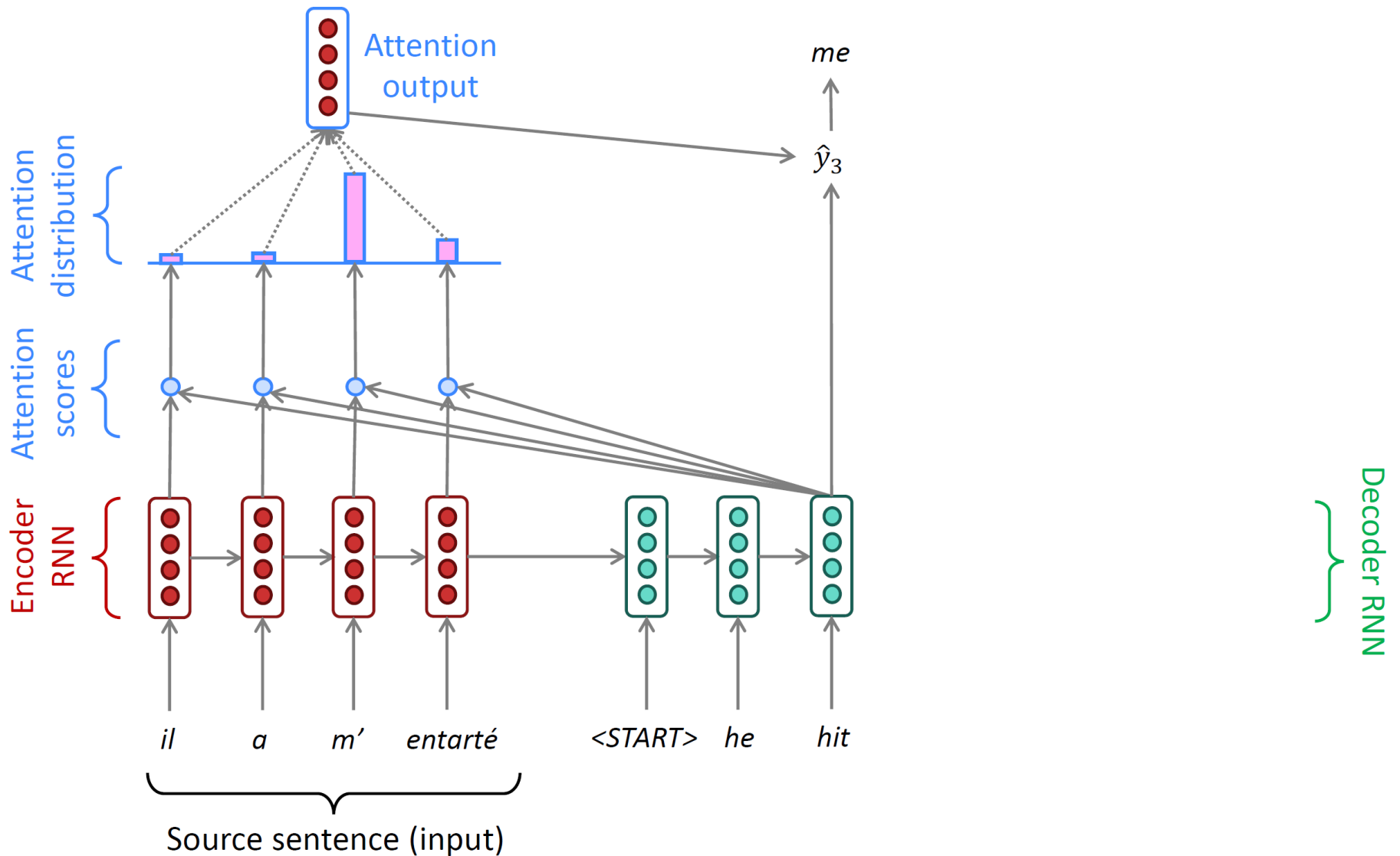
# Seq2Seq with Attention



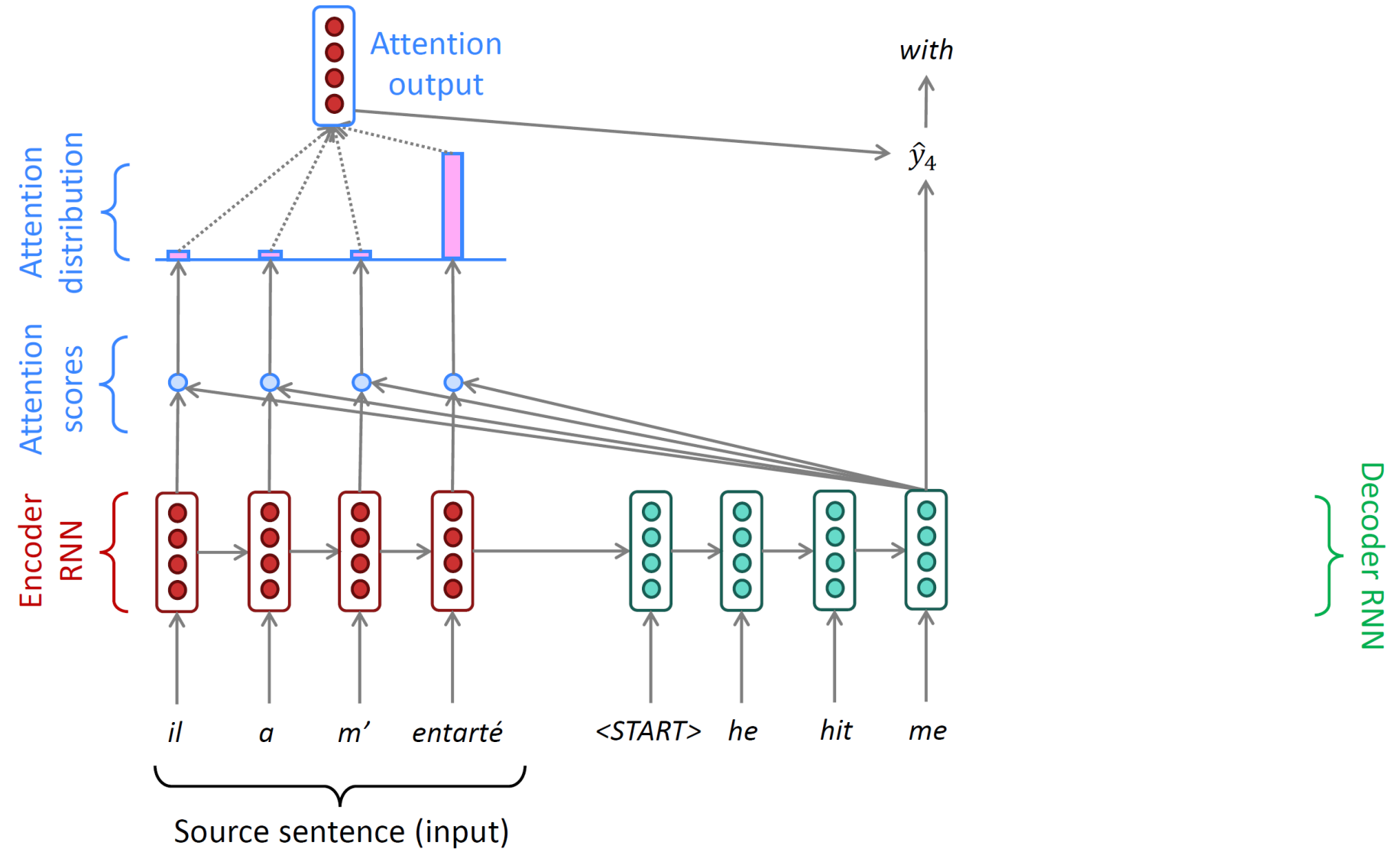
# Seq2Seq with Attention



# Seq2Seq with Attention

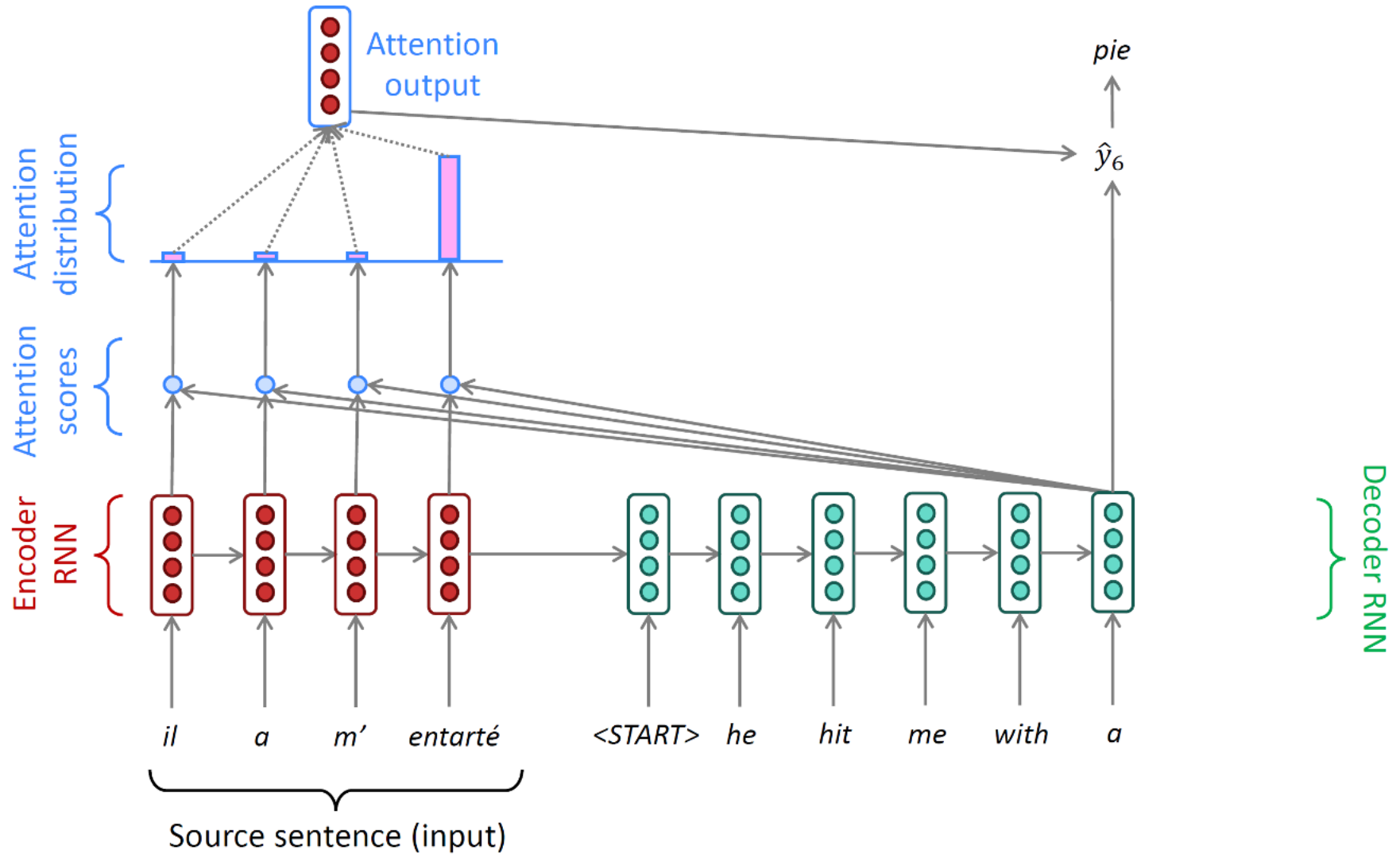


# Seq2Seq with Attention





# Seq2Seq with Attention



# Seq2Seq with Attention

## Summary

- Input sequence  $X$ , encoder  $f_{enc}$ , and decoder  $f_{dec}$
- $f_{enc}(X)$  produces hidden states  $h_1^{enc}, h_2^{enc}, \dots, h_N^{enc}$
- 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  $q$

	he	hit	me	with	a	pie
il						
a						
m'						
entarté						

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)

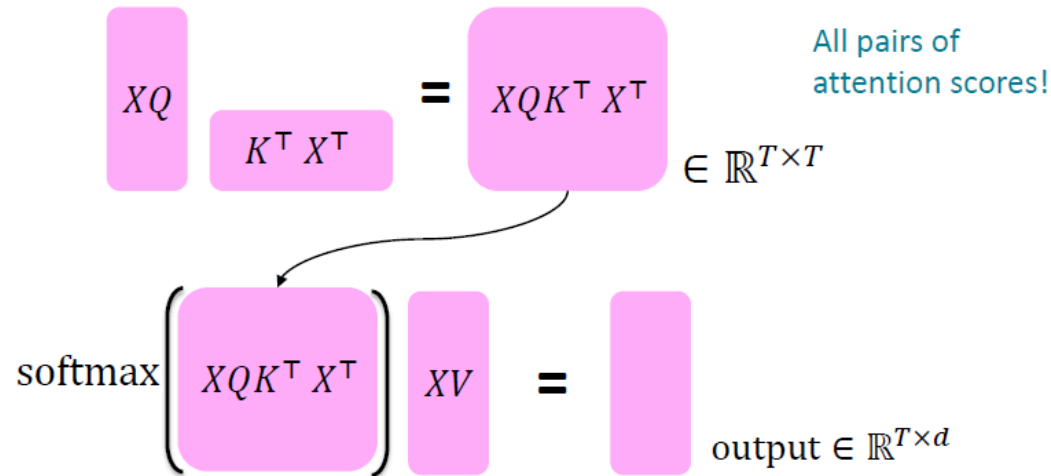
# Attention

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- 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:  $f(v_i, q) = u^\top \tanh(W_1 v_i + W_2 q)$

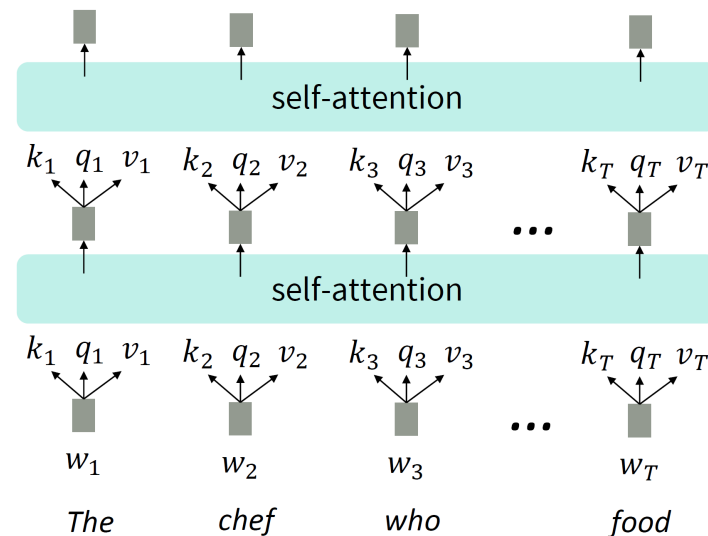
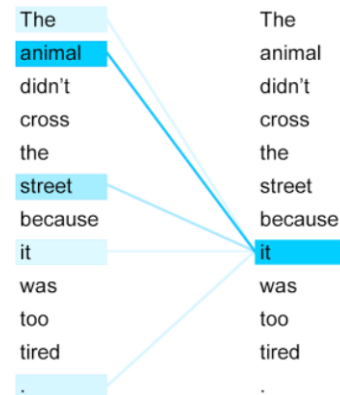
# Key-query-value attention

- 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
- $\alpha_{i,j} = \text{softmax}(q_i^\top k_j); \text{out}_i = \sum_k \alpha_{i,j} v_j$
- Intuition: key, query, and value can focus on different parts of input



# Attention is all you need (Vaswani '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

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- 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

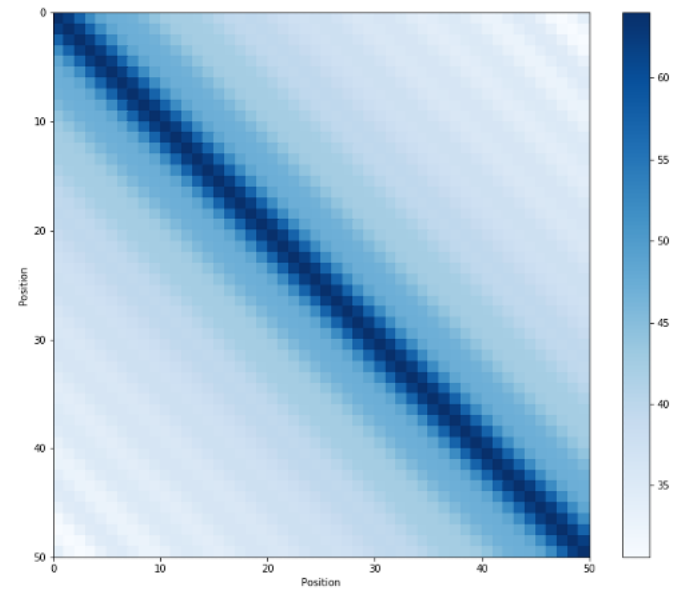
- Vanilla self-attention
  - $(k_t, v_t, q_t) = g_1(X_t; \theta)$
  - $\alpha_{t,j} = \text{softmax}(q_t^\top k_j)$
  - Attention output  $out_t = \sum_j \alpha_{t,j} v_j$
- Idea: position encoding:
  - $p_i$ : an embedding vector (feature) of position  $i$
  - $(k_t, v_t, q_t) = g_1([X_t, p_t]; \theta)$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

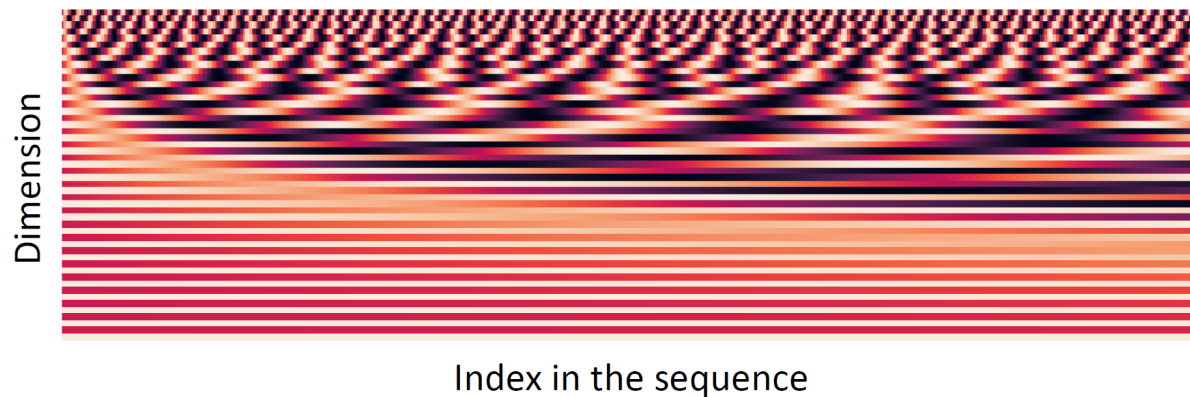
## $p_t$ design 1: Sinusoidal position representation

- 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

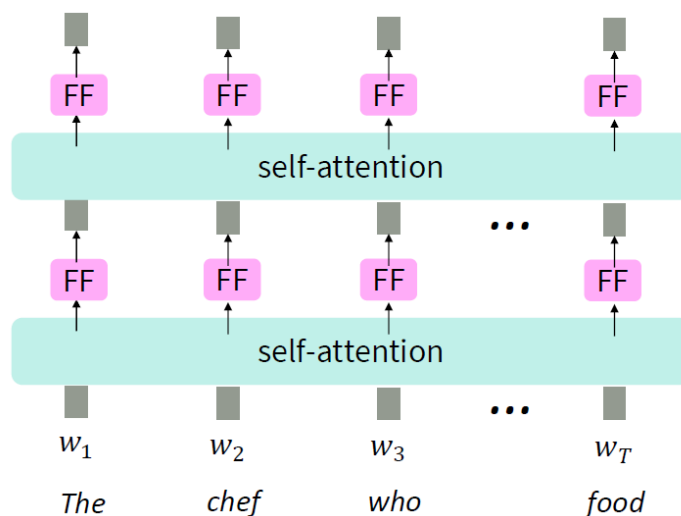
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## $p_t$ design 2: **Learned representation**

- 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  $L$

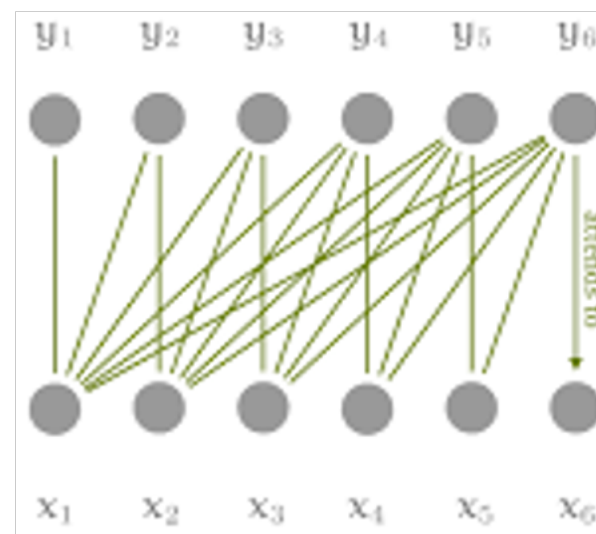
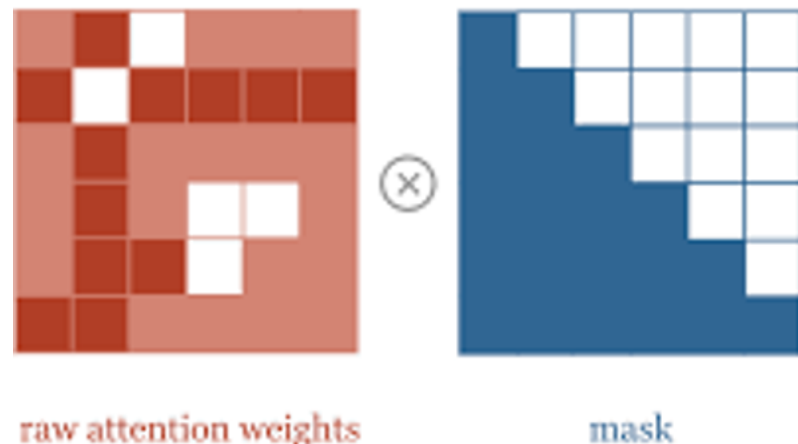
# Combine Self-Attention with Nonlinearity

- 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 softmax



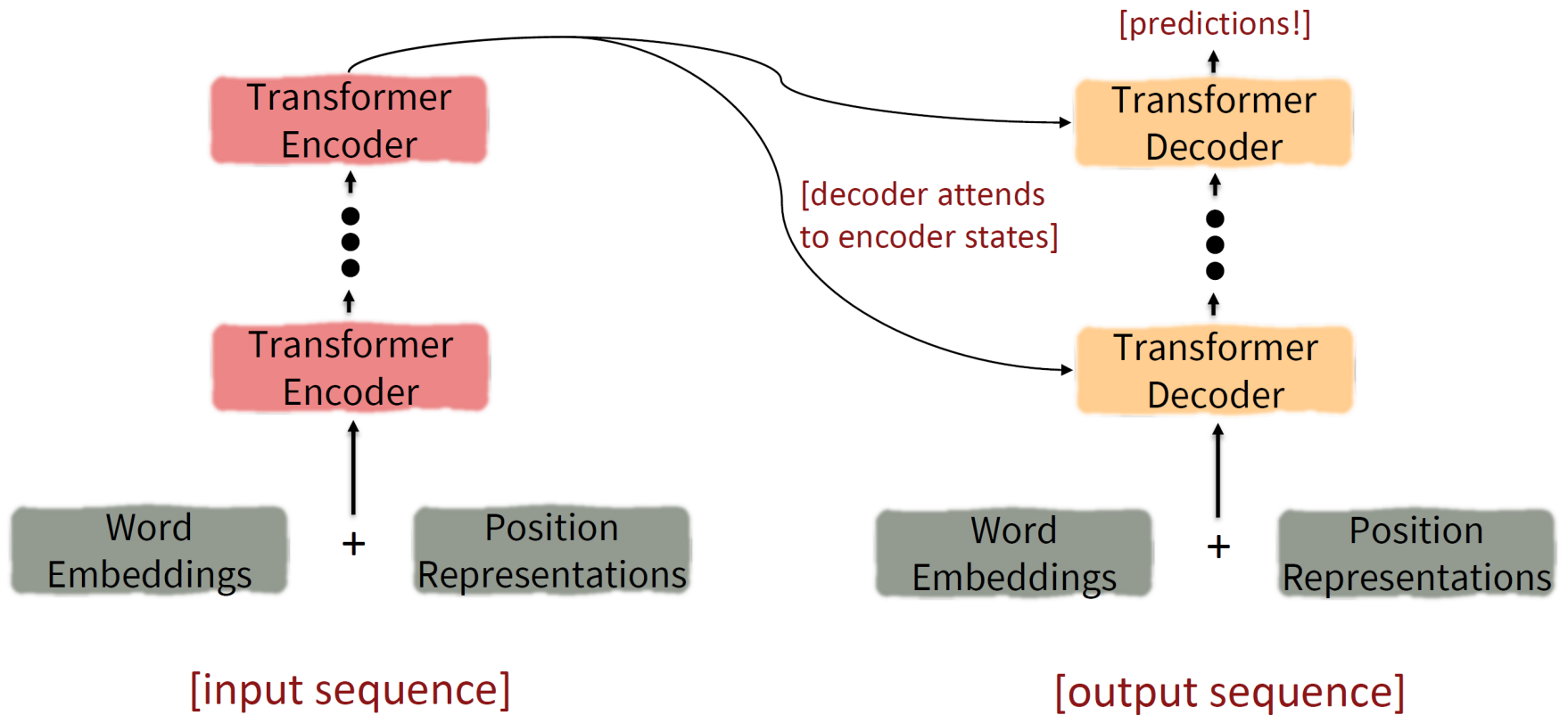
# Masked Attention

- 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 usual
  - 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



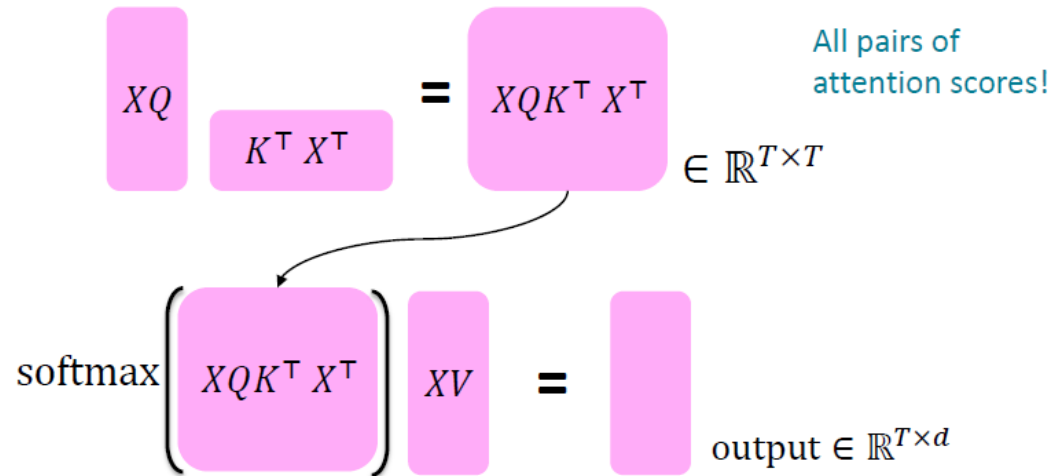
# Transformer

## Transformer-based sequence-to-sequence modeling



# Key-query-value attention

- Obtain  $q_t, v_t, k_t$  from  $X_t$
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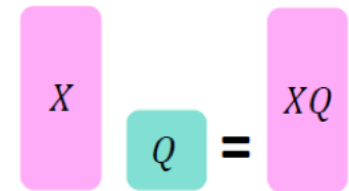


# Multi-headed attention

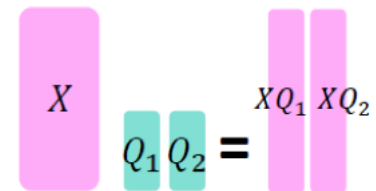
- Standard attention: single-headed attention
  - $X_t \in \mathbb{R}^d, Q, K, V \in \mathbb{R}^{d \times d}$
  - We only look at a single position  $j$  with high  $\alpha_{i,j}$
  - What if we want to look at different  $j$  for different reasons?
- Idea: define  $h$  separate attention heads
  - $h$  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!**

**Single-head attention**  
(just the query matrix)

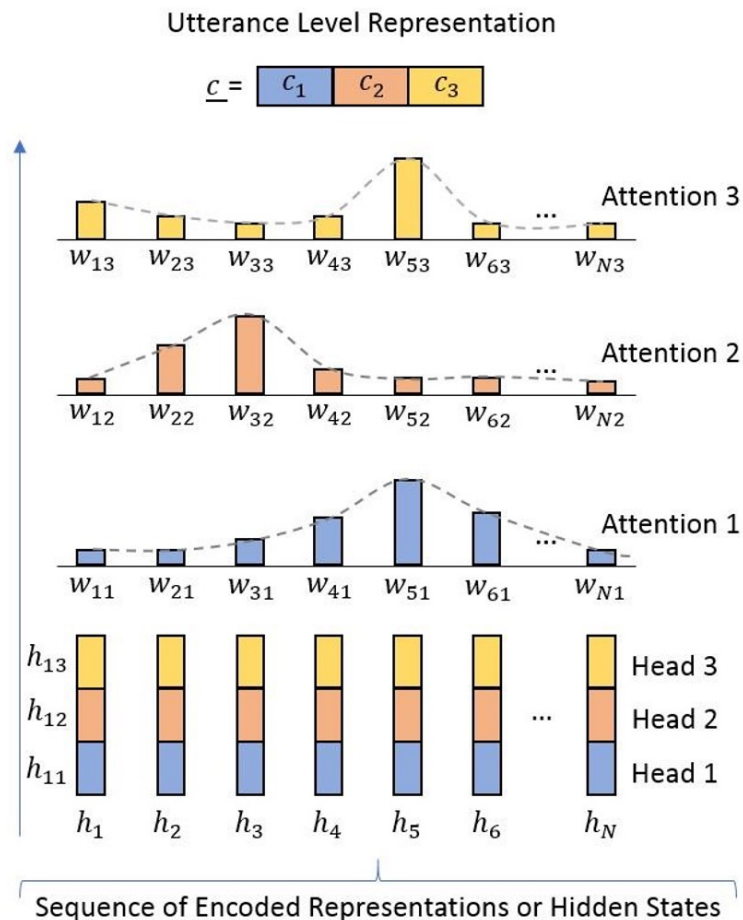


**Multi-head attention**  
(just two heads here)



# 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  $\alpha_{i,j}$
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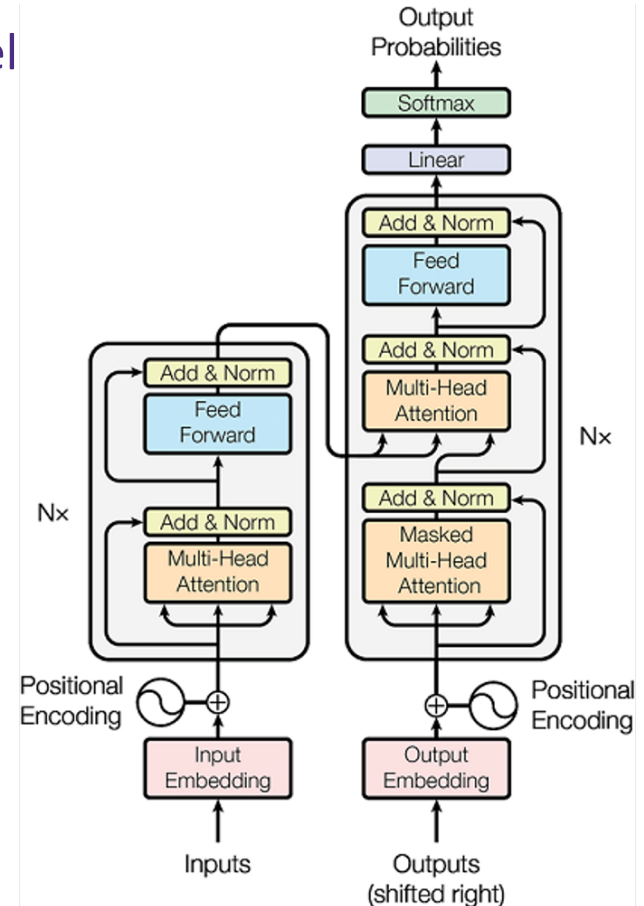




# Transformer

## 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	<b>41.29</b>	$7.7 \cdot 10^{19}$	$1.2 \cdot 10^{21}$
Transformer (base model)	27.3	38.1	<b><math>3.3 \cdot 10^{18}</math></b>	
Transformer (big)	<b>28.4</b>	<b>41.8</b>	$2.3 \cdot 10^{19}$	

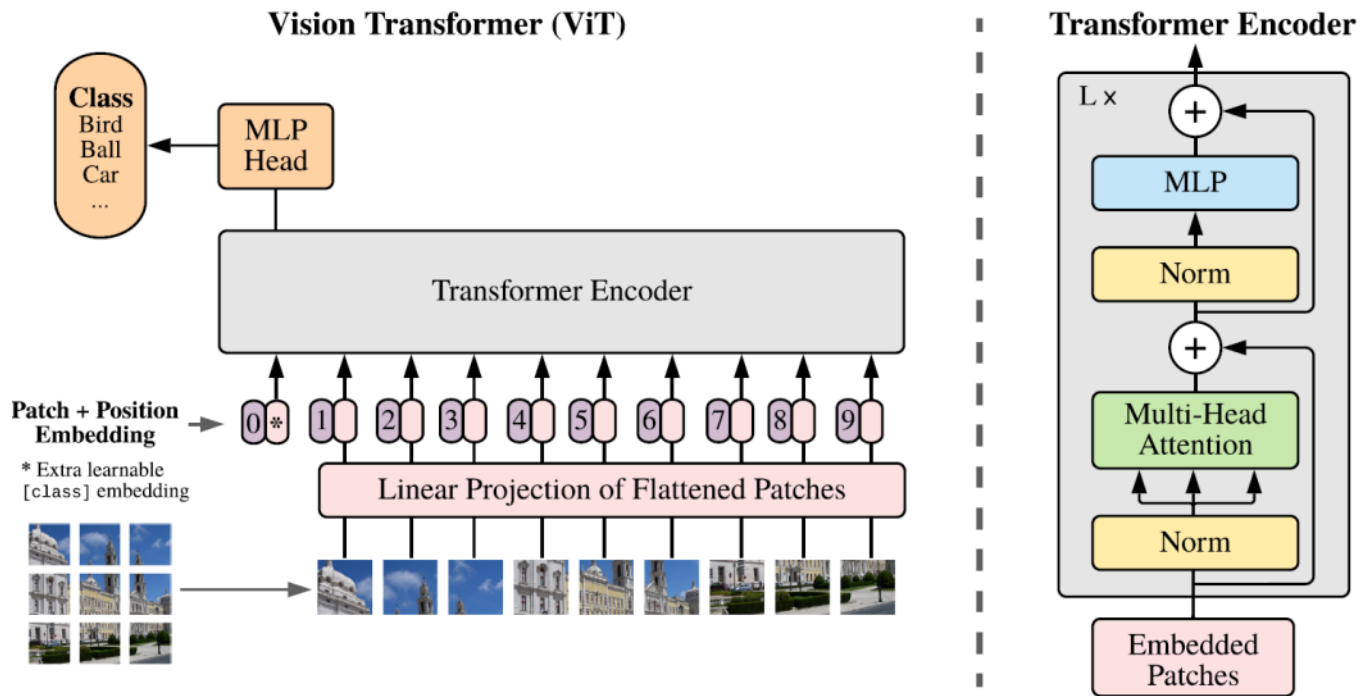
# Transformer

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- 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)

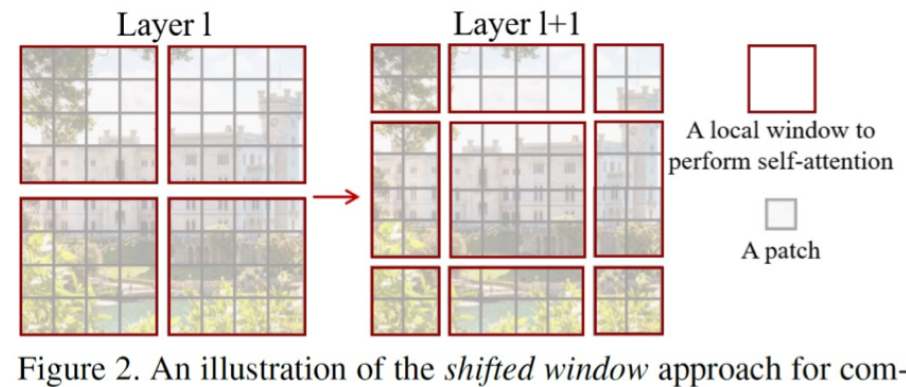
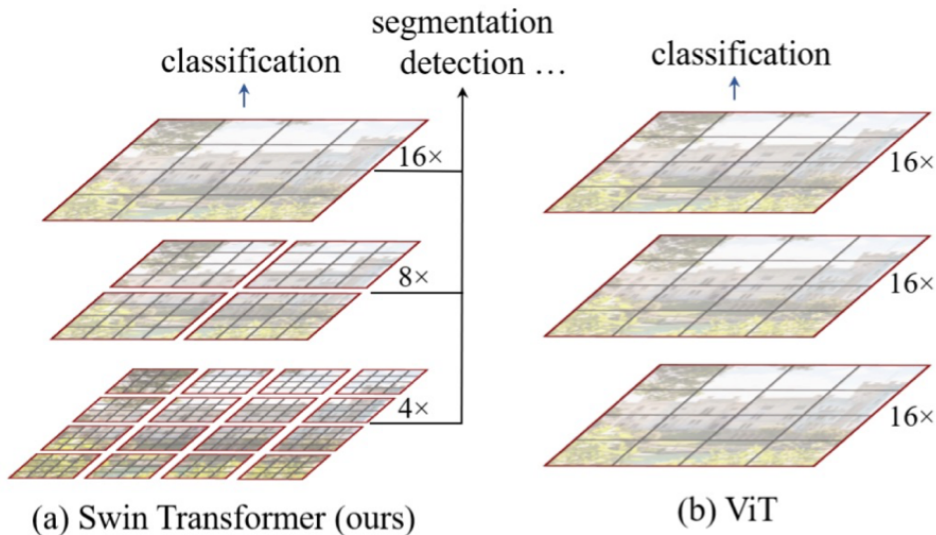
# Transformer for Images

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

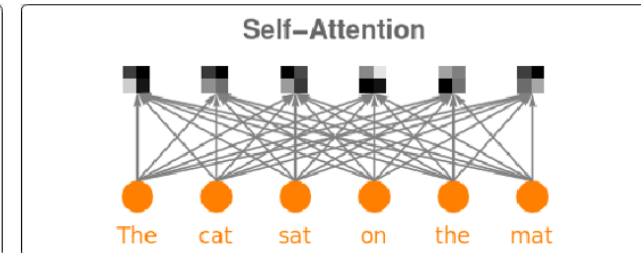
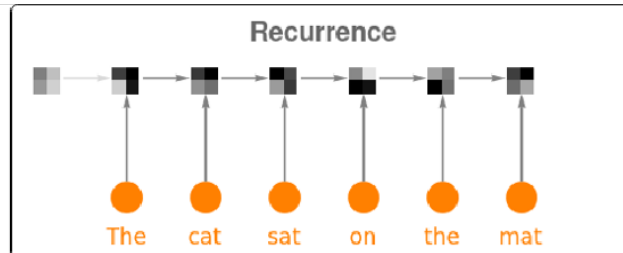
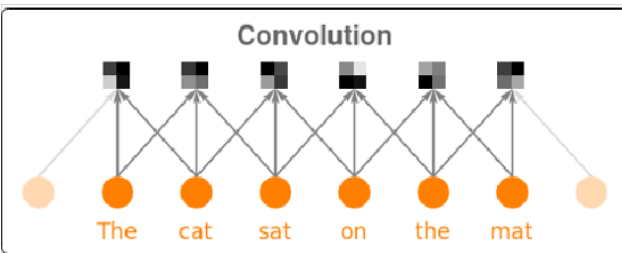


# Transformer for Images

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



# CNN vs. RNN vs. Attention



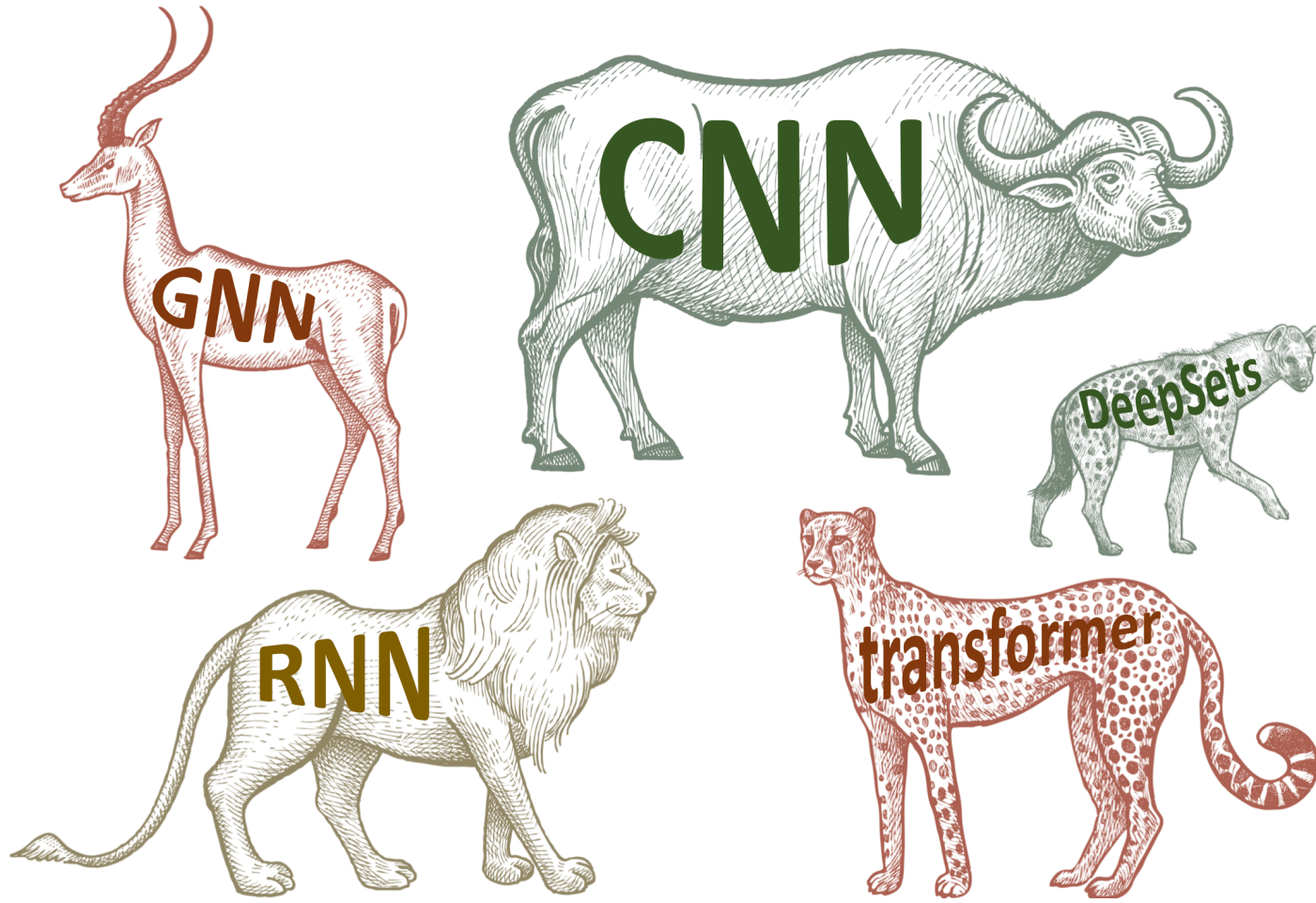
# Summary

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- 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

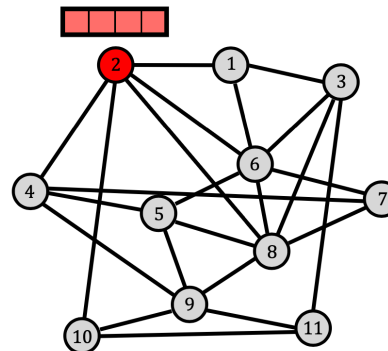
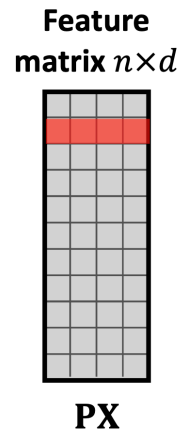
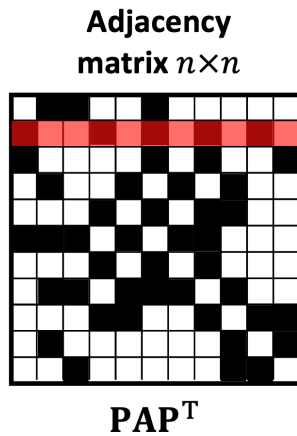
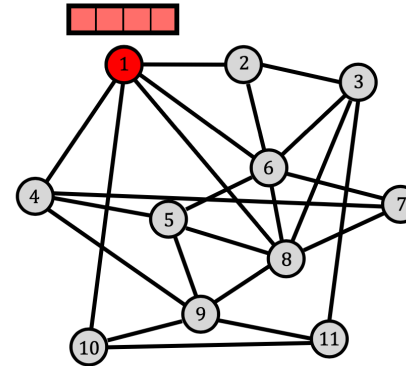
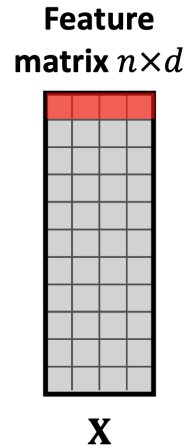
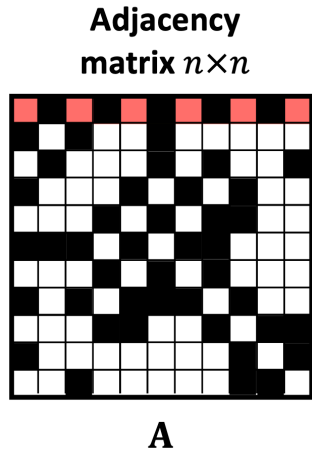
# Other architectures

---





# Graph Neural Networks



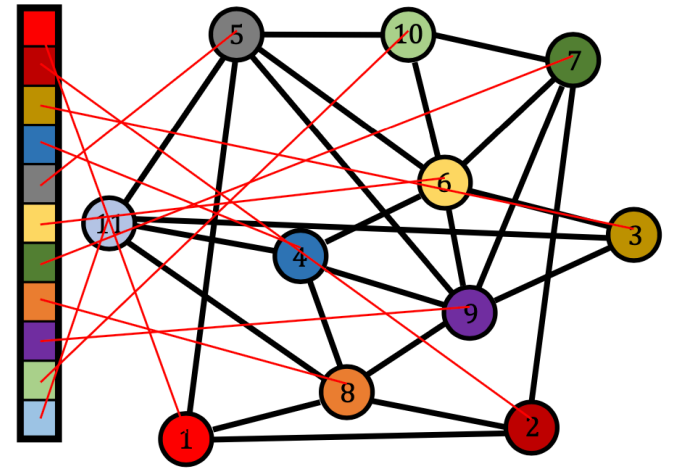
arbitrary ordering of nodes

# Graph Neural Networks

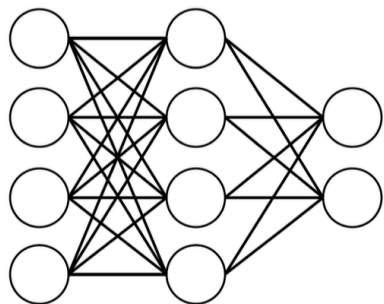
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permutation-equivariant

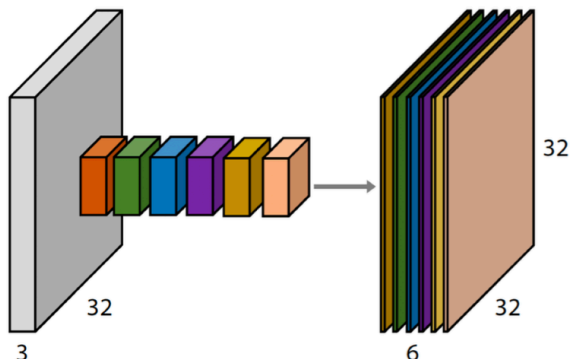
$$\mathbf{F}(\mathbf{P}\mathbf{X}, \mathbf{P}\mathbf{A}\mathbf{P}^{\top}) = \mathbf{P}\mathbf{F}(\mathbf{X}, \mathbf{A})$$



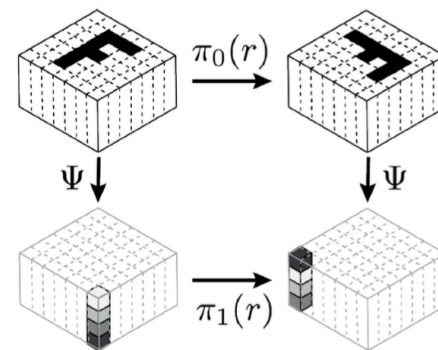
# Geometric Deep Learning



**Perceptrons**  
Function regularity



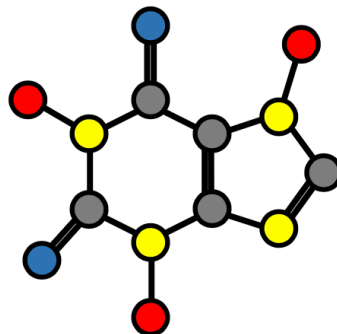
**CNNs**  
Translation



**Group-CNNs**  
Translation+Rotation



**DeepSets / Transformers**  
Permutation



**GNNs**  
Permutation



**Intrinsic CNNs**  
Local frame choice

# Supervised Learning Process

---

Collect a **dataset**

Decide on a **model**

Find the function which fits the data best

**Choose a loss function**

**Pick the function which minimizes loss  
on data**

Use function to make prediction on new  
examples

# Framework

---

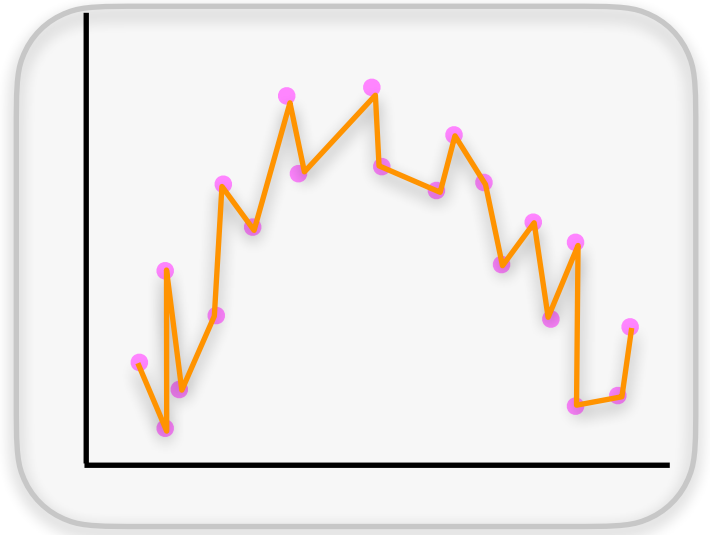
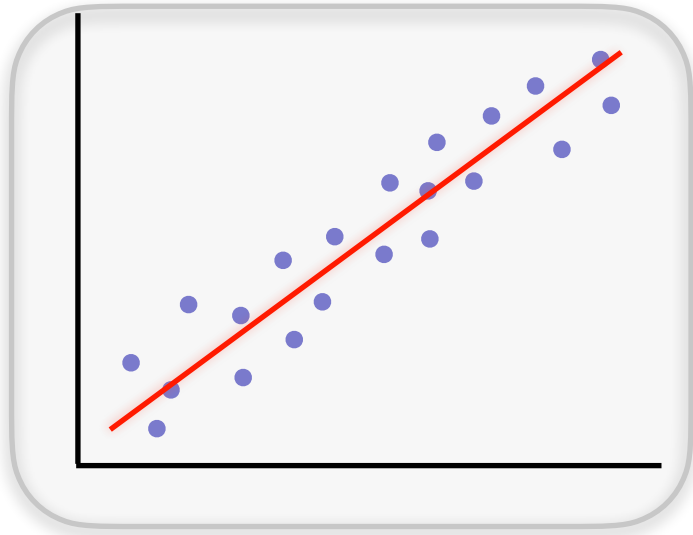
# Approximation Theory

---



# Expressivity / Representation Power

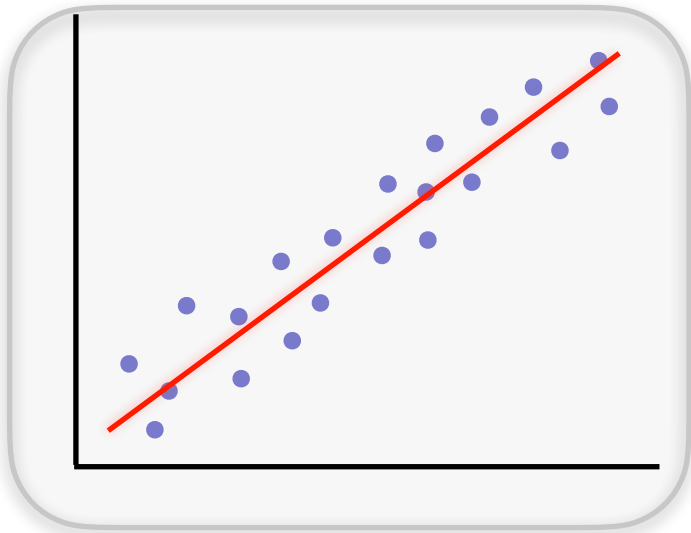
---



Expressive: Functions in class can represent “complicated” functions.

# Linear Function

---



best linear fit



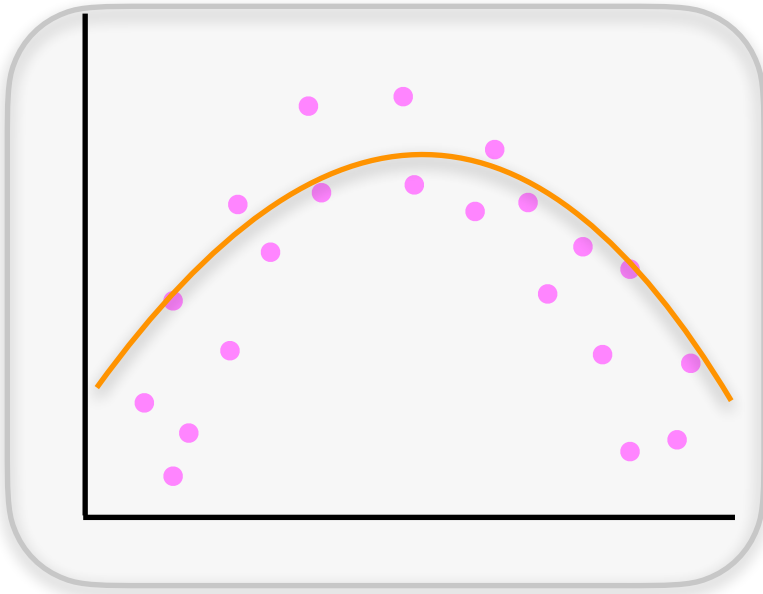
# Review: generalized linear regression

Transformed data:

$$h(x) = \begin{bmatrix} h_1(x) \\ h_2(x) \\ \vdots \\ h_p(x) \end{bmatrix}$$

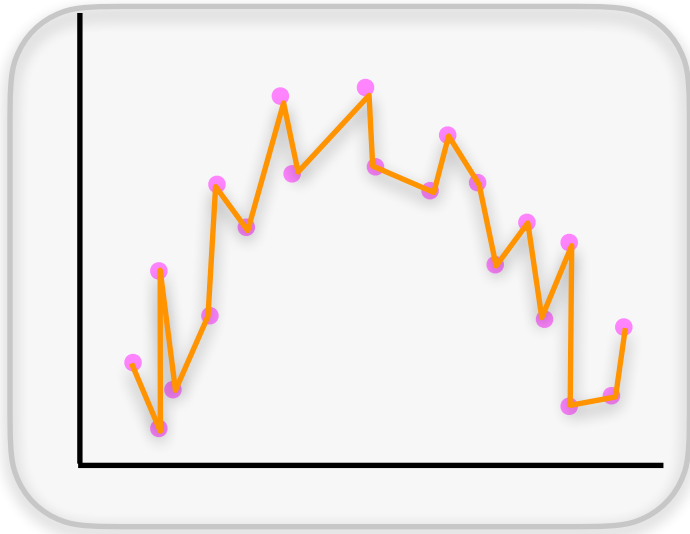
Hypothesis: linear in  $h$

$$y_i \approx h(x_i)^T w$$



# Review: Polynomial Regression

---



# Approximation Theory Setup

---

- Goal: to show there exists a neural network that has small error on training / test set.

- Set up a natural baseline:

$$\inf_{f \in \mathcal{F}} L(f) \text{ v.s. } \inf_{g \in \text{continuous functions}} L(g)$$

# Example

---

# Decomposition

---

# Specific Setups

---

- “Average” approximation: given a distribution  $\mu$

$$\|f - g\|_{\mu} = \int_x |f(x) - g(x)| d\mu(x)$$

- “Everywhere” approximation

$$\|f - g\|_{\infty} = \sup_x |f(x) - g(x)| \geq \|f - g\|_{\mu}$$

# Polynomial Approximation

---

**Theorem (Stone-Weierstrass):** for any function  $f$ , we can **approximate it** on any compact set  $\Omega$  by a sufficiently high degree polynomial: for any  $\epsilon > 0$ , there exists a polynomial  $p$  of sufficient high degree, s.t.,

$$\max_{x \in \Omega} |f(x) - p(x)| \leq \epsilon.$$

Intuition: **Taylor expansion!**

# Kernel Method

---

**Polynomial kernel**

**Gaussian Kernel**



# 1D Approximation

---

**Theorem:** Let  $g : [0,1] \rightarrow \mathbb{R}$ , and  $\rho$ -Lipschitz. For any  $\epsilon > 0$ ,  $\exists$  2-layer neural network  $f$  with  $\lceil \frac{\rho}{\epsilon} \rceil$  nodes, threshold activation:  $\sigma(z) : z \mapsto \mathbf{1}\{z \geq 0\}$  such that

$$\sup_{x \in [0,1]} |f(x) - g(x)| \leq \epsilon.$$

# Proof of 1D Approximation

---

# Multivariate Approximation

**Theorem:** Let  $g$  be a continuous function that satisfies  $\|x - x'\|_\infty \leq \delta \Rightarrow |g(x) - g(x')| \leq \epsilon$  (Lipschitzness). Then there exists a **3-layer ReLU neural network** with  $O(\frac{1}{\delta^d})$  nodes that satisfy

$$\int_{[0,1]^d} |f(x) - g(x)| dx = \|f - g\|_1 \leq \epsilon$$

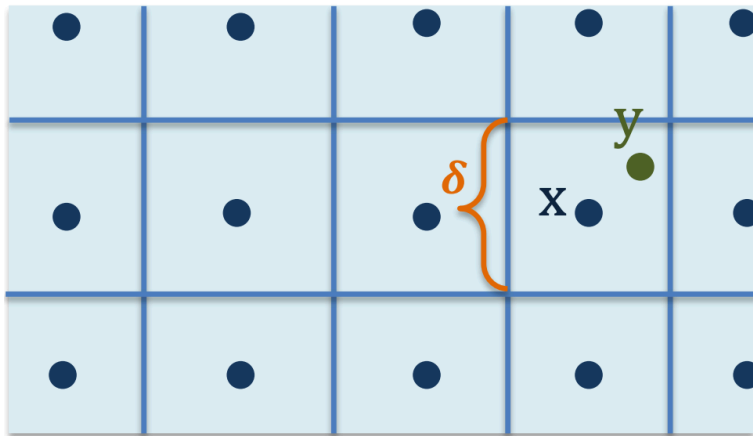
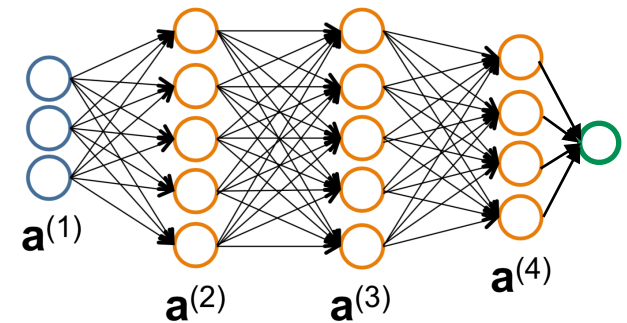


Figure credit to Andrej Risteski



# Partition Lemma

**Lemma:** let  $g, \delta, \epsilon$  be given. For any partition  $P$  of  $[0,1]^d$ ,  $P = (R_1, \dots, R_N)$  with all side length smaller than  $\delta$ , there exists  $(\alpha_1, \dots, \alpha_N) \in \mathbb{R}^N$  such that

$$\sup_{x \in [0,1]^d} |g(x) - h(x)| \leq \epsilon \text{ with } h(x) := \sum_{i=1}^N \alpha_i \mathbf{1}_{R_i}(x).$$

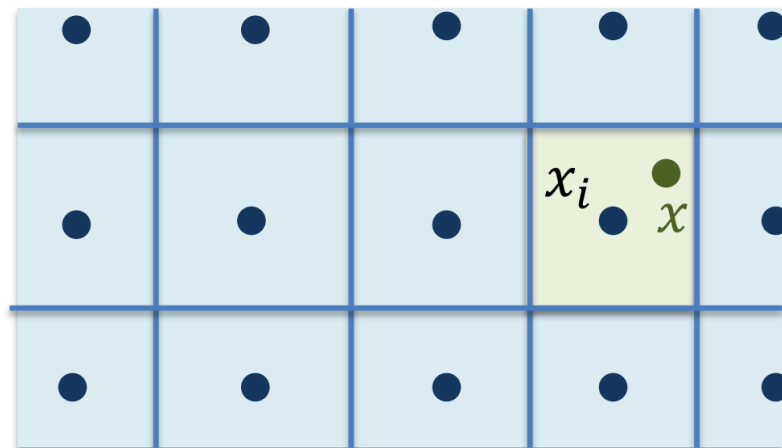


Figure credit to Andrej Risteski

# Proof of Partition Lemma

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# Proof of Multivariate Approximation Theorem

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# Proof of Multivariate Approximation Theorem

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# Proof of Multivariate Approximation Theorem

---



# Universal Approximation

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**Definition:** A class of functions  $\mathcal{F}$  is **universal approximator** over a compact set  $S$  (e.g.,  $[0,1]^d$ ), if for every continuous function  $g$  and a target accuracy  $\epsilon > 0$ , there exists  $f \in \mathcal{F}$  such that

$$\sup_{x \in S} |f(x) - g(x)| \leq \epsilon$$

# Stone-Weierstrass Theorem

---

**Theorem:** If  $\mathcal{F}$  satisfies

1. Each  $f \in \mathcal{F}$  is continuous.
2.  $\forall x, \exists f \in \mathcal{F}, f(x) \neq 0$
3.  $\forall x \neq x', \exists f \in \mathcal{F}, f(x) \neq f(x')$
4.  $\mathcal{F}$  is closed under multiplication and vector space operations,

Then  $\mathcal{F}$  is a universal approximator:

$$\forall g : S \rightarrow R, \epsilon > 0, \exists f \in \mathcal{F}, \|f - g\|_{\infty} \leq \epsilon.$$

# Example: cos activation

---

# Example: cos activation

---

# Other Examples

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**Exponential activation**

**ReLU activation**

# Curse of Dimensionality

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- Unavoidable in the worse case

# Barron's Theory

---

- Can we avoid the curse of dimensionality for “nice” functions?
- What are nice functions?
  - Fast decay of the Fourier coefficients
- Fourier basis functions:  
 $\{e_w(x) = e^{i\langle w, x \rangle} = \cos(\langle w, x \rangle) + i \sin(\langle w, x \rangle) \mid w \in \mathbb{R}^d\}$
- Fourier coefficient:  $\hat{f}(w) = \int_{\mathbb{R}^d} f(x) e^{-i\langle w, x \rangle} dx$
- Fourier integral / representation:  $f(x) = \int_{\mathbb{R}^d} \hat{f}(w) e^{i\langle w, x \rangle} dw$

# Barron's Theorem

**Definition:** The Barron constant of a function  $f$  is:

$$C \triangleq \int_{\mathbb{R}^d} \|w\|_2 |\hat{f}(w)| dw.$$

**Theorem (Barron '93):** For any  $g : \mathbb{B}_1 \rightarrow \mathbb{R}$  where  $\mathbb{B}_1 = \{x \in \mathbb{R} : \|x\|_2 \leq 1\}$  is the unit ball, there exists a

3-layer neural network  $f$  with  $O(\frac{C^2}{\epsilon})$  neurons and

sigmoid activation function such that

$$\int_{\mathbb{B}_1} (f(x) - g(x))^2 dx \leq \epsilon.$$



# Examples

---

- Gaussian function:  $f(x) = (2\pi\sigma^2)^{d/2} \exp\left(-\frac{\|x\|_2^2}{2\sigma^2}\right)$
- Other functions:
  - Polynomials
  - Function with bounded derivatives

# Proof Ideas for Barron's Theorem

---

**Step 1:** show any continuous function can be written as an **infinite neural network** with cosine-like activation functions.

(Tool: Fourier representation.)

**Step 2:** Show that a function with small Barron constant can be **approximated** by a convex combination of a **small number** of cosine-like activation functions.

(Tool: subsampling / probabilistic method.)

**Step 3:** Show that the cosine function can be approximated by sigmoid functions.

(Tool: classical approximation theory.)

# Simple Infinite Neural Nets

**Definition:** An infinite-wide neural network is defined by a signed measure  $\nu$  over neuron weights  $(w, b)$

$$f(x) = \int_{w \in \mathbb{R}^d, b \in \mathbb{R}} \sigma(w^\top x + b) d\nu(w, b).$$

**Theorem:** Suppose  $g : \mathbb{R} \rightarrow \mathbb{R}$  is differentiable, if  $x \in [0, 1]$ , then  $g(x) = \int_0^1 \mathbf{1}\{x \geq b\} \cdot g'(b) db + g(0)$

# Step 1: Infinite Neural Nets

---

The function can be written as

$$f(x) = f(0) + \int_{\mathbb{R}^d} |\hat{f}(w)| (\cos(b_w + \langle w, x \rangle) - \cos(b_w)) dw.$$

## Step 2: Subsampling

---

Writing the function as the expectation of a random variable:

$$f(x) = f(0) + \int_{\mathbb{R}^d} \frac{|\hat{f}(w)| \|w\|_2}{C} \left( \frac{C}{\|w\|_2} (\cos(b_w + \langle w, x \rangle) - \cos(b_w)) \right) dw.$$

Sample one  $w \in \mathbb{R}^d$  with probability  $\frac{|\hat{f}(w)| \|w\|_2}{C}$  for  $r$  times.

## Step 3: Approximating the Cosines

---

**Lemma:** Given  $g_w(x) = \frac{C}{\|w\|_2}(\cos(b_w + \langle w, x \rangle) - \cos(b_w))$ , there exists a 2-layer neural network  $f_0$  of size  $O(1/\epsilon)$  with sigmoid activations, such that  $\sup_{x \in [-1, 1]} |f_0(y) - h_w(y)| \leq \epsilon$ .

# Depth Separation

---

So far we only talk about 2-layer or 3-layer neural networks.

Why we need **Deep** learning?

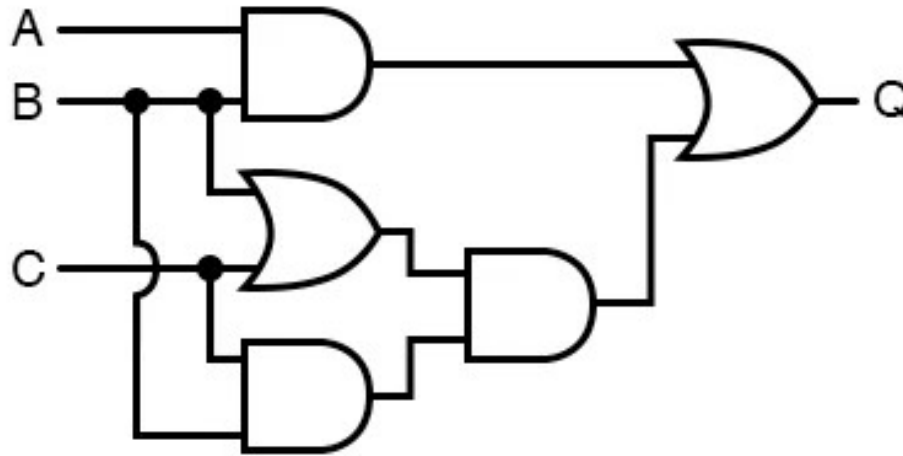
Can we show deep neural networks are **strictly** better than shallow neural networks?

# A brief history of depth separation

---

Early results from theoretical computer science

**Boolean circuits:** a directed acyclic graph model for computation over binary inputs; each node (“gate”) performs an operation (e.g. OR, AND, NOT) on the inputs from its predecessors.





# A brief history of depth separation

---

Early results from theoretical computer science

**Boolean circuits:** a directed acyclic graph model for computation over binary inputs; each node (“gate”) performs an operation (e.g. OR, AND, NOT) on the inputs from its predecessors.

**Depth separation:** the difference of the computation power: shallow vs deep Boolean circuits.

**Håstad ('86):** **parity** function cannot be approximated by a small **constant-depth** circuit with OR and AND gates.

# Modern depth-separation in neural networks

---

- **Related architectures / models of computation**
  - Sum-product networks [Bengio, Delalleau '11]
- **Heuristic measures of complexity**
  - Bound of number of linear regions for ReLU networks [Montufar, Pascanu, Cho, Bengio '14]
- **Approximation error**
  - A small deep network cannot be approximated by a small shallow network [Telgarsky '15]

# Shallow Nets Cannot Approximate Deep Nets

---

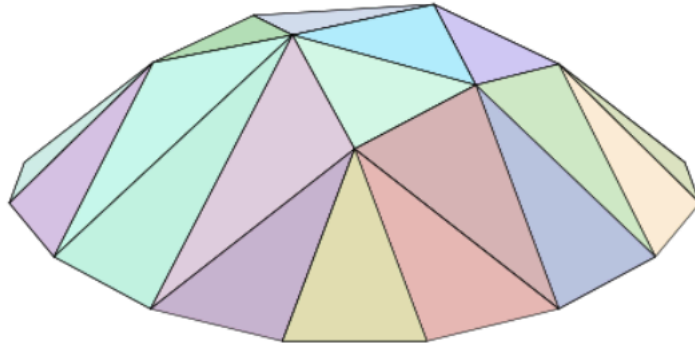
**Theorem (Telgarsky '15):** For every  $L \in \mathbb{N}$ , there exists a function  $f : [0,1] \rightarrow [0,1]$  representable as a network of depth  $O(L^2)$ , with  $O(L^2)$  nodes, and ReLU activation such that, for every network  $g : [0,1] \rightarrow \mathbb{R}$  of depth  $L$  and  $\leq 2^L$  nodes, and ReLU activation, we have

$$\int_{[0,1]} |f(x) - g(x)| dx \geq \frac{1}{32}.$$

# Intuition

---

A ReLU network  $f$  is **piecewise linear**, we can subdivide domain into a finite number of polyhedral pieces  $(P_1, P_2, \dots, P_N)$  such that in each piece,  $f$  is linear:  $\forall x \in P_i, f(x) = A_i x + b_i$ .



Deeper neural networks can make exponentially more regions than shallow neural networks.

Make each region has different values, so shallow neural networks cannot approximate.

# Benefits of depth for smooth functions

**Theorem (Yarotsky '15):** Suppose  $f : [0,1]^d \rightarrow \mathbb{R}$  has all partial derivatives of order  $r$  with coordinate-wise bound in  $[-1,1]$ , and let  $\epsilon > 0$  be given. Then there exists a  $O(\ln \frac{1}{\epsilon})$  - depth and  $\left(\frac{1}{\epsilon}\right)^{O(\frac{d}{r})}$  -size network so that  $\sup_{x \in [0,1]^d} |f(x) - g(x)| \leq \epsilon$ .

# Remarks

---

- All results discussed are **existential**: they prove that a good approximator exists. Finding one efficiently (e.g., using gradient descent) is the next topic (optimization).
- The choices of non-linearity are usually very flexible: most results we saw can be re-proven using different non-linearities.
- There are other approximation error results: e.g., deep and narrow networks are universal approximators.
- Depth separation for optimization and generalization is widely open.

# Recent Advances in Representation Power

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- Analyses of different architectures
  - Graph neural network
  - Attention-based neural network
- Separation between transformers and RNNs (especially for programming tasks)
- Finite data approximation
- In-context learning for specific tasks
- Chain-of-thought
- ...