Deep Learning
lecture 9
Sequence Modeling (2)

Yi Wu, IIIS

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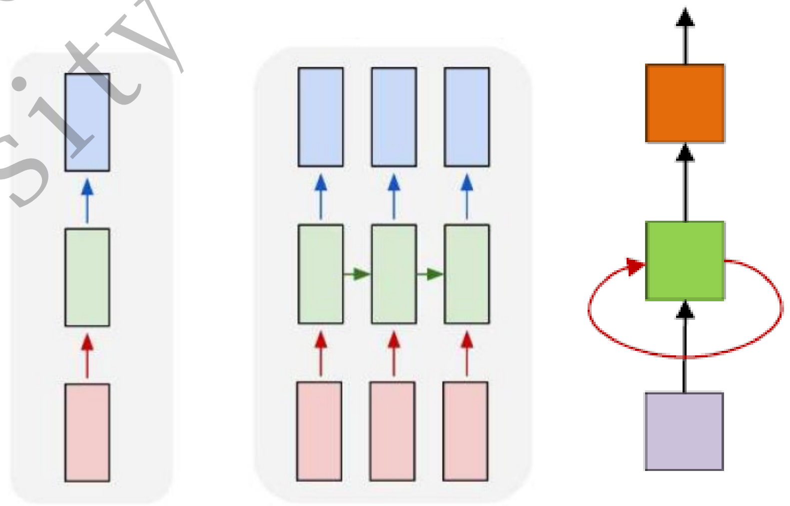
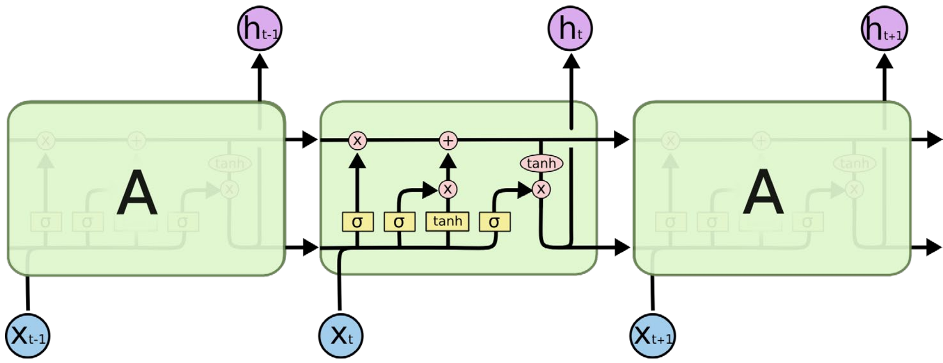
Today's Topic

- Sequence to Sequence Model and Attention Mechanism
- The Transformer Model
- Generation Speedup for Transformer Model

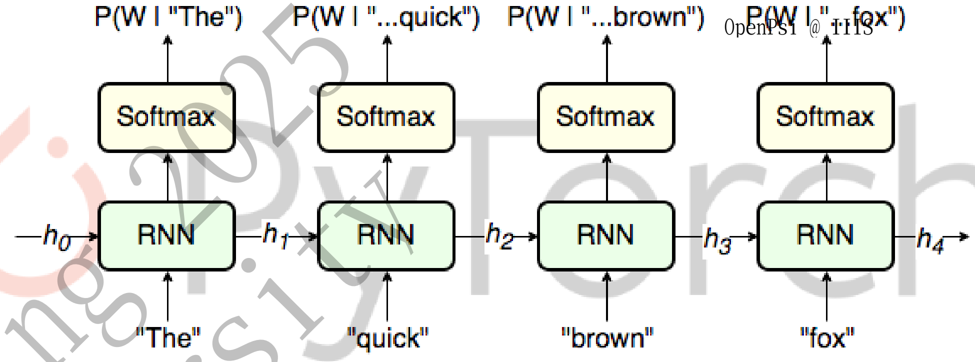
RNN Recap

- Recurrent Neural Network
  - Same MLP network over a sequence (i.e., "loops")
    - Arbitrarily long sequences → fixed-sized vector
  - Training: backpropagation through time (BPTT)
  - Practical Issues
    - Weights/Gradient explosion and saturation
  - A few tricks for gradient explosion
    - Gradient clipping, truncated BPTT, careful initialization
- Long Short-Term Memory (LSTM) Network
  - A specialized RNN for long-term dependency (~100 timesteps)
    - Key ideas: elementary gates
  - Variants: bidirectional LSTM; Peephole LSTM; GRU; etc

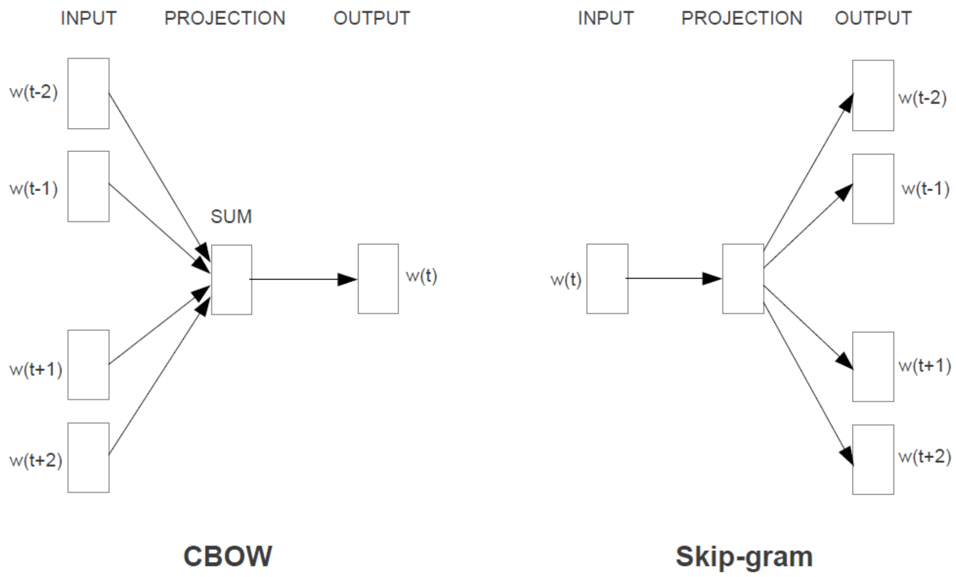




RNN Recap

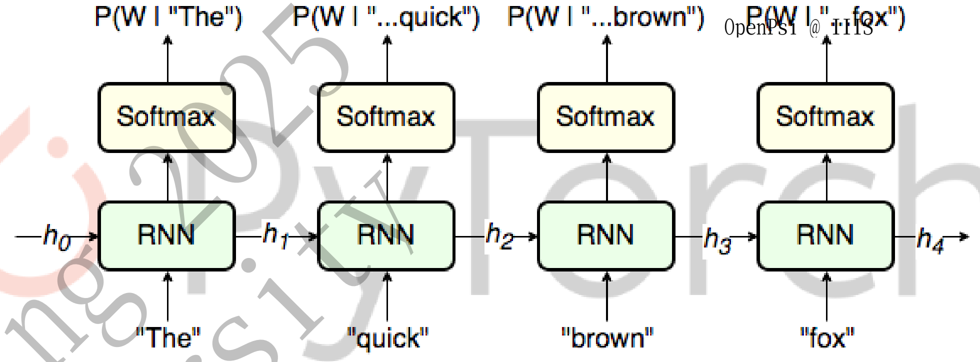


- Autoregressive Language Model
  - Generative model over texts: $P(X) = \prod_t P(X_t | X_{i<t})$
    - LSTM language model: $Y_t, h_t = LSTM(h_{t-1}, X_t)$; $P(X_t | X_{i<t}) = \text{Softmax}(Y_t)$
  - Word Embedding
    - A distributed representation for word semantics
- Word2Vec: a tool for word embedding
  - Objective: from context c to predict word w
    - CBOW and Skip-Gram
    - Negative Sampling
      - Multi-class prediction → binary classification
      - D training corpus; V vocabulary



$$L(W,C) = \sum_{(c,w)\in D} \log \frac{1}{\exp(-w^T c) + 1} + \sum_{c\in D, \tilde{w}\sim V} \log \frac{\exp(-\tilde{w}^T c)}{\exp(-\tilde{w}^T c) + 1}$$

RNN Recap



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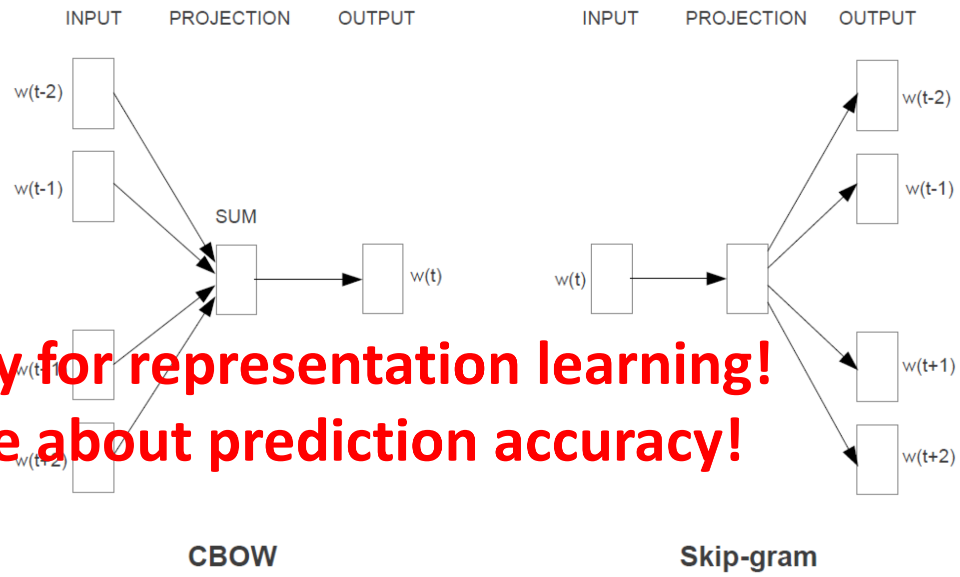
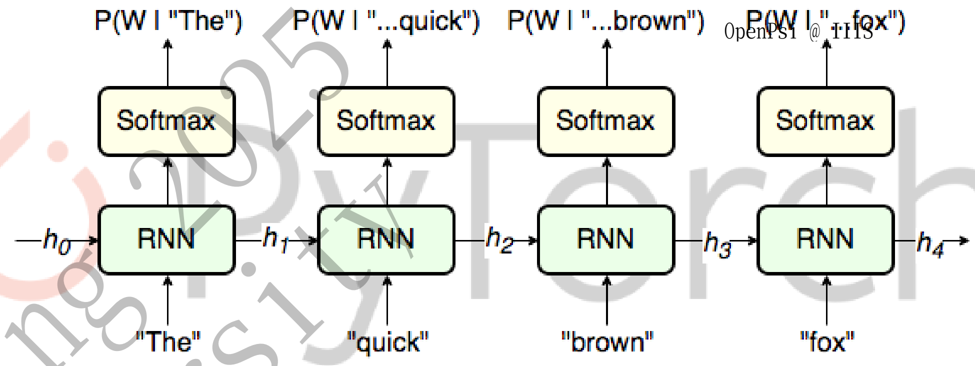


Word2Vec is only for representation learning!
It does not care about prediction accuracy!

$$L(W,C) = \sum_{(c,w)\in D} \log \frac{1}{\exp(-w^T c) + 1} + \sum_{c\in D, \tilde{w}\sim V} \log \frac{\exp(-\tilde{w}^T c)}{\exp(-\tilde{w}^T c) + 1}$$

RNN Recap



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  - Word Embedding
    - A distributed representation for word semantics
- Word2Vec: a tool for word embedding
- More Techniques
  - Hierarchical softmax
  - Beam search
  - ELMo for contextualized embeddings

Language Model Applications

- Text Classification
  - Supervised learning
- Text Generation
  - $p(X;\theta)$: the probability for X
  - Unconditioned Generation
    - E.g., AI作诗
  - **Conditioned generation?**
    - E.g., Machine translation

深度之梦

在数据的海洋里遨游，
算法如风，吹散迷雾。
神经元闪烁似星辰，
连接着未来的道路。

梯度回溯千重浪，
优化求解万象生。
一行代码塑乾坤，
模型自我去提升。

Machine Translation

- A task of translating a sentence from a source language to the target language

x: *L'homme est né libre, et partout il est dans les fers*

y: *Man is born free, but everywhere he is in chains*

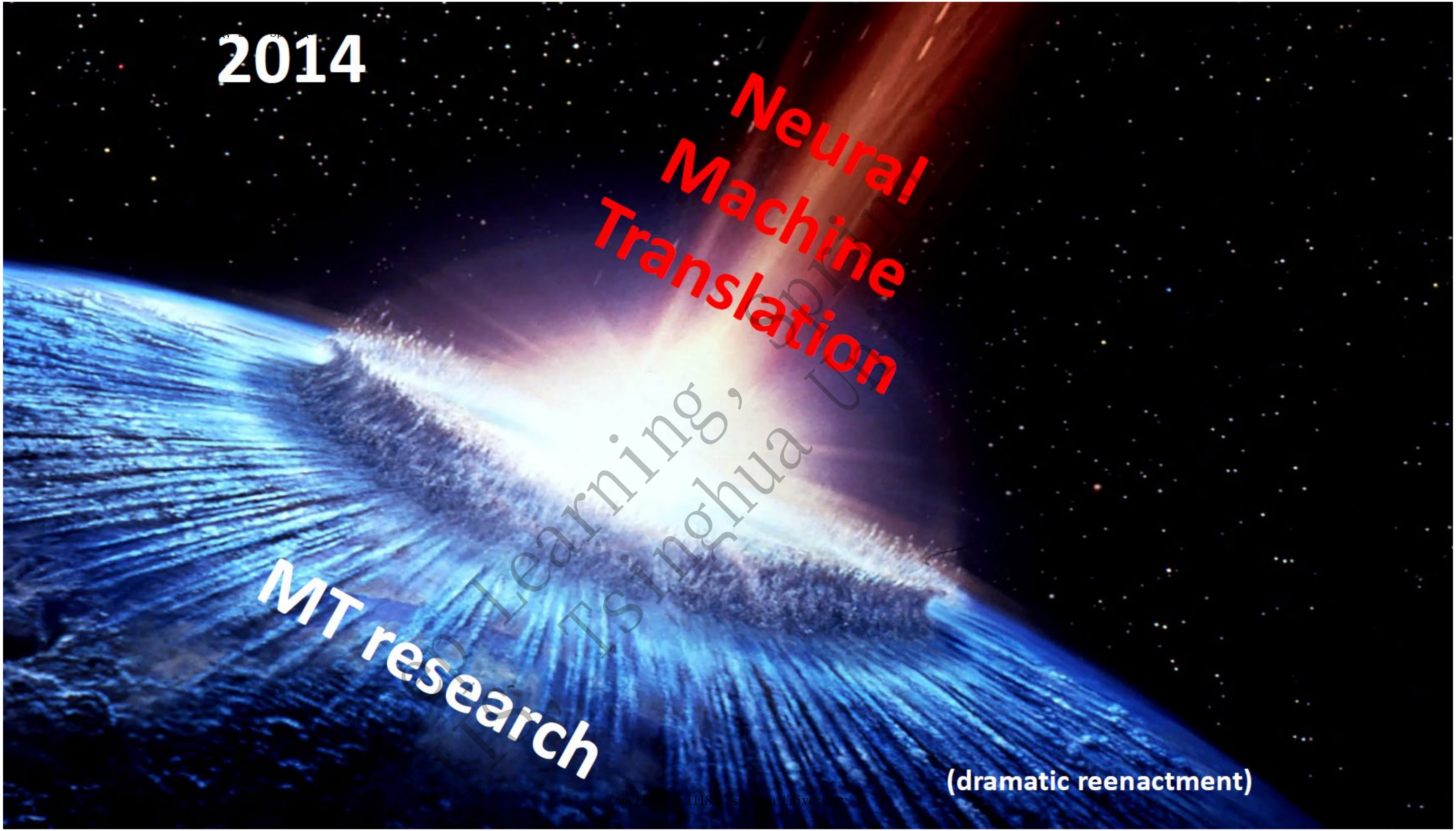
人生而自由，却无往不在枷锁之中。——卢梭《社会契约论》 – Rousseau

Machine Translation

- Before 2014: Statistical Machine Translation
  - Extremely complex systems that require massive human efforts
  - Separately designed components
  - A lot of feature engineering
  - Lots of linguistics domain knowledge and expertise
- Before 2016:
  - Google's commercial translation product is based on statistical machine translation
- What happened in 2014?
  - A borrowed slide from Stanford CS224

2014

(dramatic reenactment)

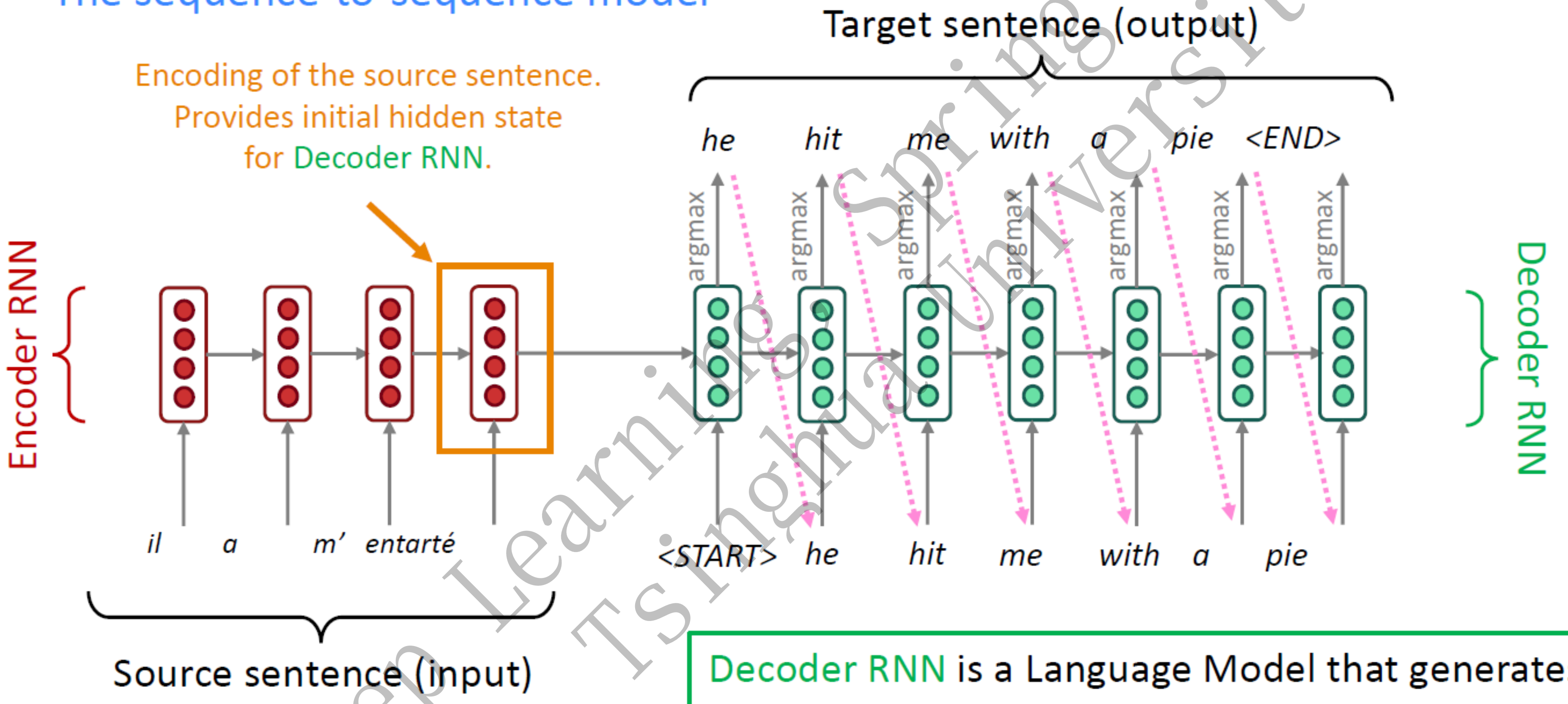

2014
Neural
Machine
Translation
MT research
(dramatic reenactment)

Sequence to Sequence Model

- Neural Machine Translation (NMT)
  - Learning to translate via single end-to-end neural network!
  - Source language X, then $Y = f(X;\theta)$
- Sequence-to-Sequence Model (Seq2Seq, Sutskever et al, NIPS2014)
  - NeurIPS 2024 test-of-time award
  - Two RNNs: f_{enc} and f_{dec}, $X \to f_{enc} \to h \to f_{dec} \to Y$
  - Encoder f_{enc}
    - It takes in X, and produce the initial hidden state h for decoder
    - We can use bidirectional RNN
  - Decoder f_{dec}
    - It takes in the hidden state h from f_{enc} to generate Y
    - Autoregressive language model

Sequence to Sequence Model

The sequence-to-sequence model



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

Encoder RNN produces an encoding of the source sentence.

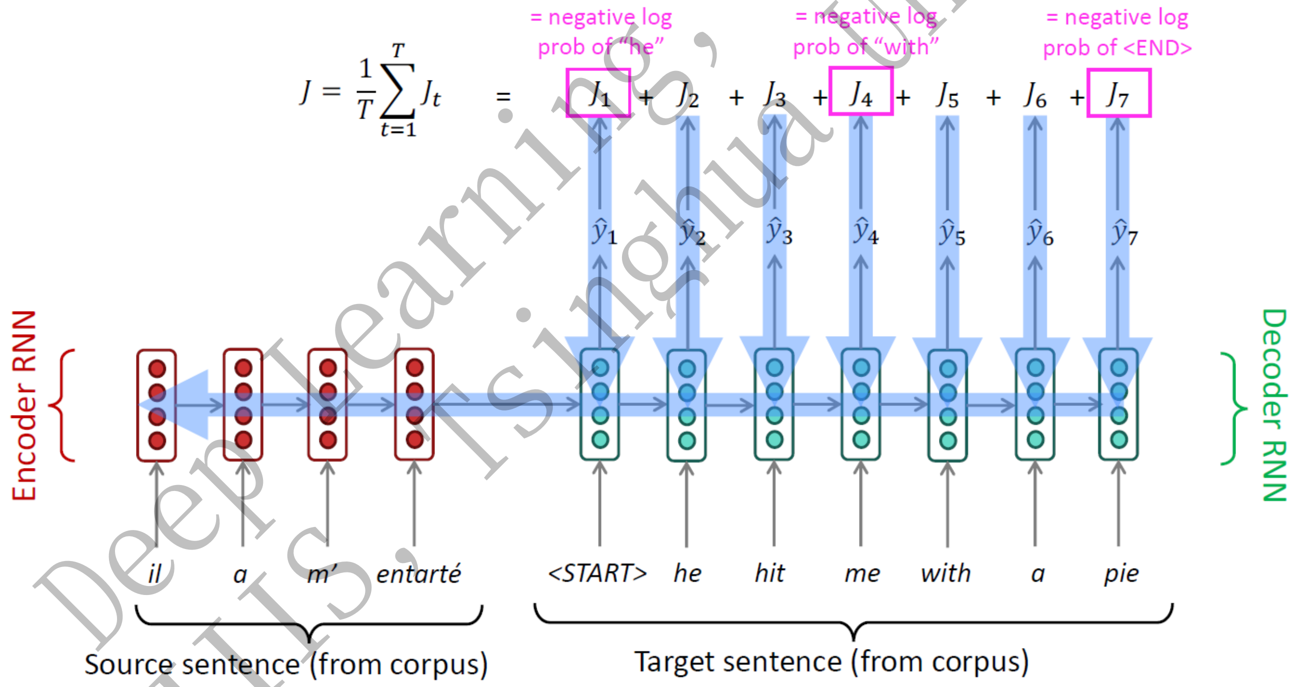
Note: This diagram shows **test time** behavior: decoder output is fed in as next step's input

Sequence to Sequence Model

- Seq2Seq is a conditioned language model
  - $h = f_{enc}(X)$ (final hidden state)
  - $Y = f_{dec}(h)$ (a LM that conditions on the initial hidden state h)
- Seq2Seq model is particularly generic for a lot of applications
  - Summarization (摘要) or Captioning (起标题)
    - Article → abstract/caption
  - Dialogue (对话)
    - Previous utterance → next utterance
  - Code generation
    - Natural language → python
  - VAE-based seq2seq model for text generation with latent variables

Sequence to Sequence Model

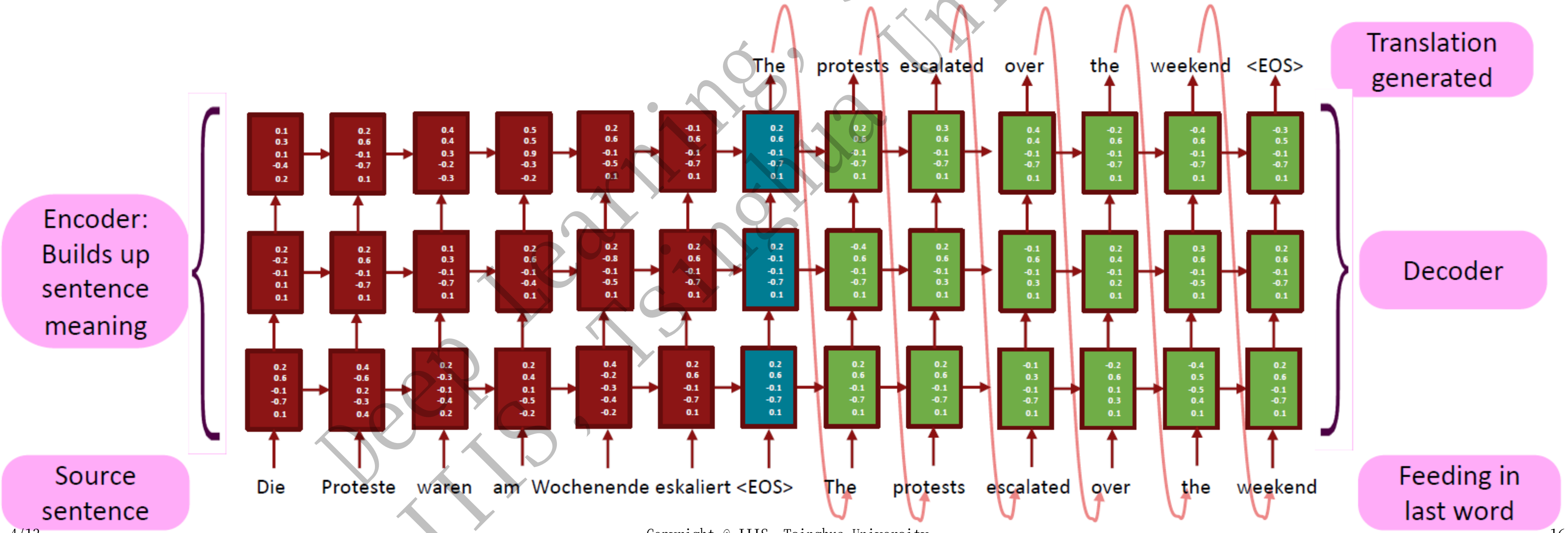
- How to train a seq2seq model?
  - Collect a huge paired dataset and train it end-to-end via BPTT!
  - MLE learning for $P(Y|X) = P(Y|f_{enc}(X))$



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

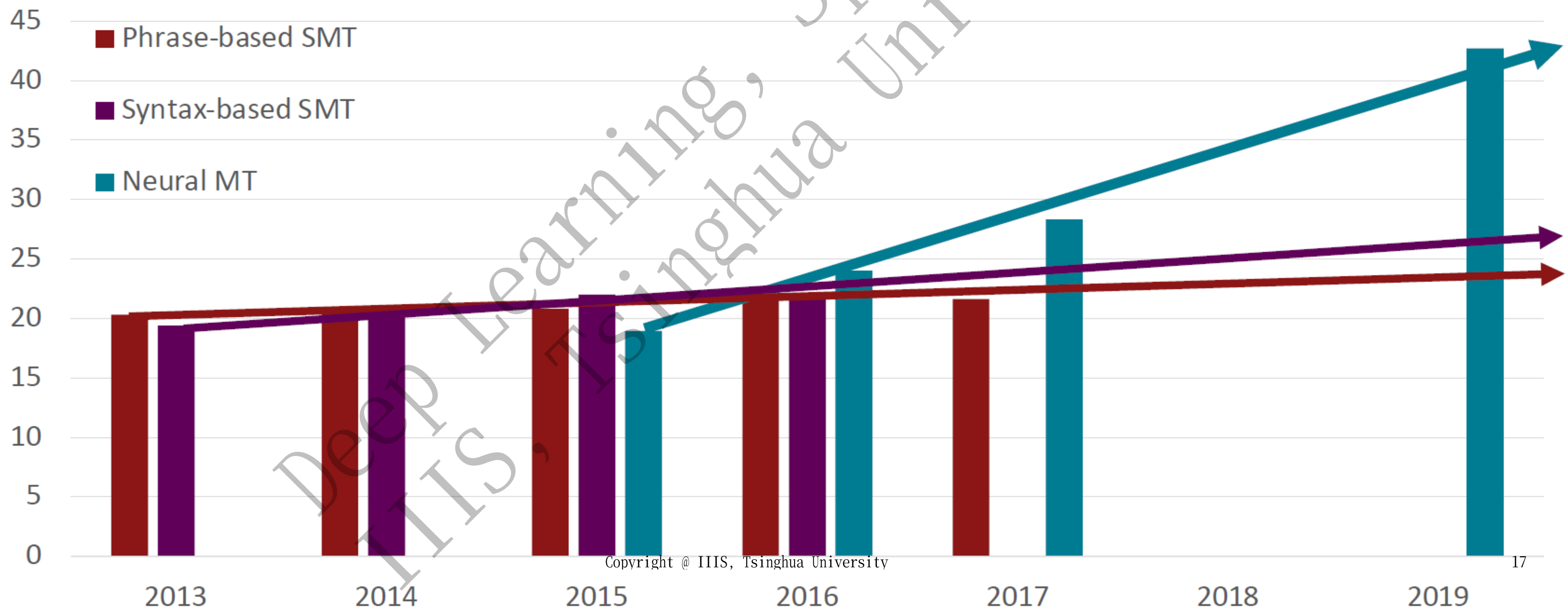
Sequence to Sequence Model

- We can also make the model deeper!
  - Stacked seq2seq model



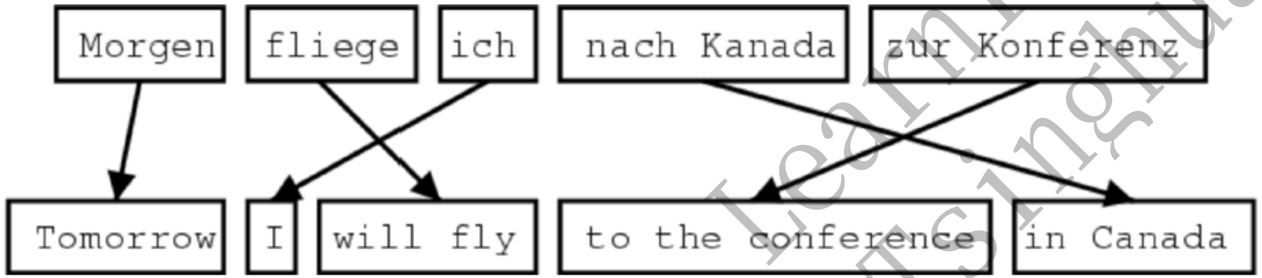
Sequence to Sequence Model

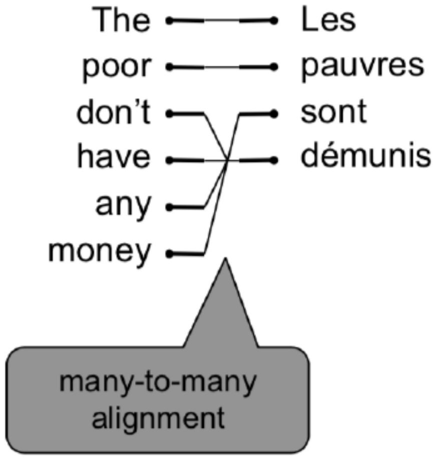
- 2016: Google switch google translate from SMT to NMT
  - Seq2Seq paper has >28.6k citations since 2014

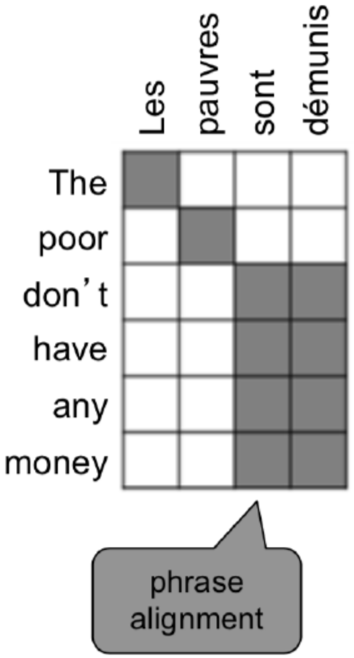


Sequence to Sequence Model

- Issue in the vanilla Seq2Seq model
  - Alignment: the word-level correspondence between X and Y
  - There are complex long-term dependencies

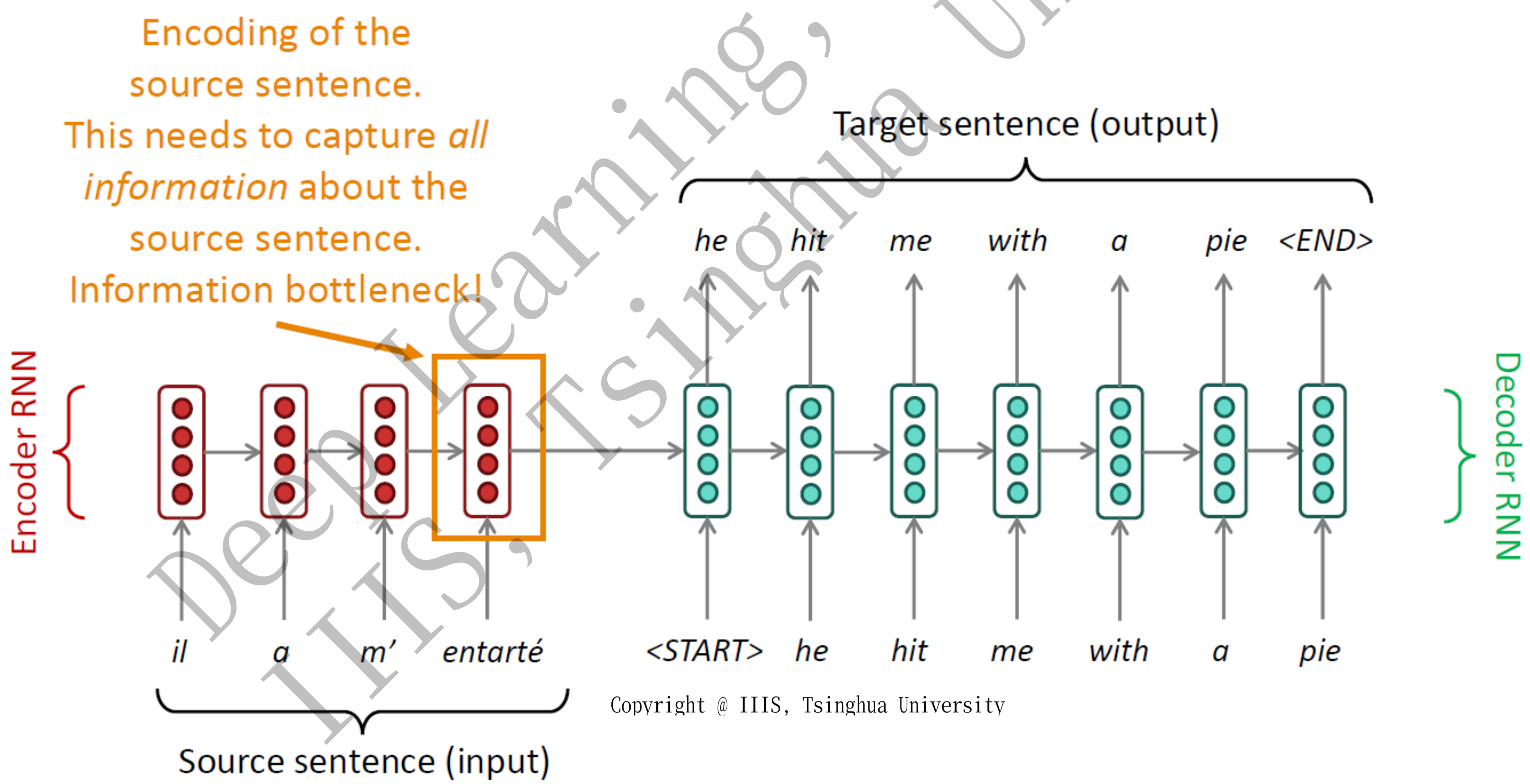






Sequence to Sequence Model

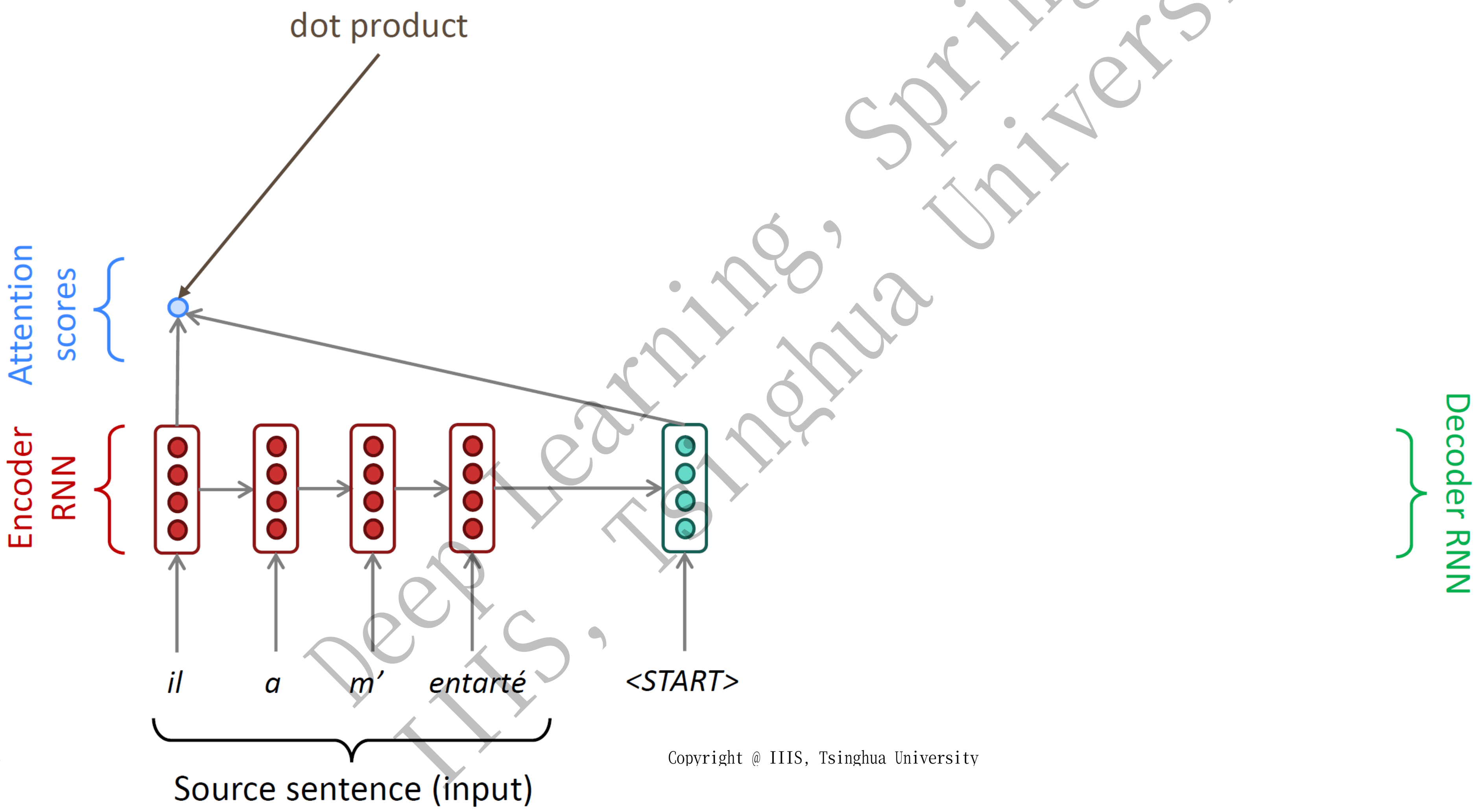
- Issue in the vanilla Seq2Seq model
  - The information bottleneck due to h
  - We want each Y_t to also focus on X_i that it is aligned with



Sequence-to-Sequence with Attention

- NMT by Jointly Learning to Align and Translate
  - Bahdanau, Cho & Bengio, ICLR 2015 (38.5k citation)
  - Core idea:
    - When decoding Y_t, we consider both hidden states and alignments
      - Hidden: h_{t-1} from $Y_{i<t}$, i.e., $h_{t-1} = f_{dec}(Y_{i<t})$
      - Alignment: a direction connection to "key" words from X
    - Which part of X to focus?
      - Learn a softmax weight over X (attention distribution P_{att})
      - $P_{att}(X_i|h_{t-1})$: how much attention you want to put on word X_i
      - attention output $h_{att} = \sum_i f_{enc}\left(X_i \middle| X_{j<i}\right) \cdot P_{att}(X_i|h_{t-1})$
      - Use h_{t-1} and h_{att} to compute Y_t
    - Let's go through the diagram before showing more details

Sequence-to-Sequence with Attention



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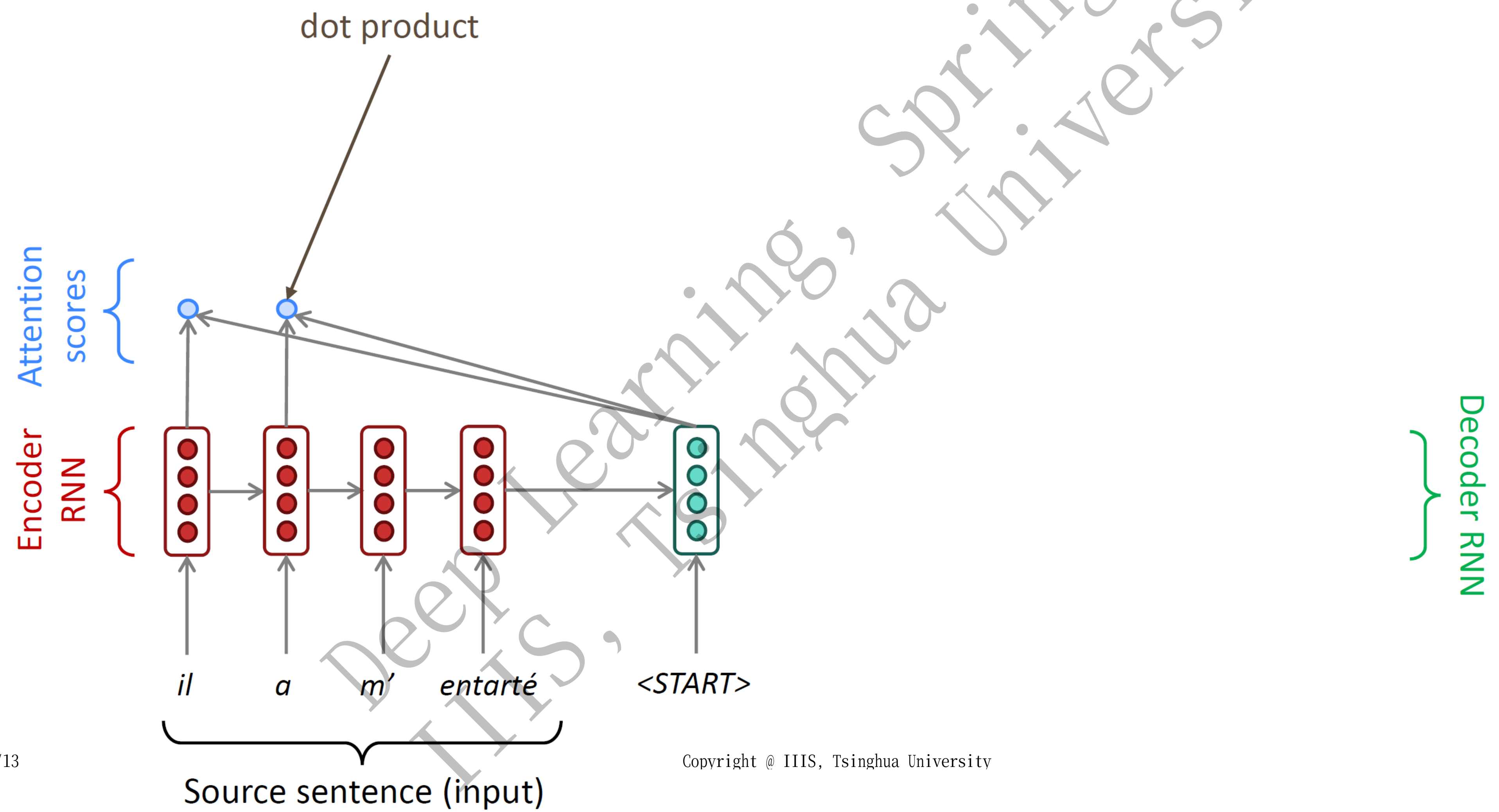

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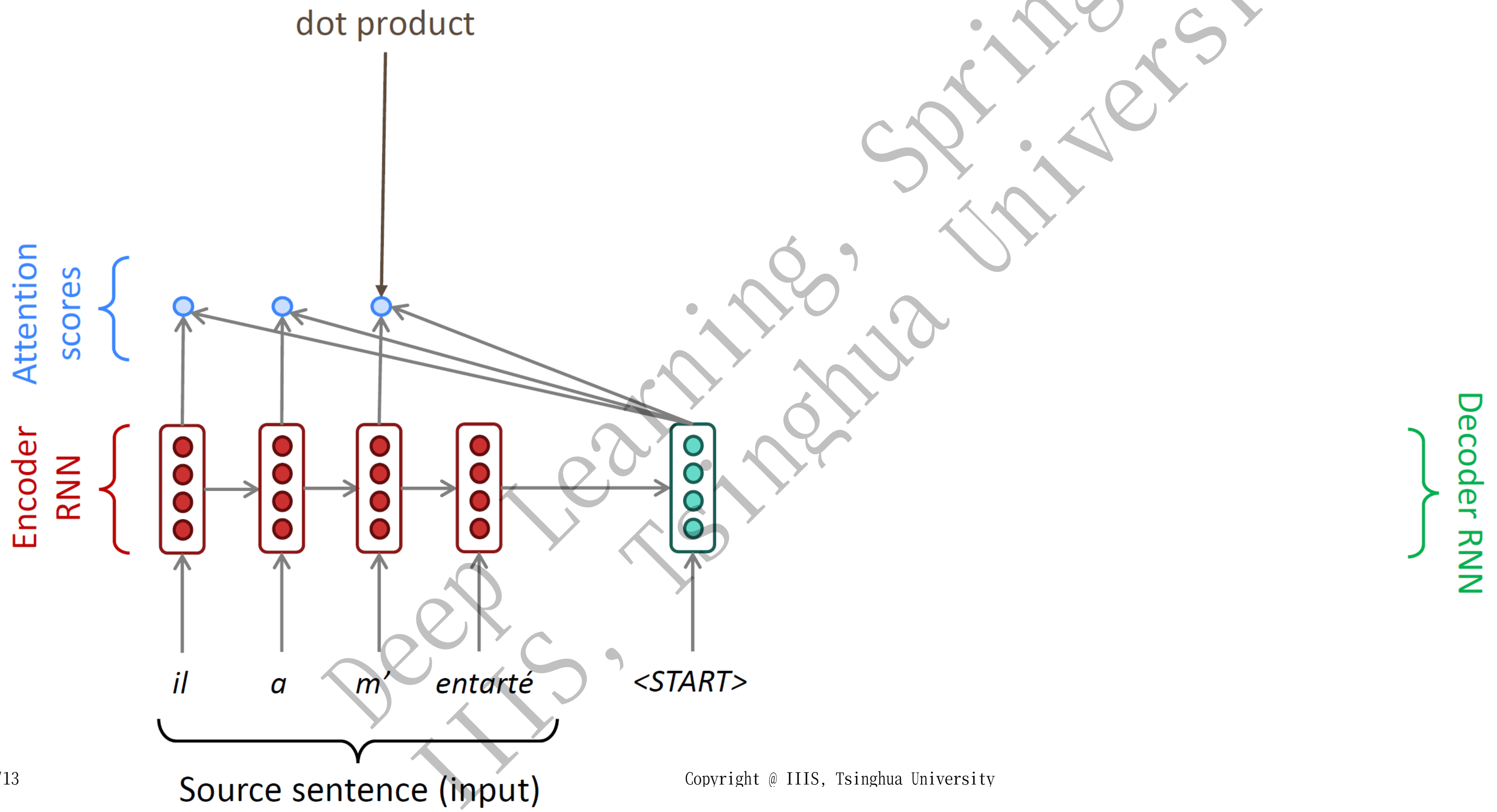

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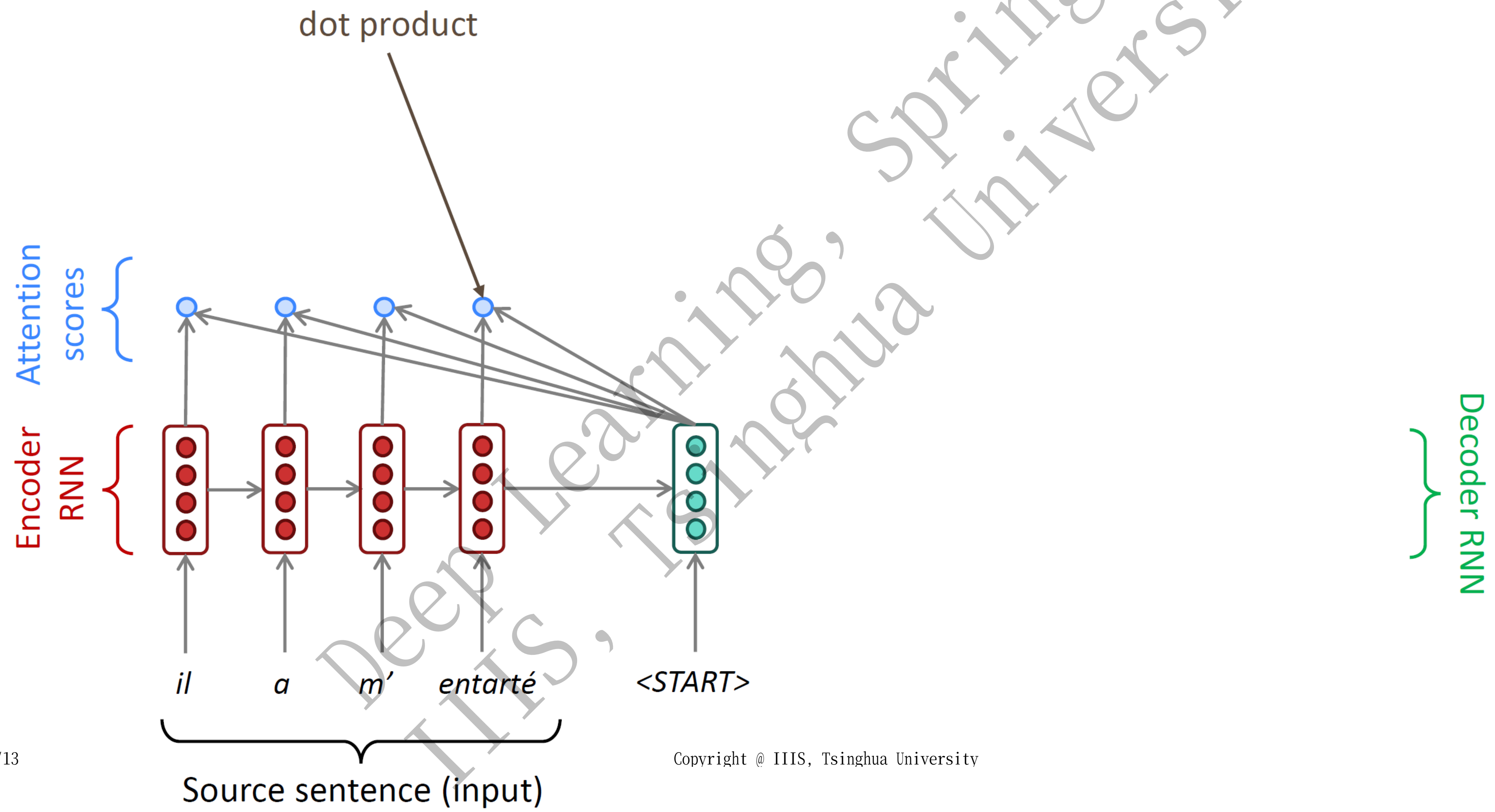

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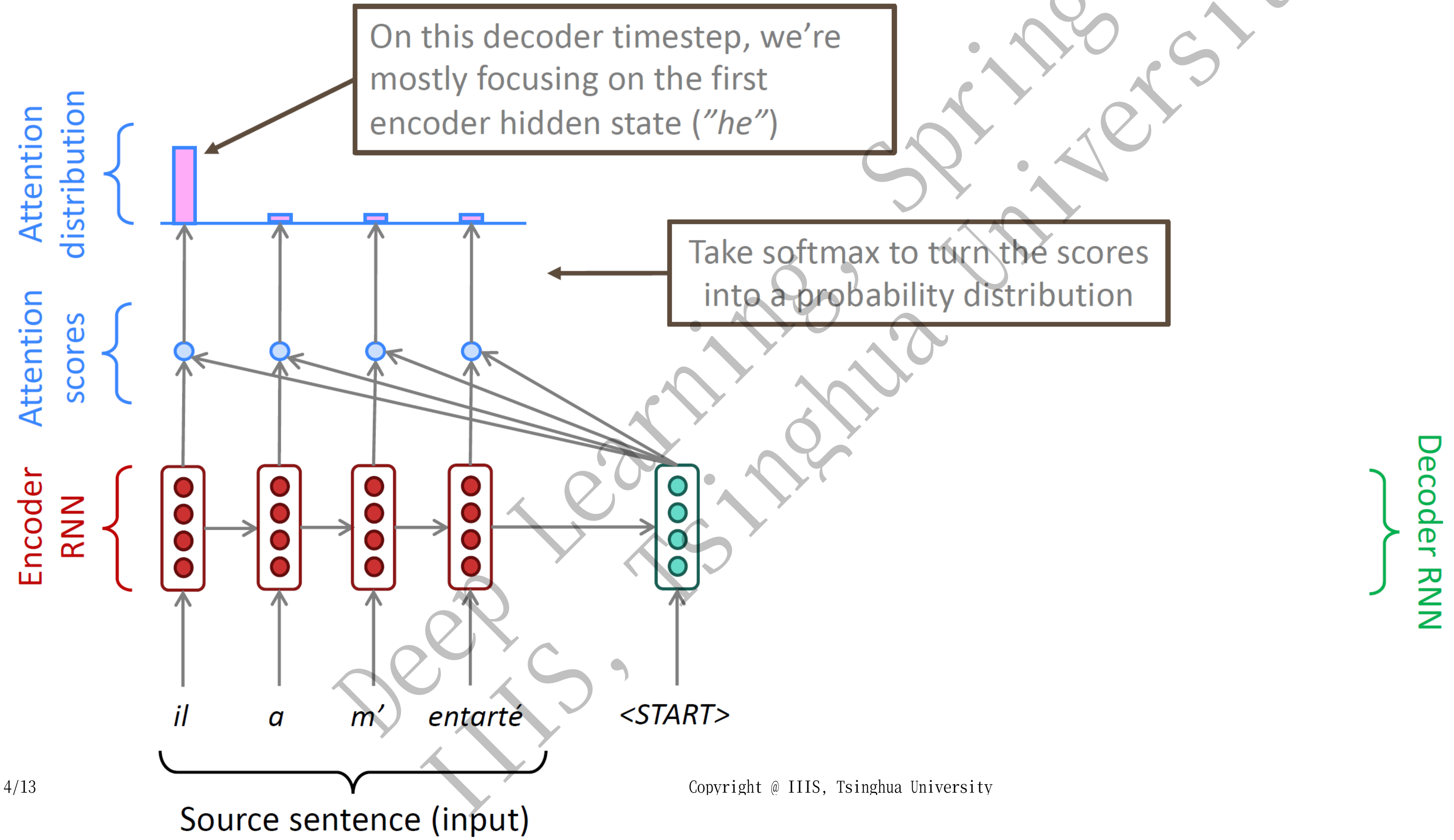

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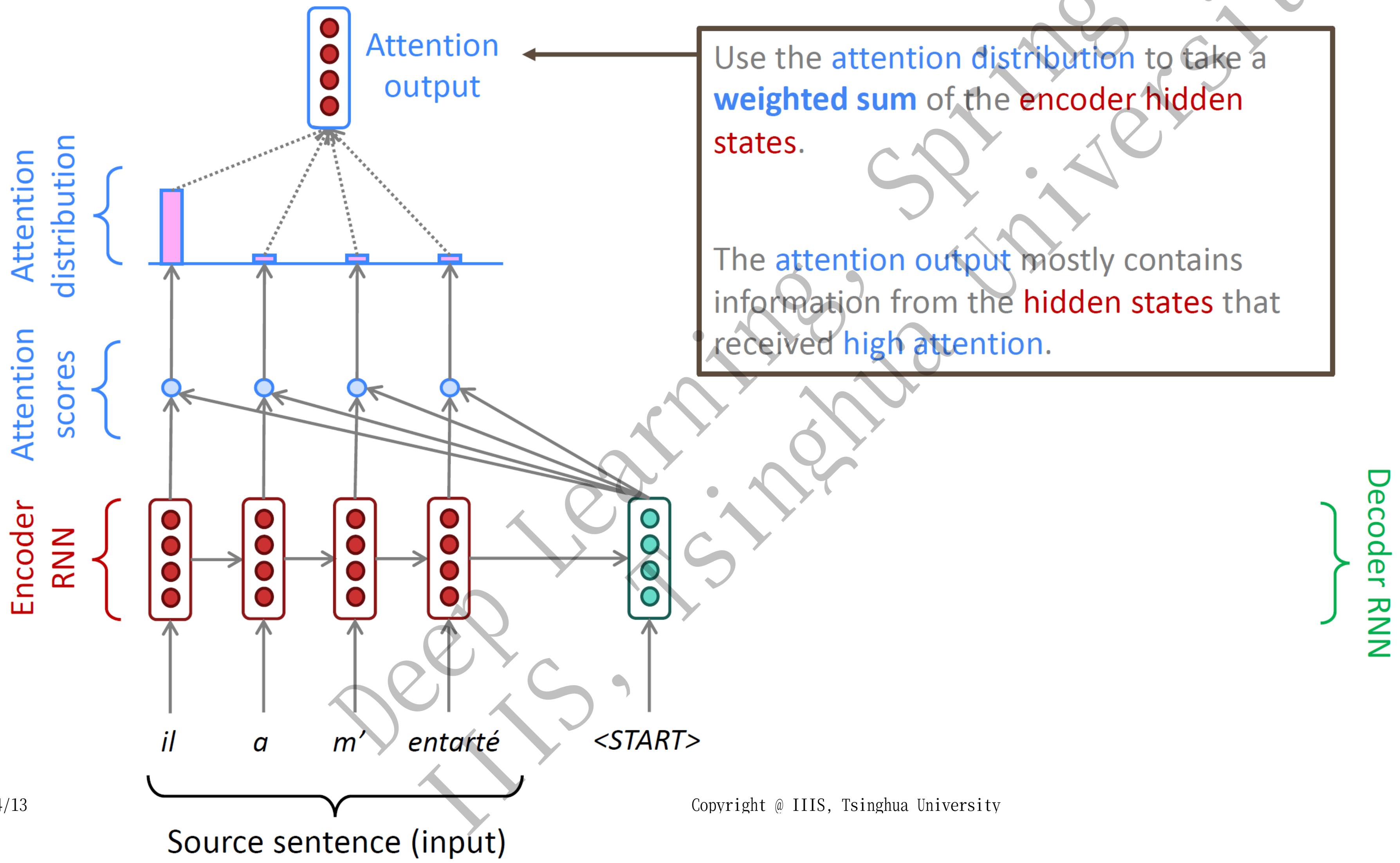
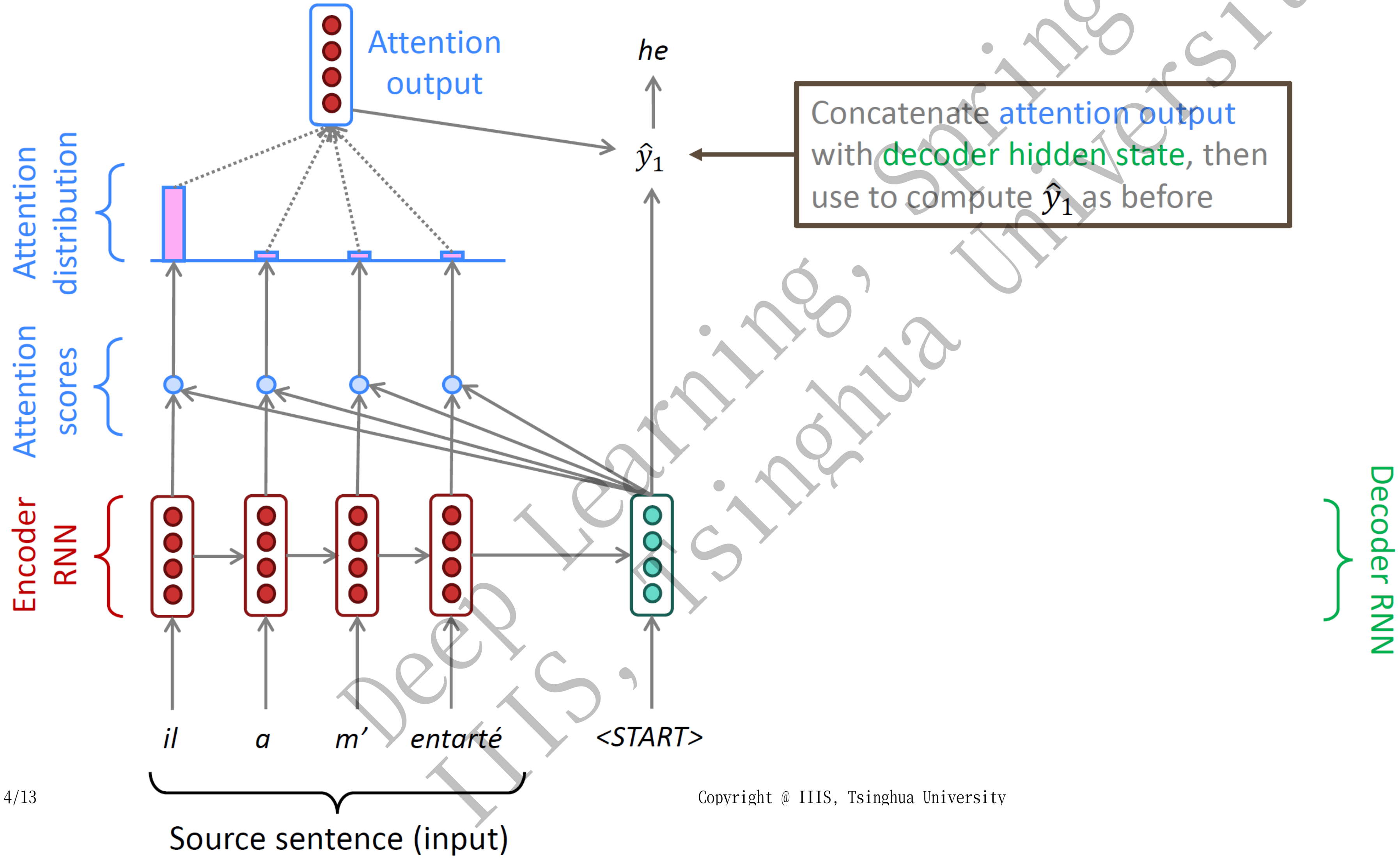


Use the attention distribution to take a **weighted sum** of the encoder hidden states.

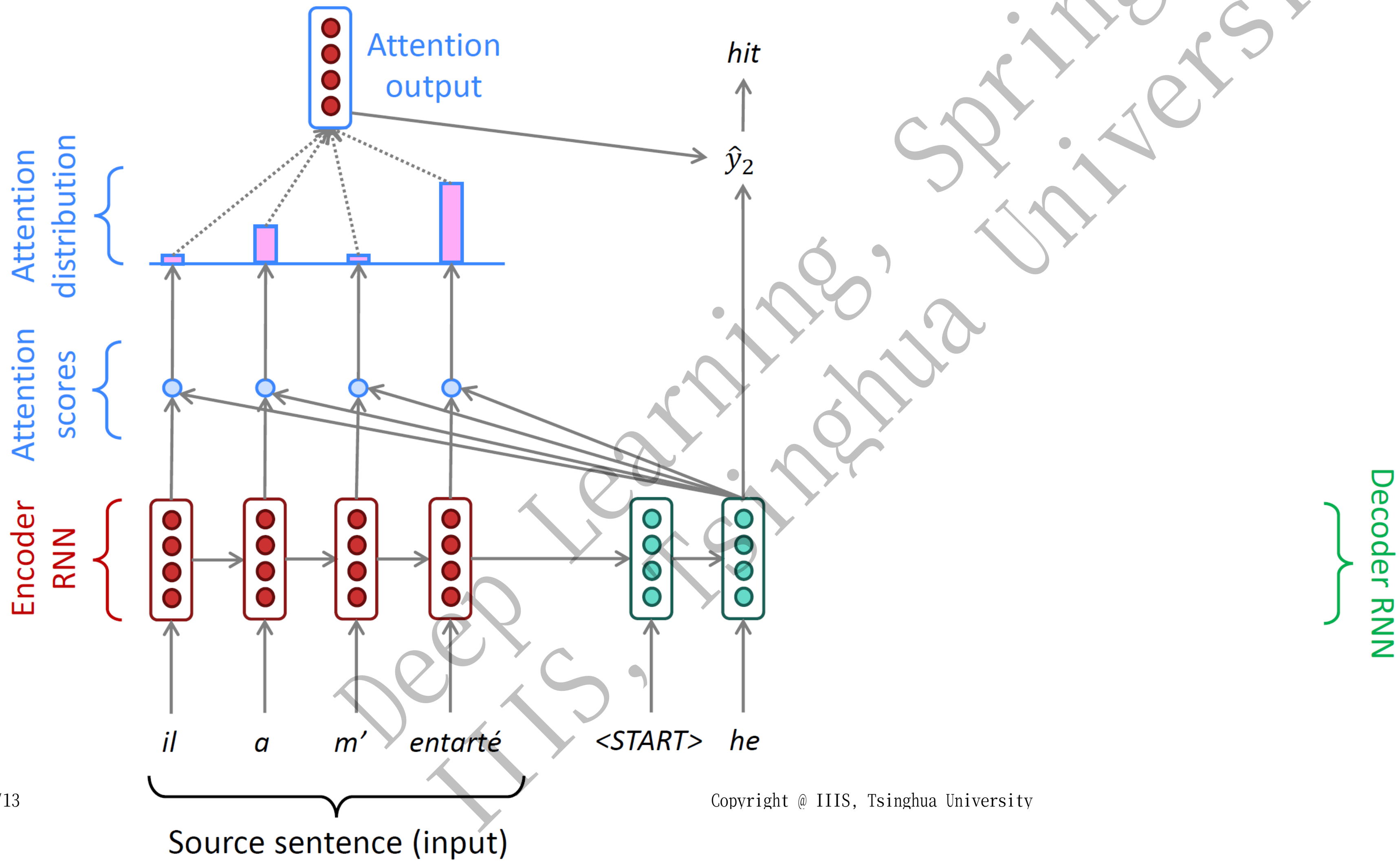
The attention output mostly contains information from the hidden states that received high attention.

Sequence-to-Sequence with Attention



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

Sequence-to-Sequence with Attention



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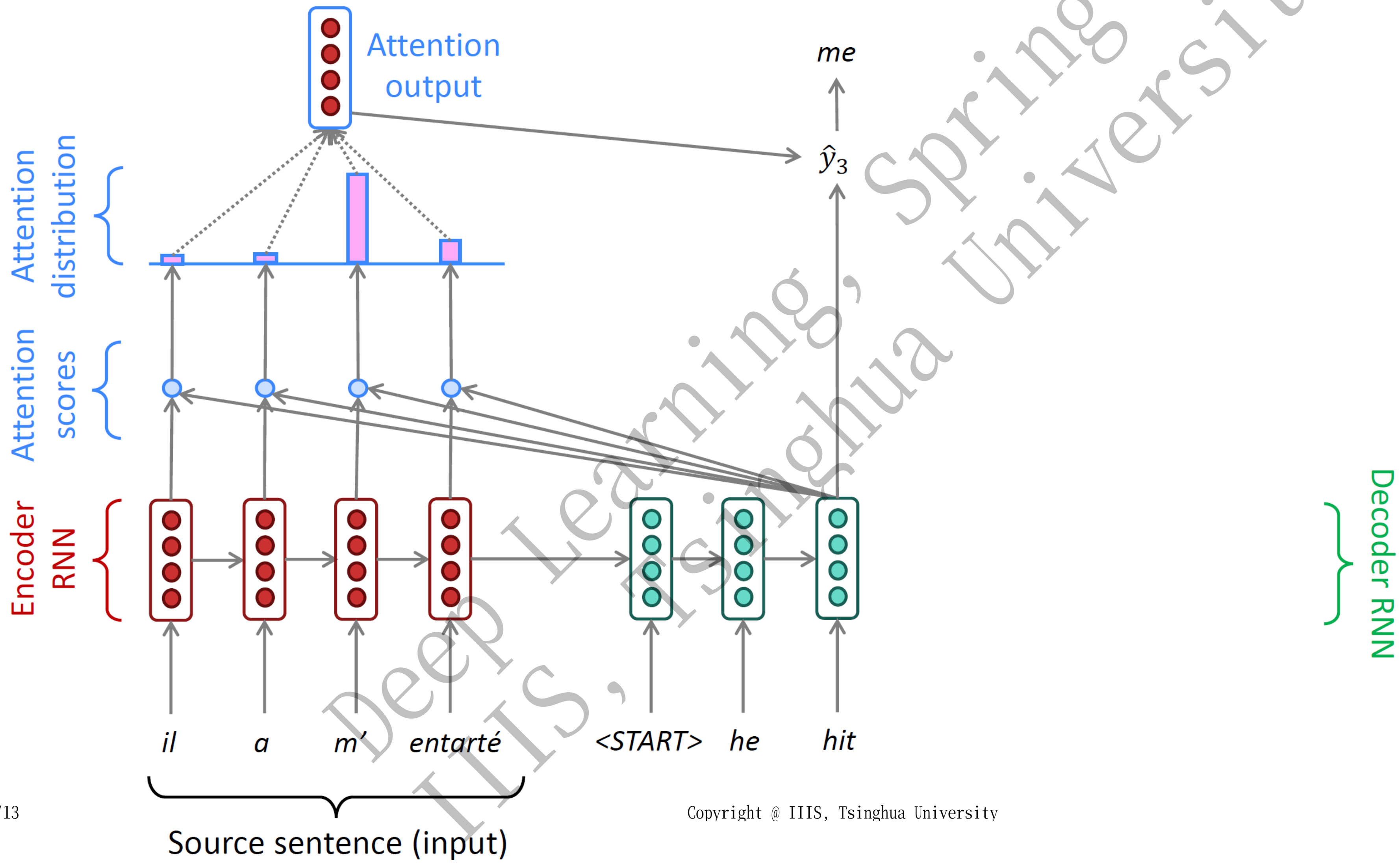

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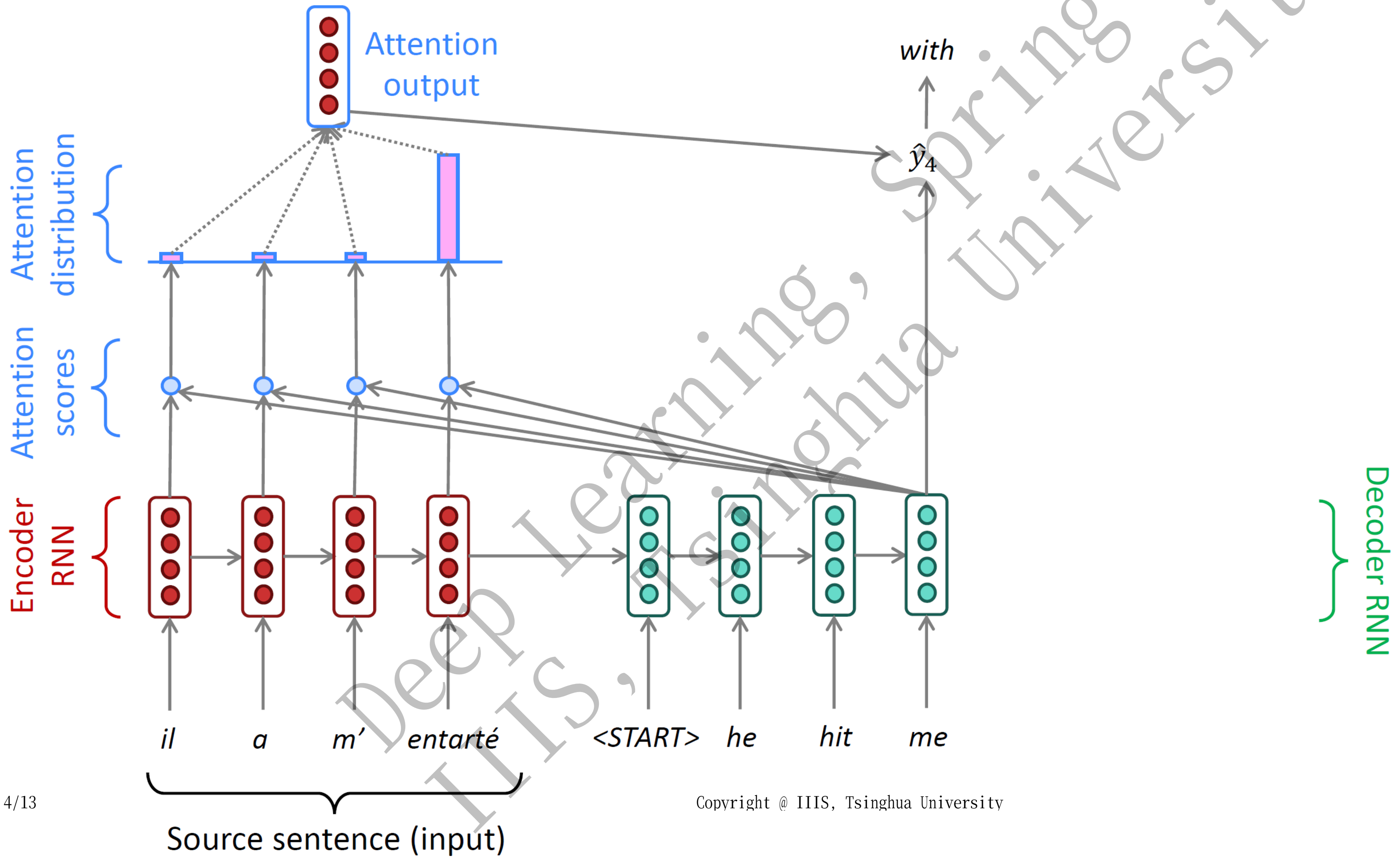

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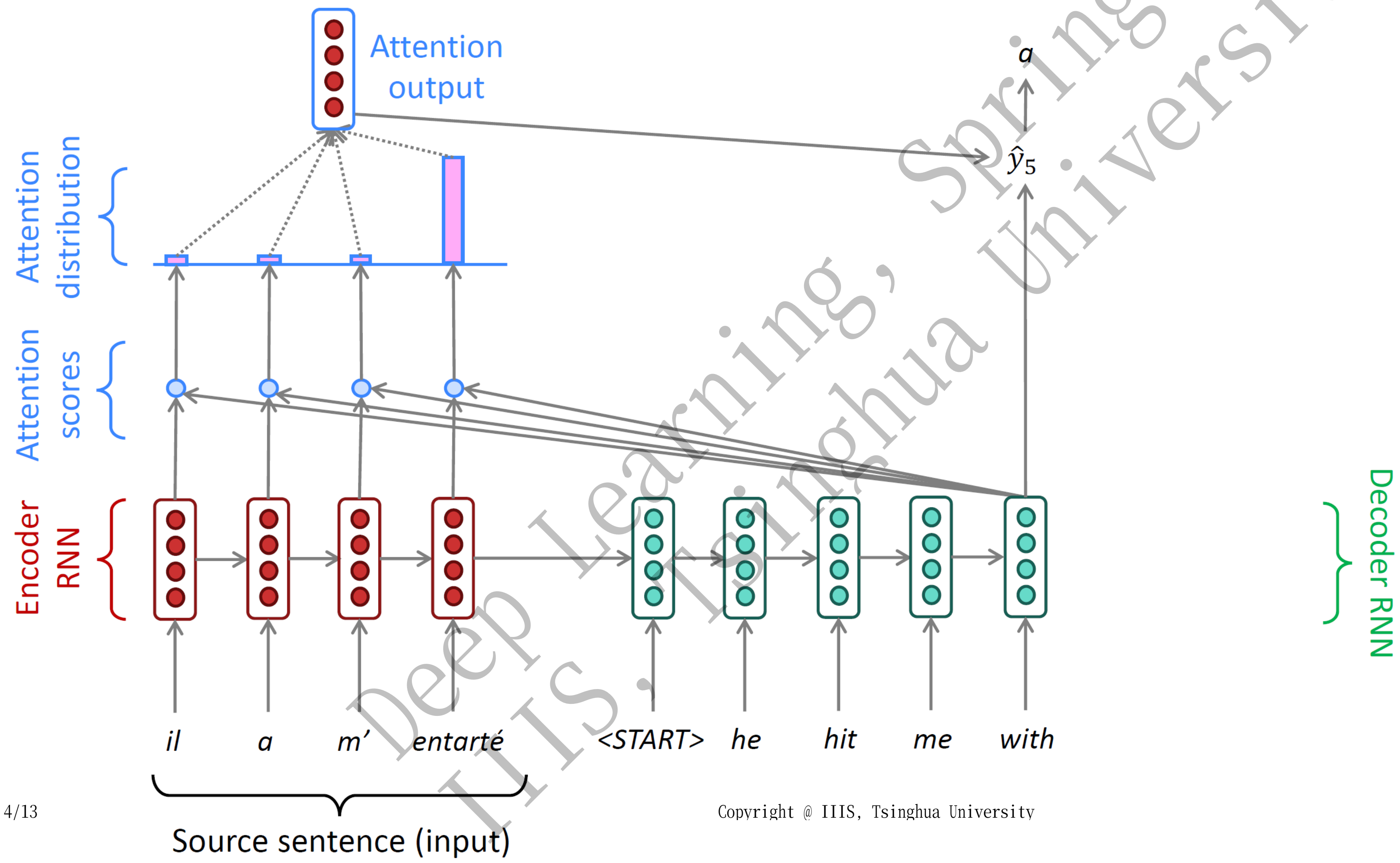

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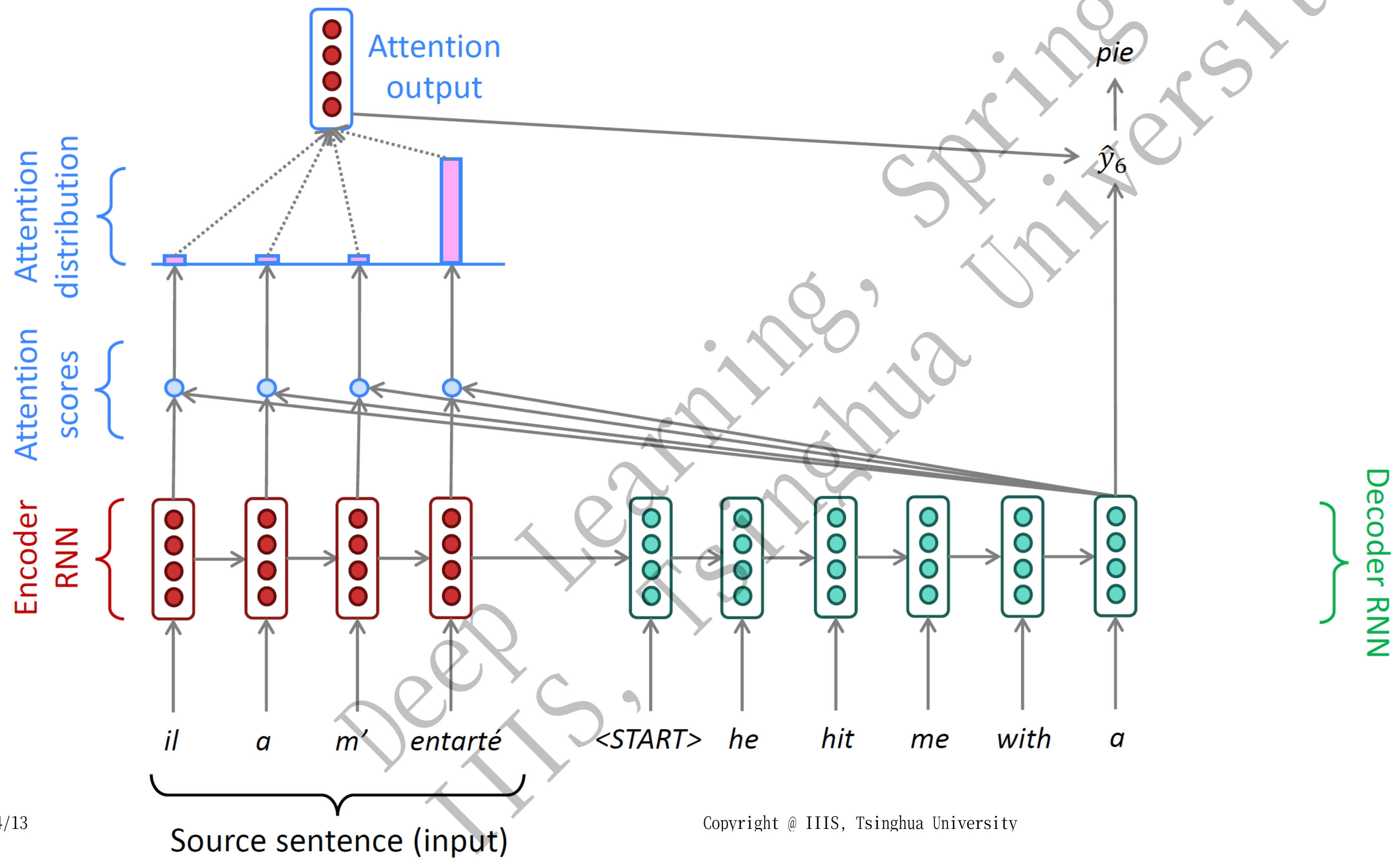


Sequence-to-Sequence with Attention

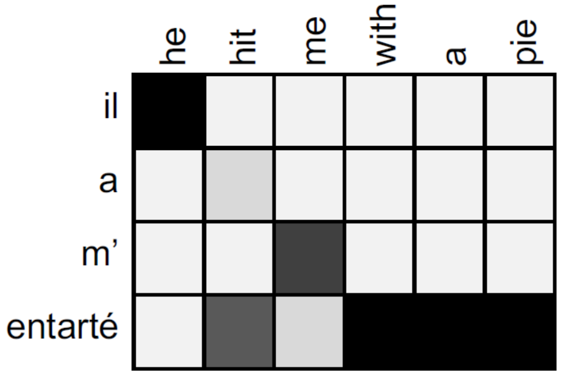
- Attention in equations
  - Input sequence X and encoder f_{enc} and decoder f_{dec}
  - $f_{enc}(X)$ produces hidden states $h_1^{enc}, h_2^{enc}, \ldots, h_N^{enc}$
  - On timestep t, we have decoder hidden state h_t
  - Attention score $e_i = h_t^T h_i^{enc}$
  - Attention distribution $\alpha_i = P_{att}(X_i) = \mathrm{softmax}(e_i)$
  - Attention output

$$h_{att}^{enc} = \sum_i \alpha_i h_i^{enc}$$

  - $Y_t \sim g(h_t, h_{att}^{enc}; \theta)$
    - Sample output using both h_t and h_{att}^{enc}

Attention

- Attention is great!
  - It significantly improves NMT!
  - It solves the bottleneck problem and long-term dependency issue
    - Also helps gradient vanishing problem
  - It provides some interpretability
    - We can understand the focus of RNN decoder



- Attention is a general technique
  - Given a set of vector values V_i and a vector query q
  - Attention computes a weighted sum of values depending on q
- Attention can learn a representation of an arbitrary set of vectors $\{v_i\}$ depending on query q

Attention

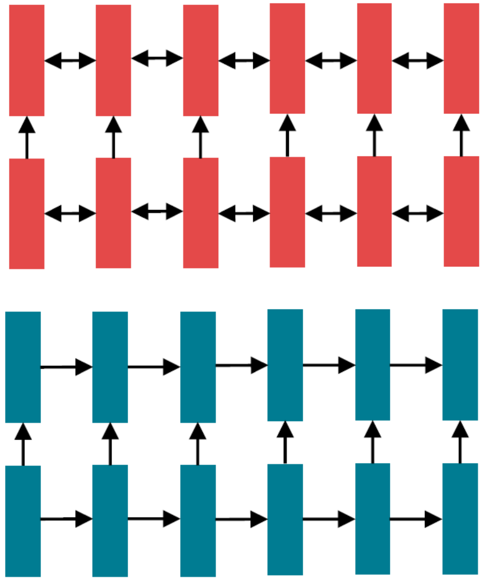
- Attention can learn a representation of an arbitrary set of vectors $\{v_i\}$ depending on query q
  - $\alpha_i = \mathrm{softmax}\big(f(v_i, q)\big)$ (attention distribution)
  - $v_{att} = \sum_i \alpha_i v_i$ (attention output)
  - Attention is *size-invariant* and *order-invariant*
- More use cases
  - E.g., a representation of a set of points (Pointer network, NIPS2015 & Deep Sets, NIPS2017)
  - E.g., include non-local information in CNN (Non-local network, CVPR18; Self-Attention GAN, ICML 19; BigGAN, ICLR 19)

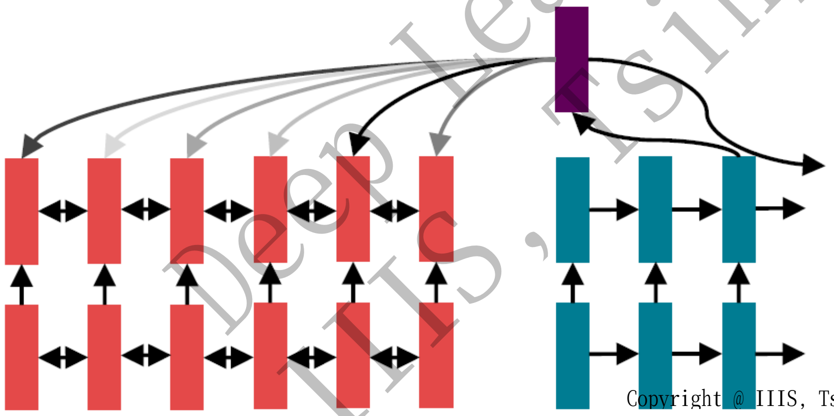
Attention

- Attention can learn a representation of an arbitrary set of vectors $\{v_i\}$ depending on query q
  - $\alpha_i = \text{softmax}\big(f(v_i, q)\big)$ (attention distribution)
  - $v_{att} = \sum_i \alpha_i v_i$ (attention output)
- Attention Variants $f(v_i, q)$
  - Multiplicative attention: $f(v_i, q) = q^T W h_i$
    - W is a weight matrix
  - Additive attention: $f(v_i, q) = u^T \tanh(W_1 v_i + W_2 q)$
    - W_1, W_2 are weight matrices
    - u is a weight vector
  - Expressiveness v.s. efficiency

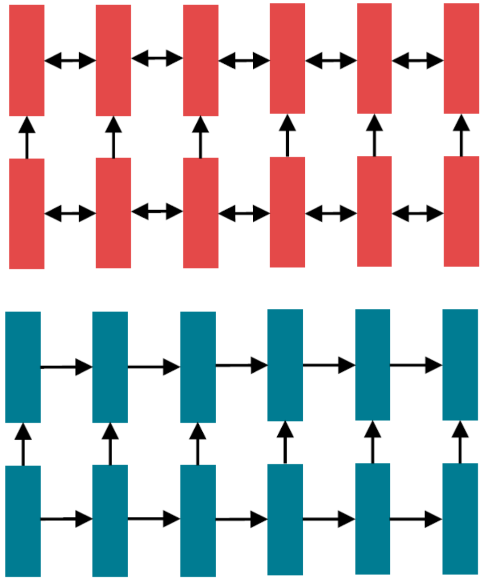
Sequence to Sequence Model with Attention

- Attention-Based Seq2Seq Model
  - Use bidirectional LSTMs as your encoder for input data
  - Use stacked LSTMs as your decoder for output data
  - Use attention for long-term dependencies

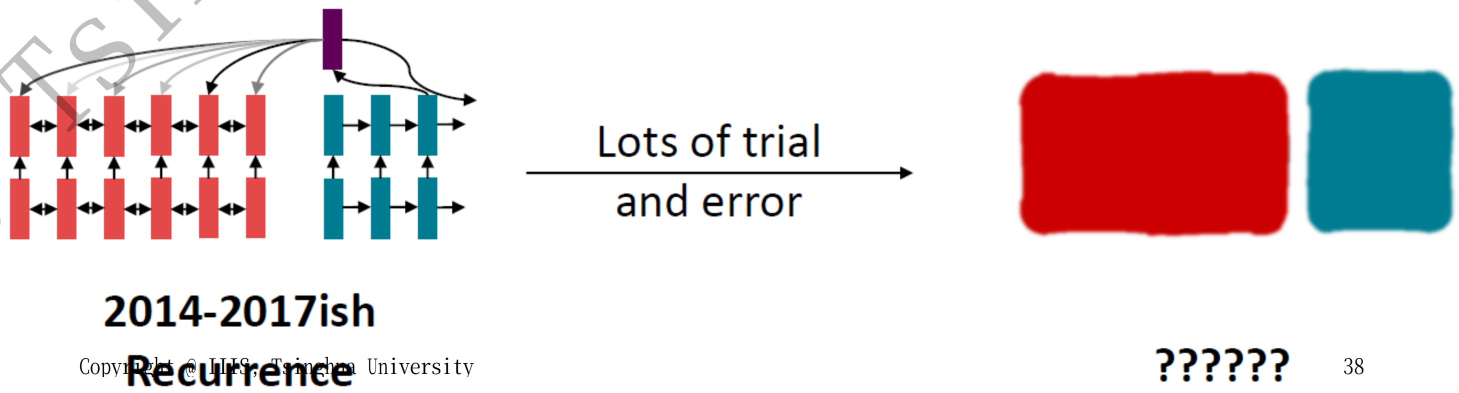




Sequence to Sequence Model with Attention

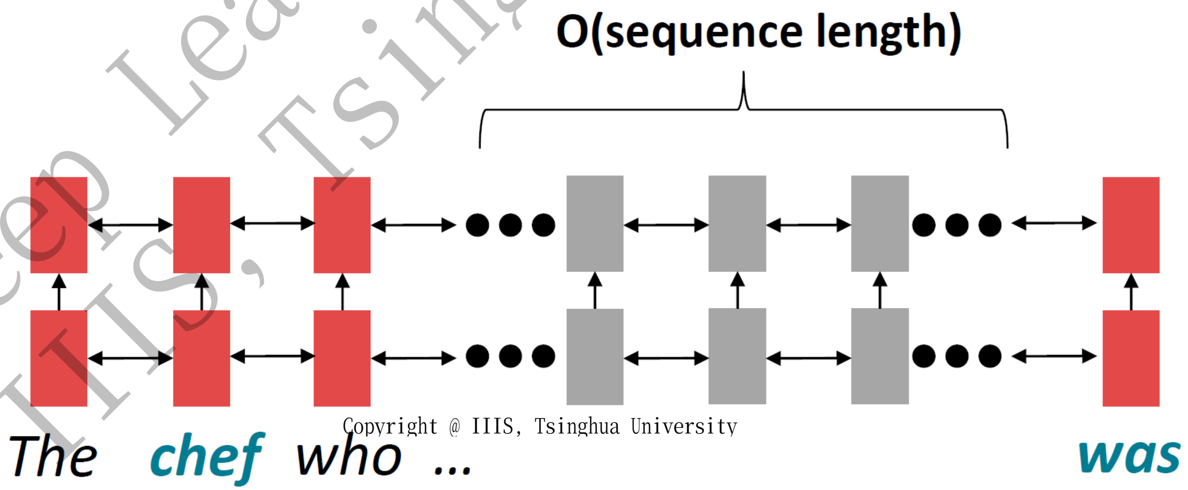


- Attention-Based Seq2Seq Model
  - Use bidirectional LSTMs as your encoder for input data
  - Use stacked LSTMs as your decoder for output data
  - Use attention for long-term dependencies
  - Most NLP applications!
    - till 2017 ☺



Sequence to Sequence Model with Attention

- Story So Far
  - RNN Models
    - Simple & Generic solution for sequence modeling
    - Issue for long-term dependencies
      - Linear computations for distant words through a single latent state
    - Lack of parallelization
      - Forced sequential computation (contrast with CNN)



Sequence to Sequence Model with Attention

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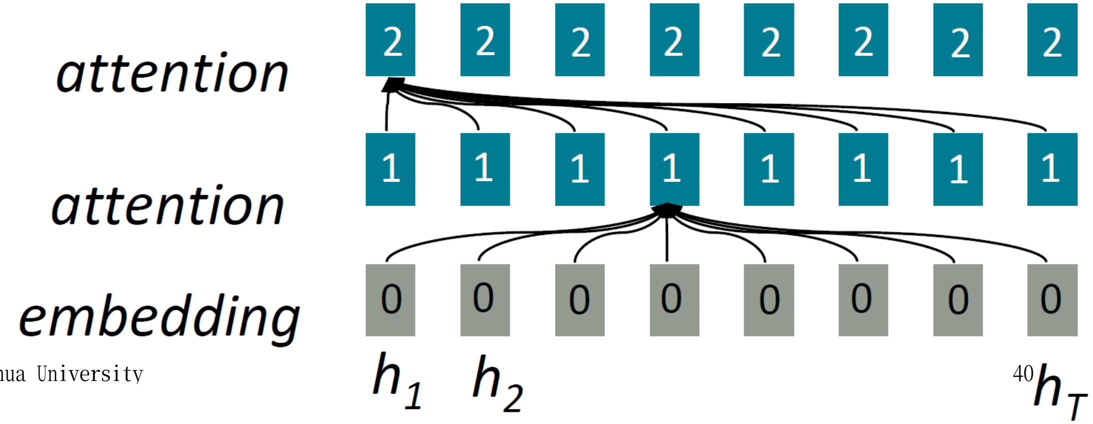
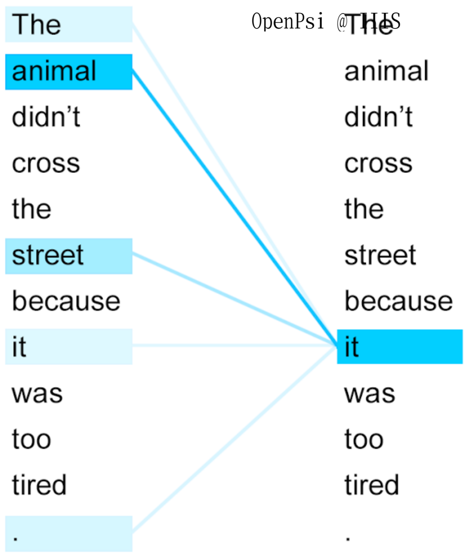
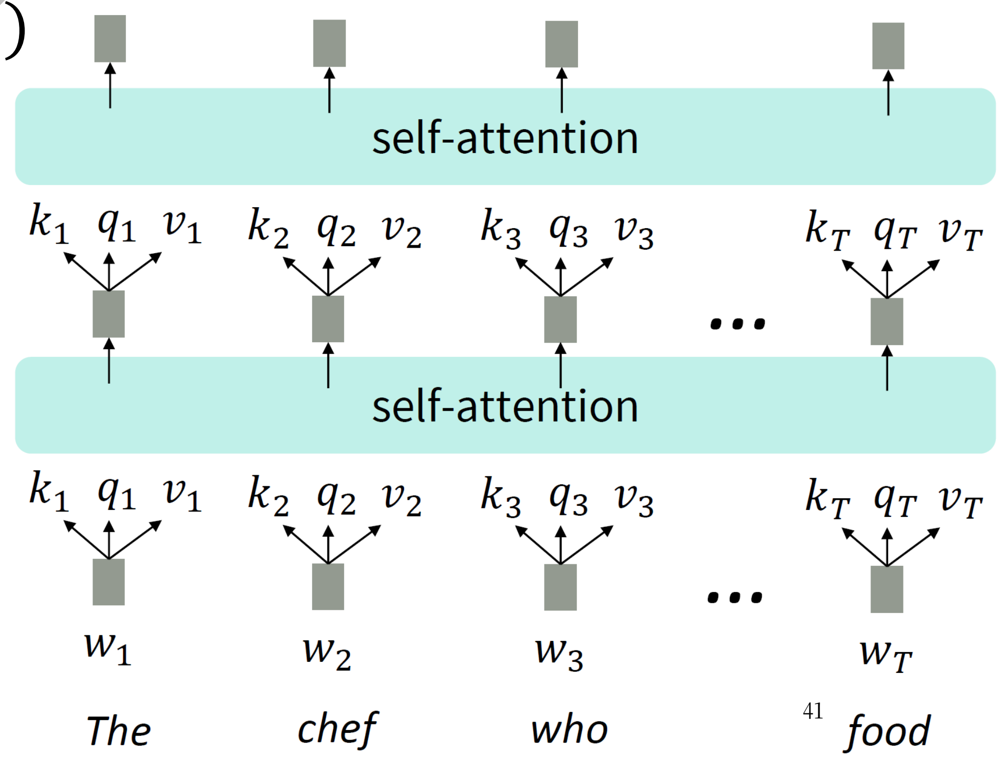
    - Simple & Generic solution for sequence modeling
    - Issue for long-term dependencies
      - Linear computations for distant words through a single latent state
    - Lack of parallelization
      - Forced sequential computation (contrast with CNN)
  - Attention
    - Direct connection to distant words
    - $O(N)$ computation but perfectly parallel!
  - Attention is all we need?



Self-Attention



- Attention is all you need (NIPS2017, Google Brain)
  - A purely attention-base architecture for sequence modeling
    - NO RNN at all
  - Basic component: Self-Attention, $Y = f_{SA}(X;\theta)$
    - Core idea:
      - X_t attends on the entire X sequence
      - Y_t computed from X_t and the attention output
    - Equations for 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 $\alpha_{t,j} = \mathrm{softmax}(q_t^T k_j)$
      - Attention output $out_t = \sum_j \alpha_{t,j} v_j$
      - $Y_t = g_2(out_t;\theta)$
- Issues of self-attention?



Self-Attention

- Issues of Vanilla Self-Attention
  - Notion of sequence order
    - Attention is order-invariant
  - Lack of non-linearities
    - All the weights are simple linear weighted average
  - Capability of autoregressive modelling
    - In generation tasks, the model cannot “look at the future”
    - E.g., text generation
      - Y_t can only depend on $X_{i<t}$
      - Vanilla self-attention focuses on the entire sequence

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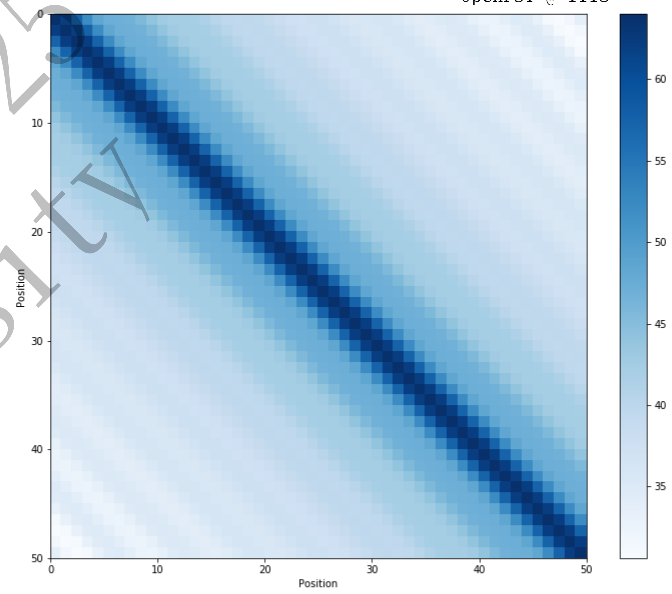
Self-Attention

- Notion of Sequence Ordering
  - Vanilla attention
    - $\tilde{\alpha}_{i,j} = \text{softmax}(\tilde{q}_i^T \tilde{k}_j);\ out_i = \sum_j \tilde{\alpha}_{i,j} \tilde{v}_j$
    - $\tilde{k}_t, \tilde{v}_t, \tilde{q}_t = g_1(X_t)$, do not contain position information
  - Idea: position encoding
    - p_i: an embedding vector of position i
    - $k_t, v_t, q_t = g_1([X_t, p_t])$ include position features
    - Practical remark:
      - Additive can be sufficient: $k_t \leftarrow \tilde{k}_t + p_t, q_t \leftarrow \tilde{q}_t + p_t, v_t \leftarrow \tilde{v}_t + p_t$
      - p_t is typically only included in the first layer
    - How to design p_i?
      - Note that the length of a sequence can be long

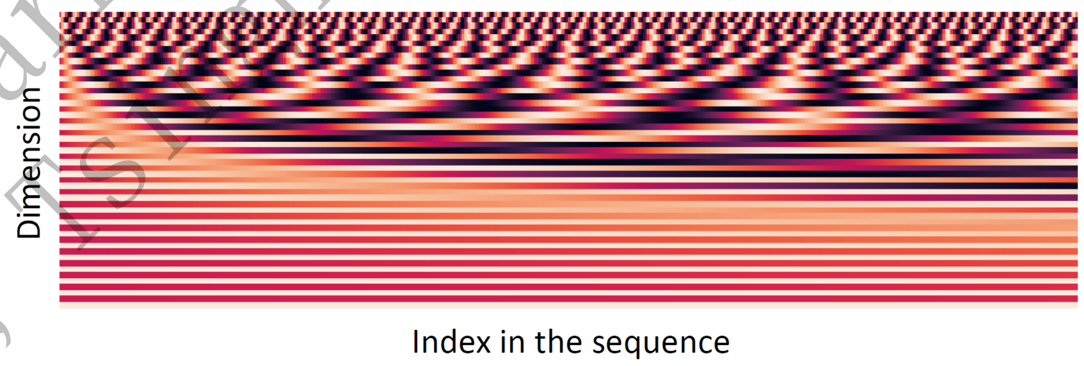
Self-Attention

- Notion of Sequence Ordering
  - Idea: position encoding p_i
    - $\tilde{k}_t, \tilde{v}_t, \tilde{q}_t = g_1(X_t)$, do not contain position information
  - Design of p_t
    - **Sinusoidal position representation**
      - Concatenate sinusoidal functions of varying periods



Heatmap of $p_i^T p_j$

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



- Pros: simple, naturally modelling “relative position”, easily applied to long sequences
- Cons: not learnable; generalization poorly to sequences longer than training data

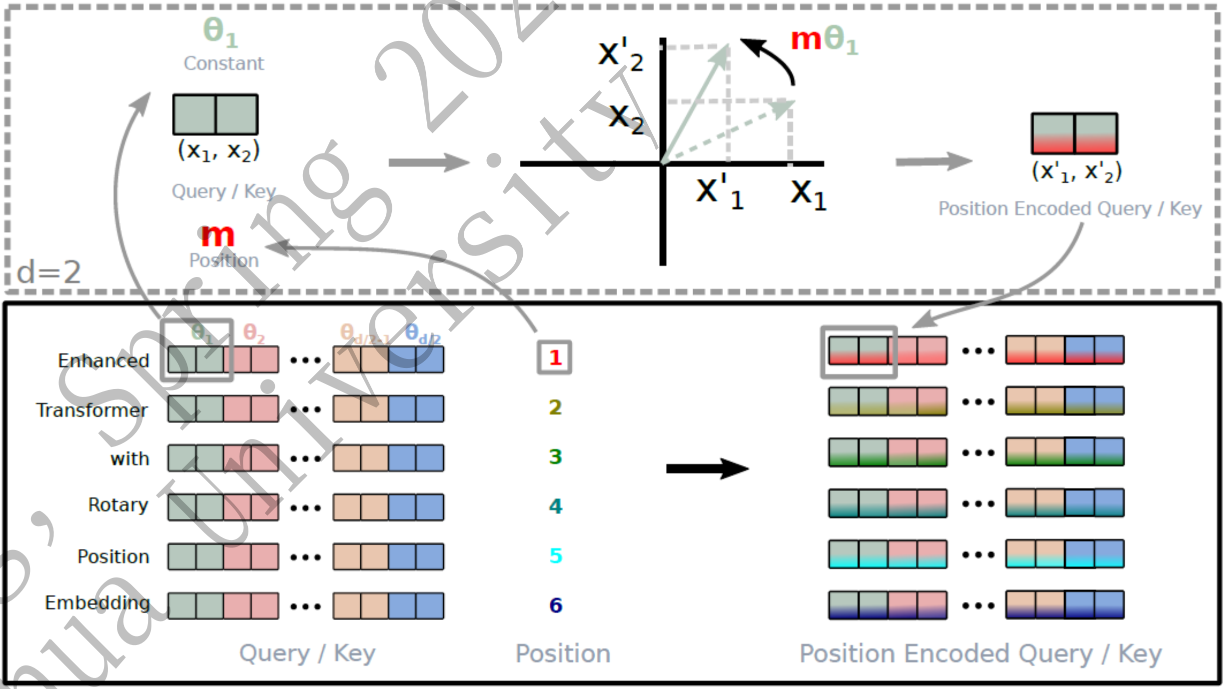
Self-Attention

- Notion of Sequence Ordering
  - Idea: position encoding p_i
    - $\tilde{k}_t, \tilde{v}_t, \tilde{q}_t = g_1(X_t)$, do not contain position information
  - Design of p_t
    - Sinusoidal position representation
    - **Learned absolute representation**
      - Let p_t become a learned parameter vector!
        - Assume maximum length L, learn a matrix $p \in \mathbb{R}^{d \times T}$, p_t is a column of p
      - A popular choice in practice!
      - Pros:
        - Flexible and learnable, more powerful
      - Cons:
        - Assume a fixed maximum length L, does not work at all for length above L

Self-Attention

- Notion of Sequence Ordering
  - Idea: position encoding p_i
    - $\tilde{k}_t, \tilde{v}_t, \tilde{q}_t = g_1(X_t)$, do not contain position information
  - Design of p_t
    - Sinusoidal position representation
    - Learned absolute representation
    - **Relative position representation (ACL2018, Google)**
      - When computing attention, relative distance is important!
        - $\alpha_{i,j} = \mathrm{softmax}\left(q_i^T\left(k_j + p_{[i-j]}\right)\right)$
        - $out_i = \sum_j \alpha_{i,j}\left(v_j + p_{[i-j]}\right)$
        - Bounded relative distance $p_t = p_{\max(-k,\min(k,t))}$
          - Truncate $t < -k$ to k and $t > k$ to k
      - Pros: learned representation and extrapolate well; More powerful.
      - Cons: computation overhead (refer to the paper for implementation tricks)

Self-Attention



$$\Theta = \{\theta_i = 10000^{-2(i-1)/d}, i \in [1, 2, ..., d/2]\}$$

- Notion of Sequence Ordering
  - Idea: position encoding p_i
    - $\tilde{k}_t, \tilde{v}_t, \tilde{q}_t = g_1(X_t)$, do not contain p
  - Design of p_t
    - Sinusoidal position representation
    - Learned absolute representation
    - Relative position representation
    - **Rotary position embedding (RoPE, Roformer, 2021)**
      - Relative position but factored computation

$$\boldsymbol{q}_m^\intercal \boldsymbol{k}_n = (\boldsymbol{R}^d_{\Theta,m} \boldsymbol{W}_q \boldsymbol{x}_m)^\intercal (\boldsymbol{R}^d_{\Theta,n} \boldsymbol{W}_k \boldsymbol{x}_n) = \boldsymbol{x}^\intercal \boldsymbol{W}_q R^d_{\Theta,n-m} \boldsymbol{W}_k \boldsymbol{x}_n$$

$$\boldsymbol{R}^d_{\Theta,n-m} = (\boldsymbol{R}^d_{\Theta,m})^\intercal \boldsymbol{R}^d_{\Theta,n}$$

$$\boldsymbol{R}^d_{\Theta,m} = \begin{pmatrix} \cos m\theta_1 & -\sin m\theta_1 & 0 & 0 & \cdots & 0 & 0 \\ \sin m\theta_1 & \cos m\theta_1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cos m\theta_2 & -\sin m\theta_2 & \cdots & 0 & 0 \\ 0 & 0 & \sin m\theta_2 & \cos m\theta_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & \cos m\theta_{d/2} & -\sin m\theta_{d/2} \\ 0 & 0 & 0 & 0 & \cdots & \sin m\theta_{d/2} & \cos m\theta_{d/2} \end{pmatrix}$$

Remark:

- Compatible with any dimension and length
- Fast computation
- Effective in practice

Self-Attention

- Issues of Vanilla Self-Attention
  - **Notion of sequence order**
    - Solution: position encoding
  - Lack of non-linearities
    - All the weights are simple linear weighted average
  - Capability of autoregressive modelling
    - In generation tasks, the model cannot “look at the future”
    - E.g., text generation
      - Y_t can only depend on $X_{i<t}$
      - Vanilla self-attention focuses on the entire sequence

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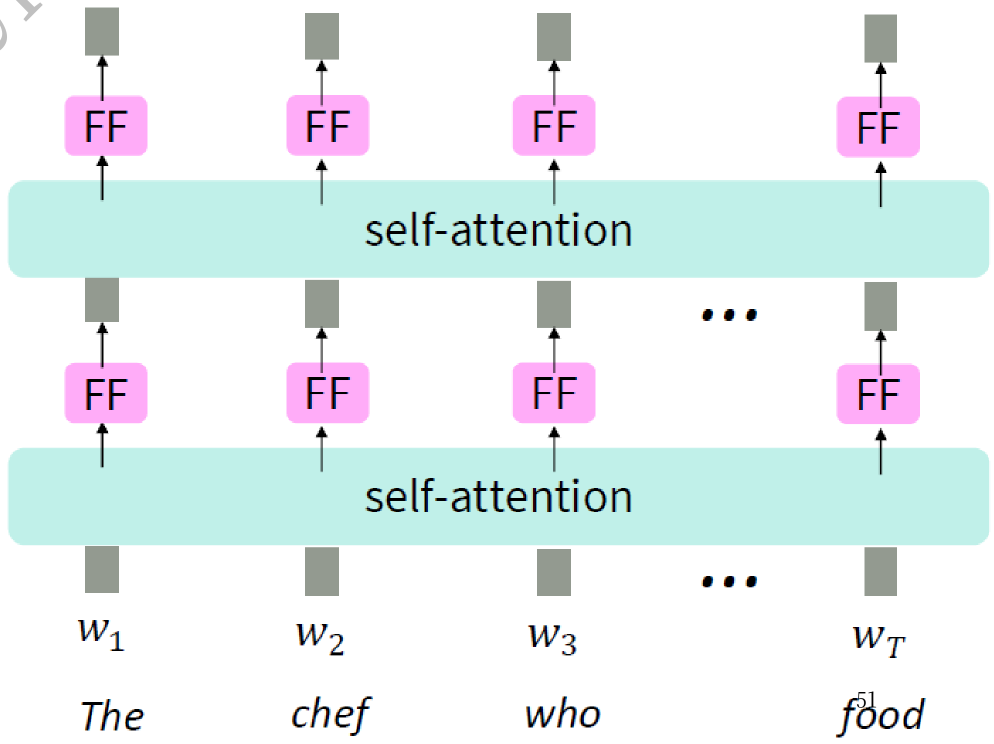
Self-Attention

- Combine nonlinearities in self-attention
  - Vanilla self-attention
    - No element-wise activation functions (e.g., ReLU, tanh)
    - Only weighted average and softmax operators
      - Essentially linear transformations of inputs
  - Easy fix:
    - Add an MLP to process out_i
    - $m_i = MLP(out_i)$
    - $\quad = W_2 \cdot \mathrm{ReLU}(W_1 \cdot out_i + b_1) + b_2$
    - Remark
      - we do not put activation layer before softmax



Self-Attention

- Issues of Vanilla Self-Attention
  - Notion of sequence order
    - Solution: position encoding
  - **Lack of non-linearities**
    - Solution: post-processing MLP layer
  - Capability of autoregressive modelling
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    - E.g., text generation
      - Y_t can only depend on $X_{i<t}$
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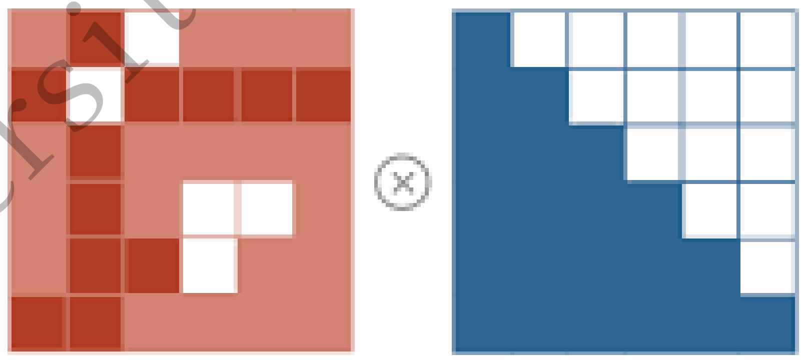
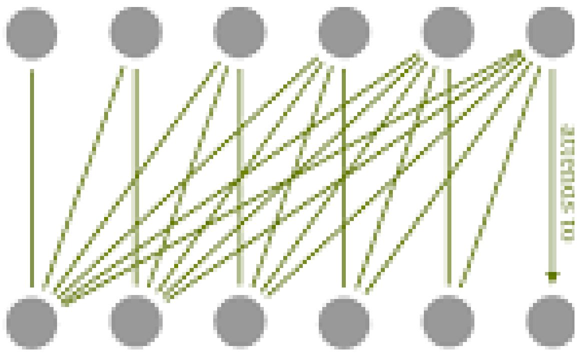
Self-Attention

- Autoregressive Modeling
  - In language mode decoder: model $P(Y_t|X_{i<t})$
    - out_t cannot loot at future $X_{i>t}$
    - Naïve solution:
      - For each t, a varying for-loop only iterating over $i \leq t$
      - Varying for-loop for each t, parallelization unfriendly
  - Masked Attention
    - Compute $e_{i,j} = q_i^T k_j$ as usual (perfect parallel)
    - Mask out $e_{i>j}$ by setting $e_{i>j} = -\infty$ (perfect parallel)
      - $e \odot (1 - M) \leftarrow -\infty$; M is a fixed 0/1 mask matrix
    - Then compute $\alpha_i = \text{softmax}(e_i)$ (perfect parallel)
    - Remark:
      - $M = 1$ for full self-attention
      - Set M for arbitrary dependency ordering





Self-Attention

- Issues of Vanilla Self-Attention
  - Notion of sequence order
    - Solution: position encoding
  - Lack of non-linearities
    - Solution: post-processing MLP layer
  - **Capability of autoregressive modelling**
    - Solution: masked self-attention

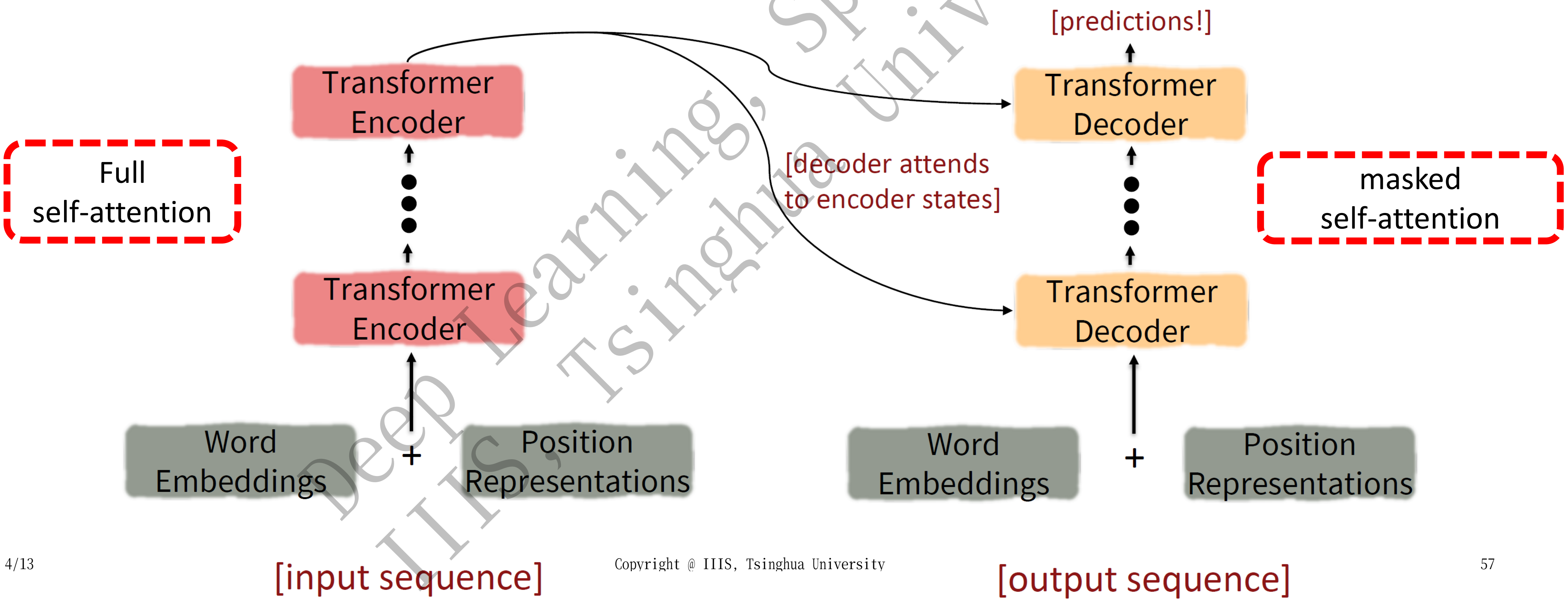
Self-Attention

- Issues of Vanilla Self-Attention
  - Notion of sequence order
    - Solution: position encoding
  - Lack of non-linearities
    - Solution: post-processing MLP layer
  - Capability of autoregressive modelling
    - Solution: masked self-attention

  - Basic building block for the famous “Transformer” model!
    - Attention is all you need (NIPS2017, Vaswani et al, Google)
      - Self-attention + **a few more other enhancements**!
    - A milestone: first pure attention-based model for effective sequence modeling
      - *Originally proposed for NMT; Soon dominates general sequence modeling problems*

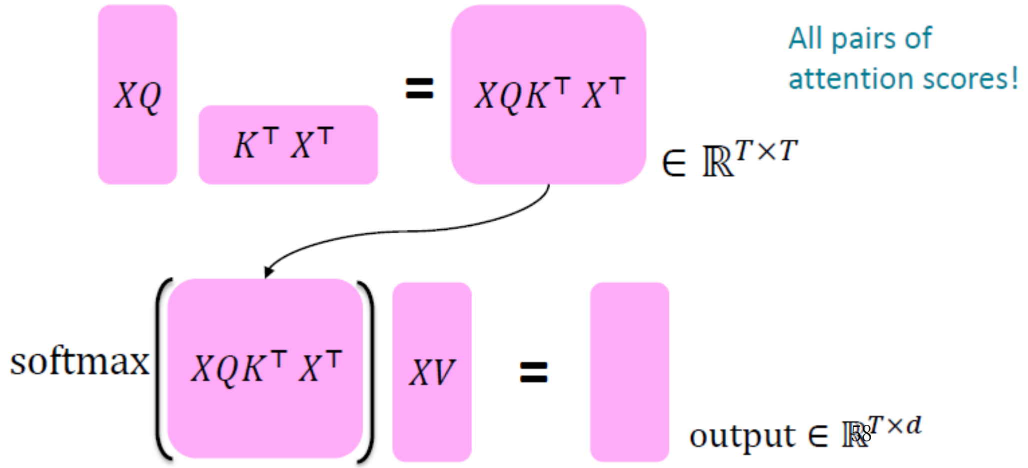
Transformer Model

- Transformer-based sequence-to-sequence modeling



Transformer Model

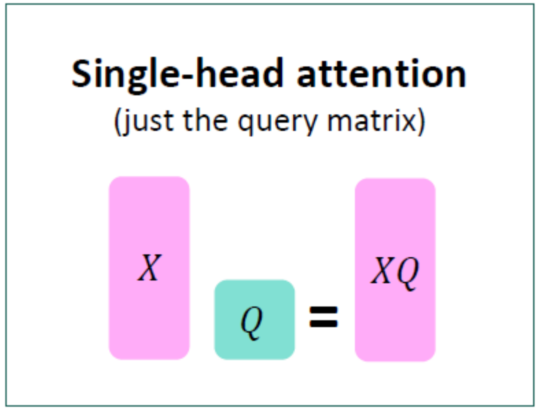
- Transformer-based sequence-to-sequence modeling
  - Basic building blocks: masked self-attention
  - Enhancements
    - **Key-query-value attention**
      - Obtain $q_t, v_t,$ k_t from X_t
      - $q_t = W^q X_t; v_t = W^v X_t; k_t = W^k X_t$ (position encoding omitted)
        - W^q, W^v, W^k are learnable weight matrices
      - $\alpha_{i,j} = \mathrm{softmax}(q_i^T k_j); out_i = \sum_j \alpha_{i,j} v_j$
      - Intuition: key, query, and value can focus on different parts of input

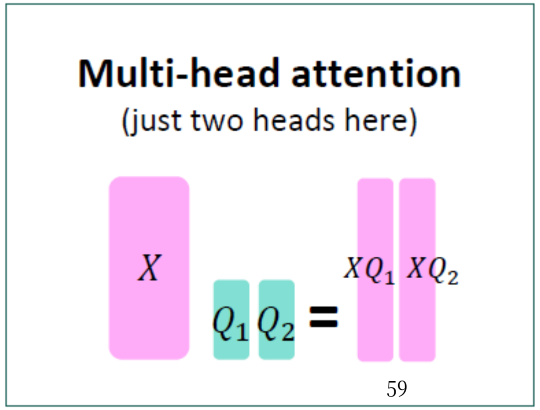


Transformer Model

- Transformer-based sequence-to-sequence modeling
  - Basic building blocks: masked self-attention
  - Enhancements
    - Key-query-value attention
    - **Multi-headed attention**
      - Standard attention → single-headed attention
        - $X_t \in \mathbb{R}^d, \quad Q, K, V \in \mathbb{R}^{d \times d}$
        - 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
        - $Q^l, K^l, V^l \in \mathbb{R}^{d \times \frac{d}{h}}$, for $1 \leq l \leq h$
        - $\alpha_{i,j}^l = \text{softmax}\left({q_i^l}^T k_j^l\right); out_i^l = \sum_j \alpha_{i,j}^l v_j^l$

#Params Unchanged!





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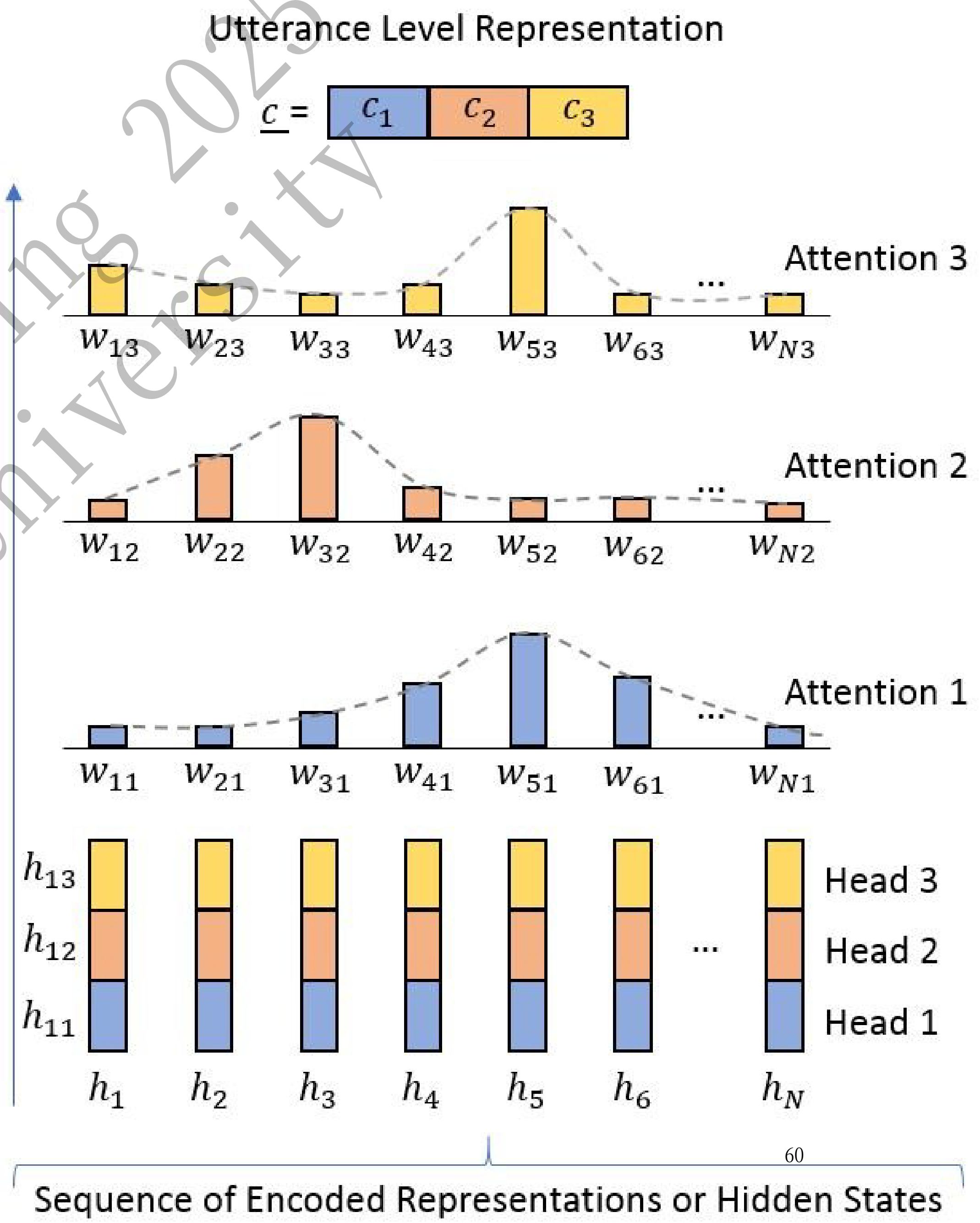
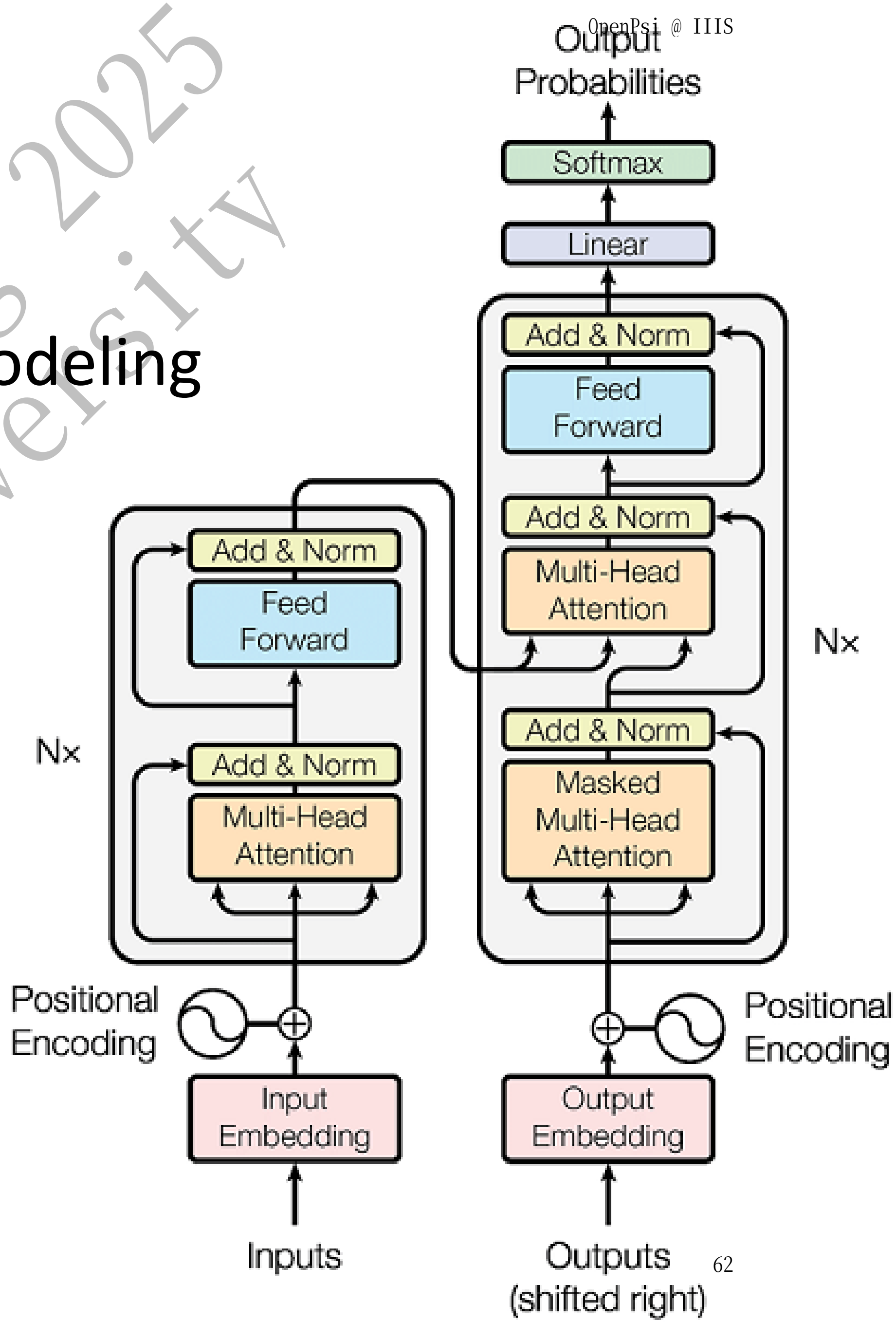


Transformer Model

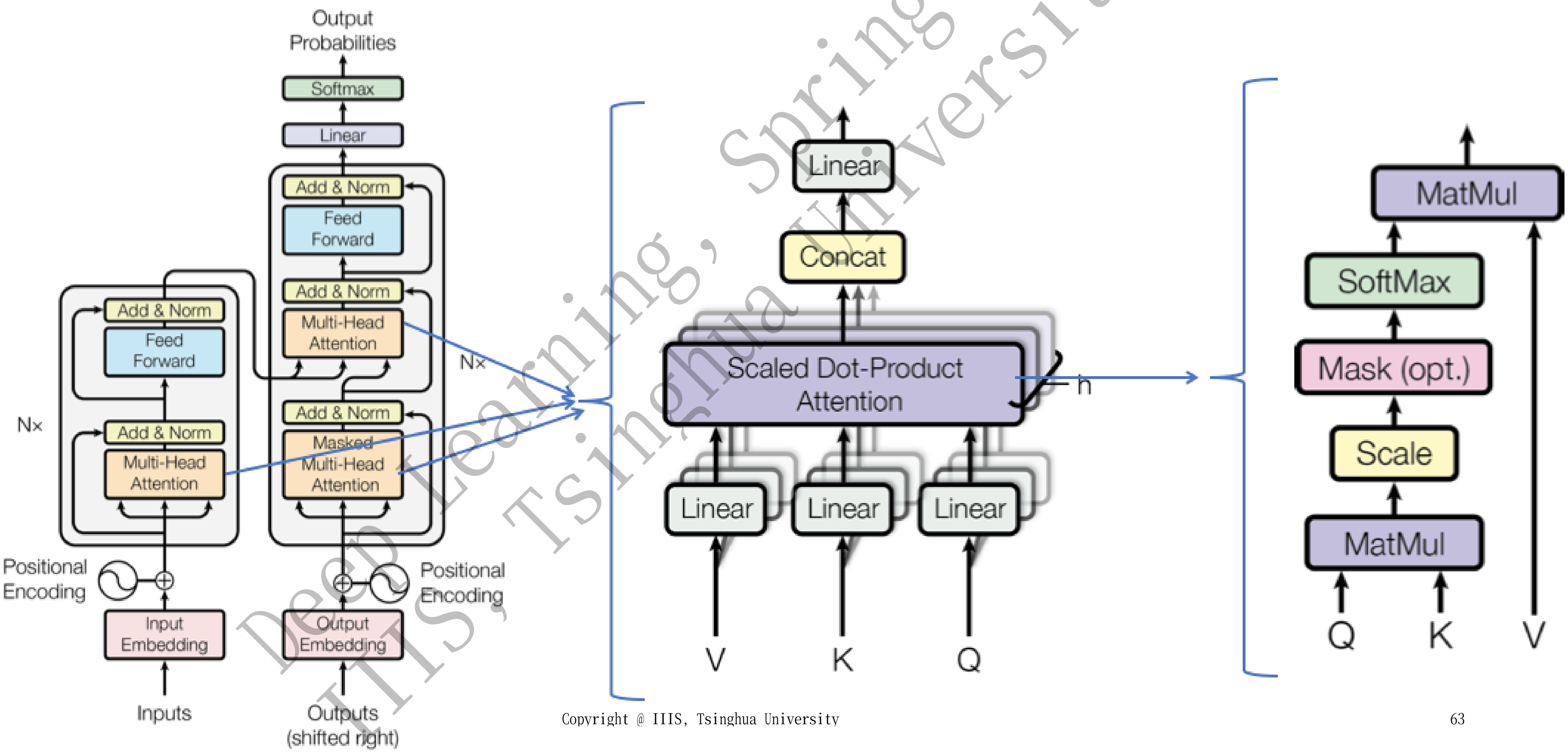
- Transformer-based sequence-to-sequence modeling
  - Basic building blocks: masked self-attention
  - Enhancements
    - Key-query-value attention
    - Multi-headed attention
    - **Architecture modifications**
      - Residual connection
      - Layer normalization
        - $out_t = \mathrm{LN}(f_{SA}(X_t, M) + X_t); m_t = \mathrm{LN}(\mathrm{MLP}(out_t) + out_t)$
      - Scaled dot product
        - Intuition: when dimension d becomes large, $q^T k$ can be large
        - Issue: input to softmax can be large and make gradient small
        - $\alpha_{i,j}^l = \mathrm{softmax}\left(\frac{{q_i^l}^T k_j^l}{\sqrt{d/h}}\right)$

Transformer Model

- Transformer-based sequence-to-sequence modeling
  - Basic building blocks: masked self-attention
    - Position encoding
    - Post-processing MLP
    - Attention mask
  - Enhancements
    - Key-query-value attention
    - Multi-headed attention
    - Architecture modifications
      - Residual connection
      - Layer normalization
      - Scaled dot product



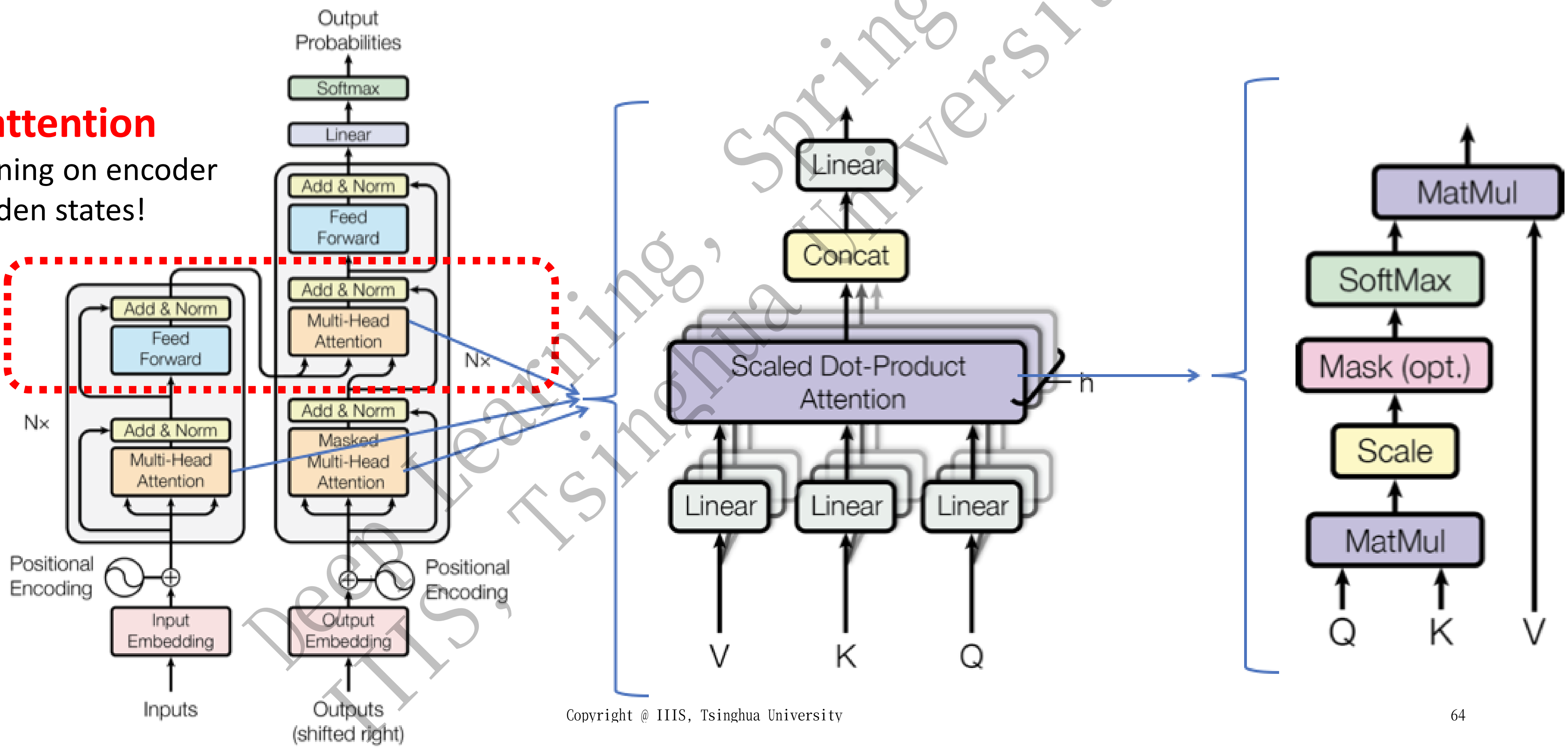
Transformer-Based Seq2Seq Model



Transformer-Based Seq2Seq Model

Cross-attention

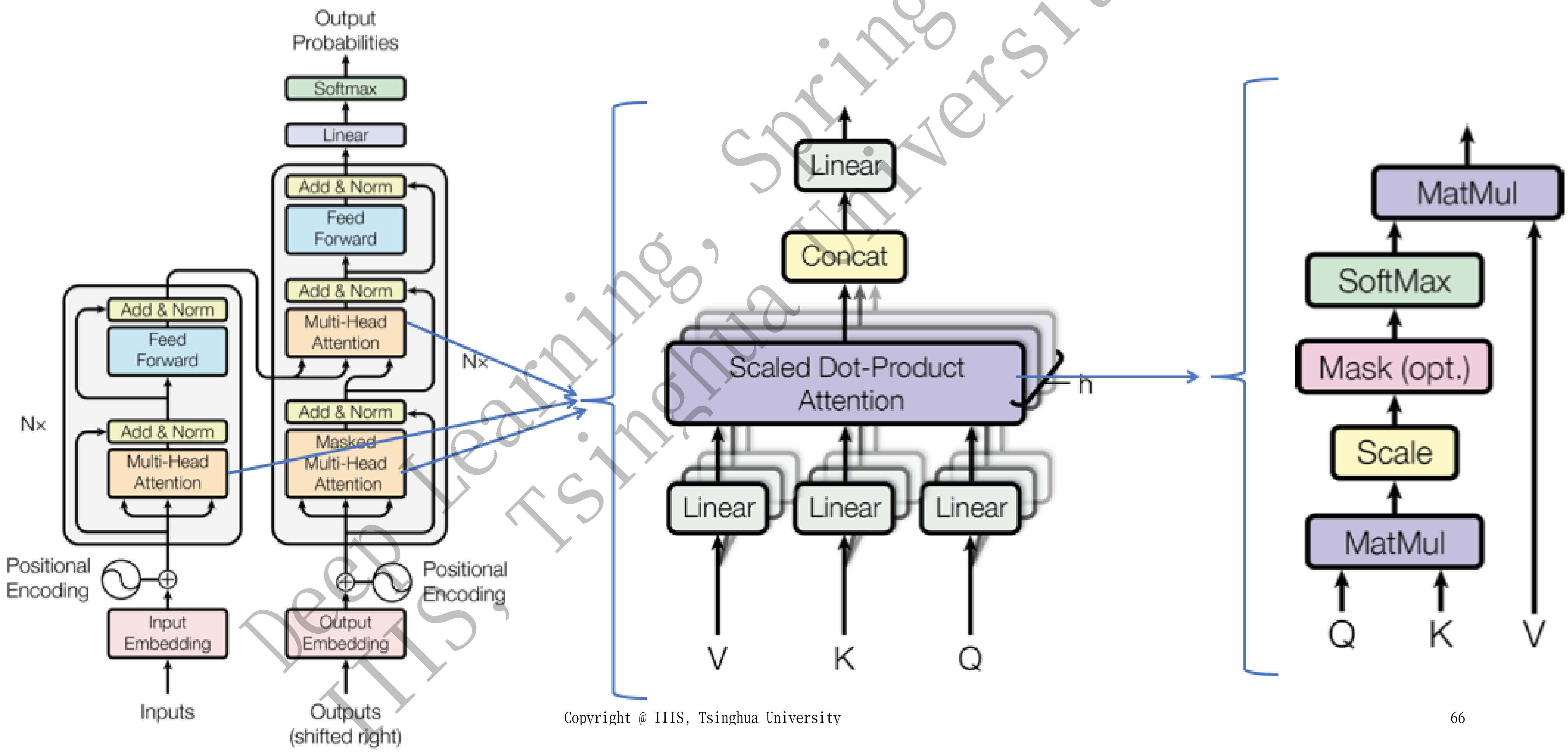
Conditioning on encoder hidden states!



Transformer-Based Seq2Seq Model

- Cross-attention
  - The conditioning part of transformer
    - Decoder can generate texts conditioning on the input sequence
    - Just like standard attention in RNN seq2seq model
  - z_t: decoder SA module inputs
  - h_t: encoder output hidden states
  - For each decoder out_t, we attend on encoder hiddens
    - Query from decoder: $q_t = W^q z_t$
    - Key and value from encoder: $k_j = W^k h_j$; $v_j = W^v h_j$
    - $\alpha_{ij} = \text{softmax}\left(\frac{q_i^T k_j}{\sqrt{d}}\right)$; $out_i = LN\left(\sum_j \alpha_{ij} v_j + z_i\right)$
      - Many practical variants can be implemented

Transformer-Based Seq2Seq Model



Transformer-Based Seq2Seq Model

- Machine translation with transformer (NIPS2017, Google)

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

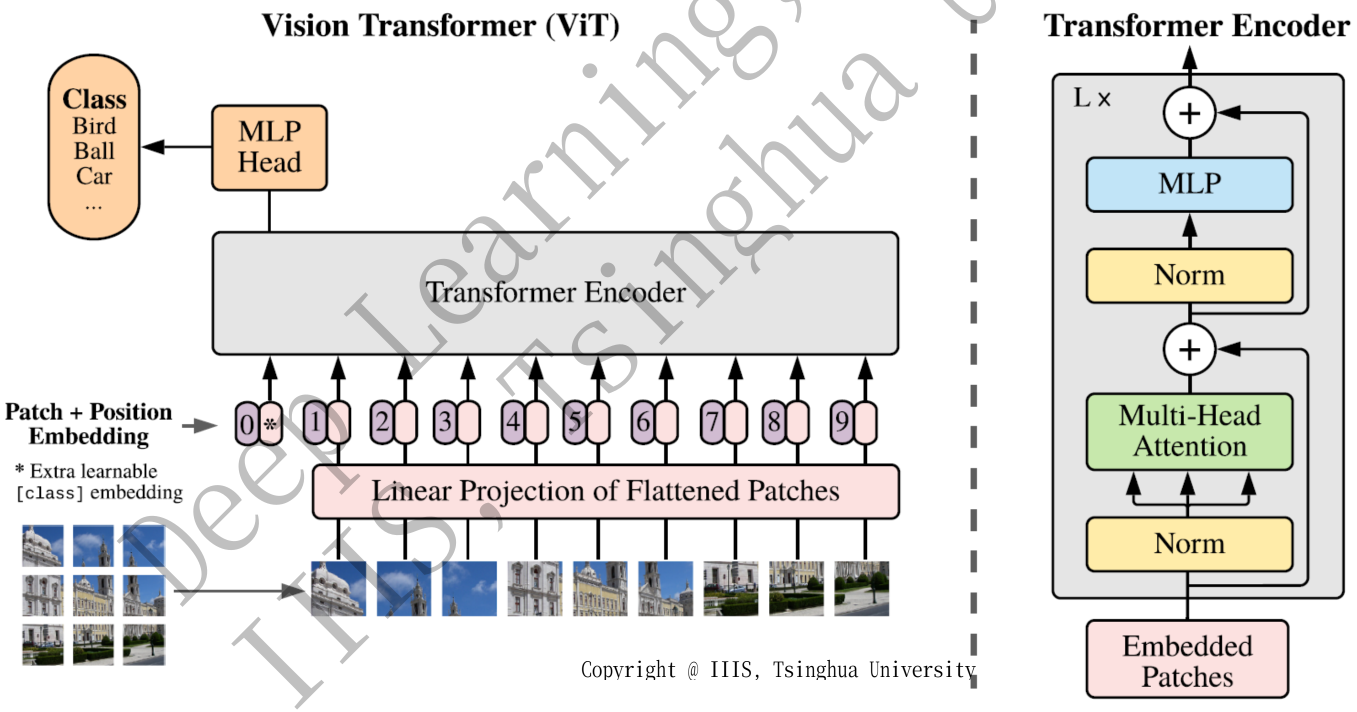
Transformer-Based Seq2Seq Model

- Generating Wikipedia by summarizing long sequences (ICLR2018, Google)
  - Document generation

Model	Test perplexity	ROUGE-L
seq2seq-attention, $L = 500$	5.04952	12.7
Transformer-ED, $L = 500$	2.46645	34.2
Transformer-D, $L = 4000$	2.22216	33.6
Transformer-DMCA, no MoE-layer, $L = 11000$	2.05159	36.2
Transformer-DMCA, MoE-128, $L = 11000$	1.92871	37.9
Transformer-DMCA, MoE-256, $L = 7500$	1.90325	38.8

Transformer Model for Images

- Vision Transformer (ViT, Google Brain, ICLR 2021, 33.4k citation)
  - *An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale*
  - Decompose an image to 16x16 patches and then apply transformer encoder



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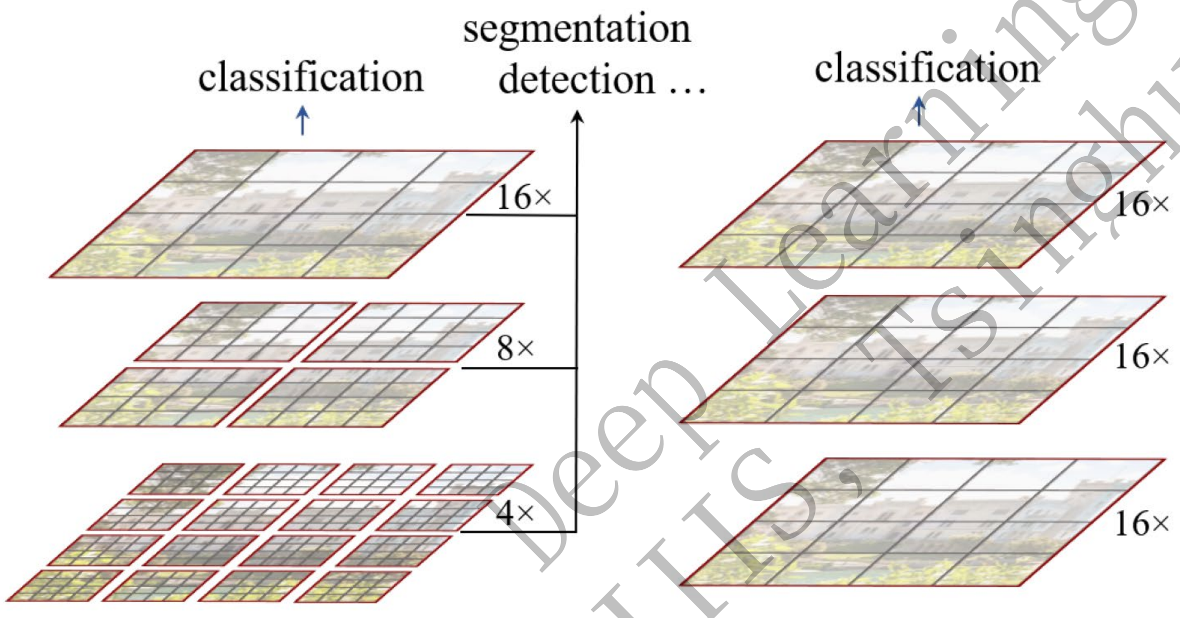
	Ours-JFT (ViT-H/14)	Ours-JFT (ViT-L/16)	Ours-I21k (ViT-L/16)	BiT-L (ResNet152x4)	Noisy Student (EfficientNet-L2)
ImageNet	**88.55** ± 0.04	87.76 ± 0.03	85.30 ± 0.02	87.54 ± 0.02	88.4/88.5*
ImageNet ReaL	**90.72** ± 0.05	90.54 ± 0.03	88.62 ± 0.05	90.54	90.55
CIFAR-10	**99.50** ± 0.06	99.42 ± 0.03	99.15 ± 0.03	99.37 ± 0.06	–
CIFAR-100	**94.55** ± 0.04	93.90 ± 0.05	93.25 ± 0.05	93.51 ± 0.08	–
Oxford-IIIT Pets	**97.56** ± 0.03	97.32 ± 0.11	94.67 ± 0.15	96.62 ± 0.23	–
Oxford Flowers-102	99.68 ± 0.02	**99.74** ± 0.00	99.61 ± 0.02	99.63 ± 0.03	–
VTAB (19 tasks)	**77.63** ± 0.23	76.28 ± 0.46	72.72 ± 0.21	76.29 ± 1.70	–
TPUv3-core-days	2.5k	0.68k	0.23k	9.9k	12.3k

Transformer Model for Images

- Swin Transformer (MSRA, CVPR 2021 best paper)
    - Build hierarchical feature maps at different resolution
        - Self-attention only within each block (linear computation for image size)
        - Shifted block partitions to encode information between blocks



(a) Swin Transformer (ours)   (b) ViT

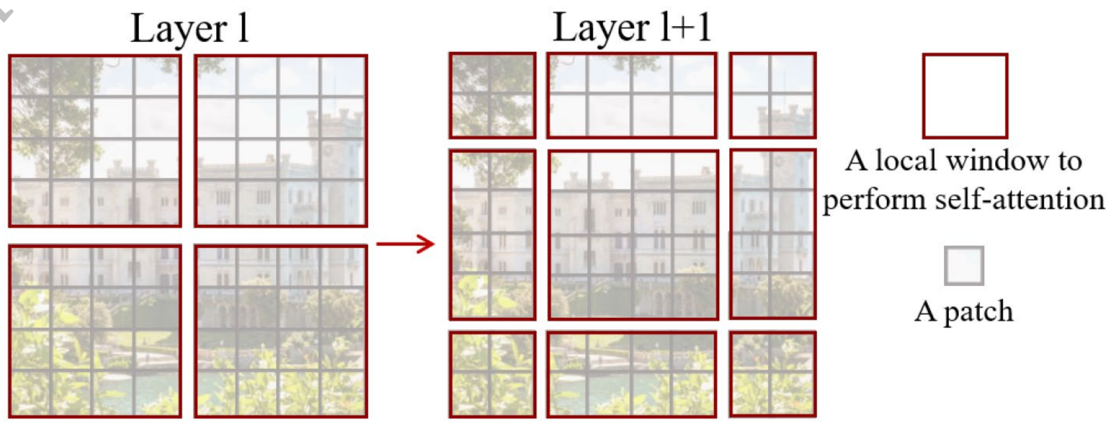


Figure 2. An illustration of the *shifted window* approach for com-

Transformer Model for Images

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  - Build hierarchical feature maps at different resolution
    - Self-attention only within each block (linear computation for image size)
    - Shifted block partitions to encode information between blocks

Method	mini-val AP^{box}	mini-val AP^{mask}	test-dev AP^{box}	test-dev AP^{mask}	#param.	FLOPs
RepPointsV2* [12]	-	-	52.1	-	-	-
GCNet* [7]	51.8	44.7	52.3	45.4	-	1041G
RelationNet++* [13]	-	-	52.7	-	-	-
SpineNet-190 [21]	52.6	-	52.8	-	164M	1885G
ResNeSt-200* [78]	52.5	-	53.3	47.1	-	-
EfficientDet-D7 [59]	54.4	-	55.1	-	77M	410G
DetectoRS* [46]	-	-	55.7	48.5	-	-
YOLOv4 P7* [4]	-	-	55.8	-	-	-
Copy-paste [26]	55.9	47.2	56.0	47.4	185M	1440G
X101-64 (HTC++)	52.3	46.0	-	-	155M	1033G
Swin-B (HTC++)	56.4	49.1	-	-	160M	1043G
Swin-L (HTC++)	57.1	49.5	57.7	50.2	284M	1470G
Swin-L (HTC++)*	**58.0**	**50.4**	**58.7**	**51.1**	284M	-

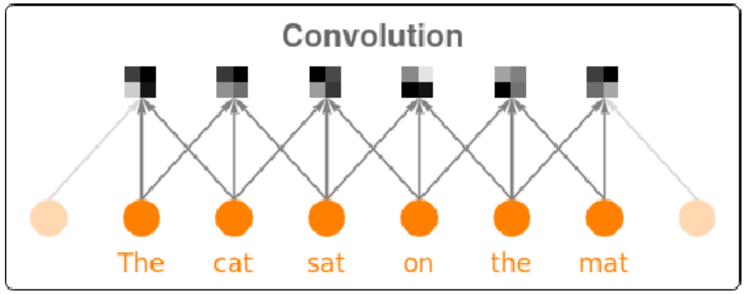
Table 2. Results on COCO object detection and instance segmentation. †denotes that additional decovolution layers are used to produce hierarchical feature maps. * indicates multi-scale testing.

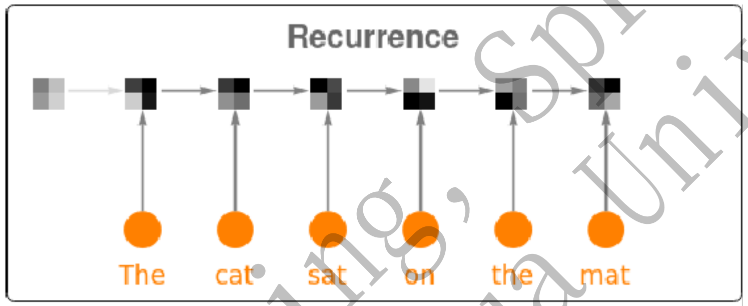
ADE20K Method	Backbone	val mIoU	test score	#param.	FLOPs	FPS
DANet [23]	ResNet-101	45.2	-	69M	1119G	15.2
DLab.v3+ [11]	ResNet-101	44.1	-	63M	1021G	16.0
ACNet [24]	ResNet-101	45.9	38.5	-		
DNL [71]	ResNet-101	46.0	56.2	69M	1249G	14.8
OCRNet [73]	ResNet-101	45.3	56.0	56M	923G	19.3
UperNet [69]	ResNet-101	44.9	-	86M	1029G	20.1
OCRNet [73]	HRNet-w48	45.7	-	71M	664G	12.5
DLab.v3+ [11]	ResNeSt-101	46.9	55.1	66M	1051G	11.9
DLab.v3+ [11]	ResNeSt-200	48.4	-	88M	1381G	8.1
SETR [81]	T-Large‡	50.3	61.7	308M	-	-
UperNet	DeiT-S†	44.0	-	52M	1099G	16.2
UperNet	Swin-T	46.1	-	60M	945G	18.5
UperNet	Swin-S	49.3	-	81M	1038G	15.2
UperNet	Swin-B‡	51.6	-	121M	1841G	8.7
UperNet	Swin-L‡	**53.5**	**62.8**	234M	3230G	6.2

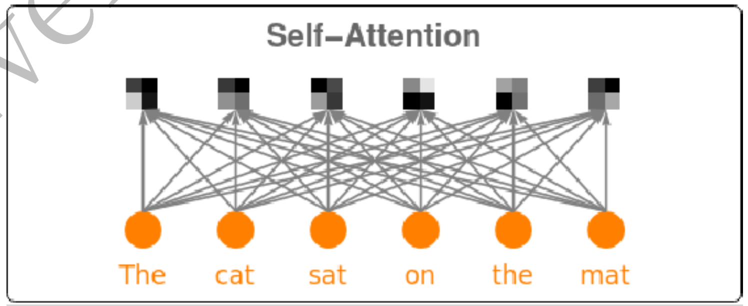
Table 3. Results of semantic segmentation on the ADE20K val and test set. † indicates additional deconvolution layers are used to produce hierarchical feature maps. ‡ indicates that the model is pre-trained on ImageNet-22K.

Comparisons

- CNN v.s. LSTM v.s. Transformer







Context length L	Temporal Convolution	RNN	Transformer
Layers			
Generation			
Inference			

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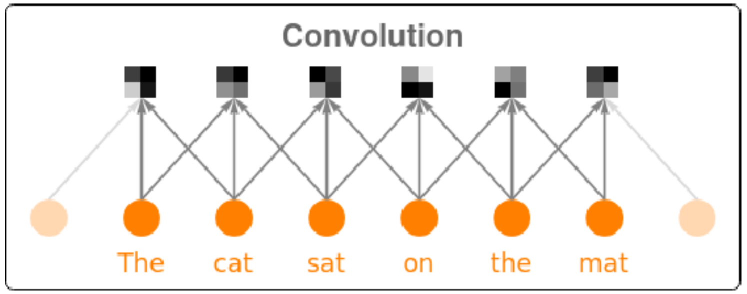

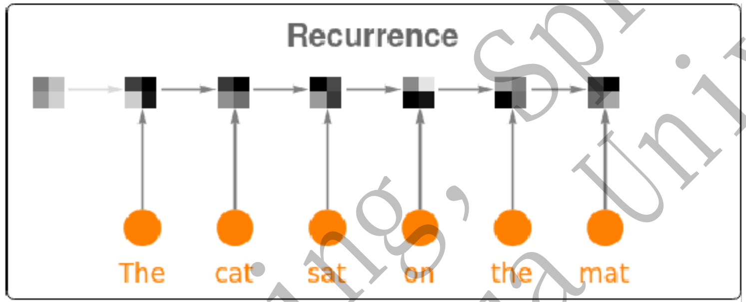

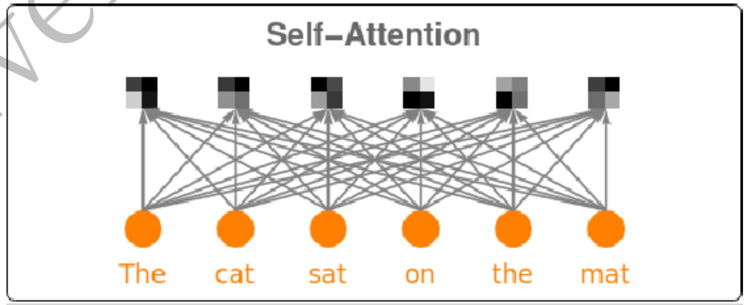

Context length L	Temporal Convolution	RNN	Transformer
Layers	$O(\log L)$	$O(1)$	$O(1)$
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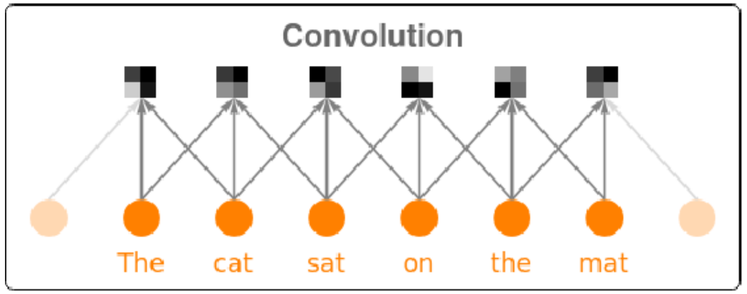

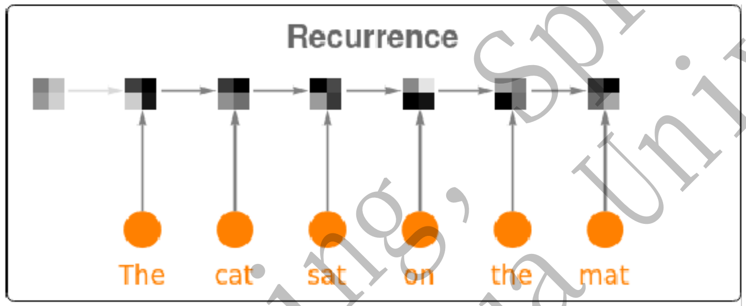

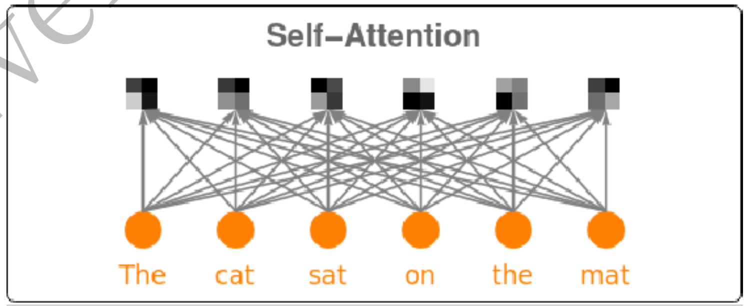

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Inference			

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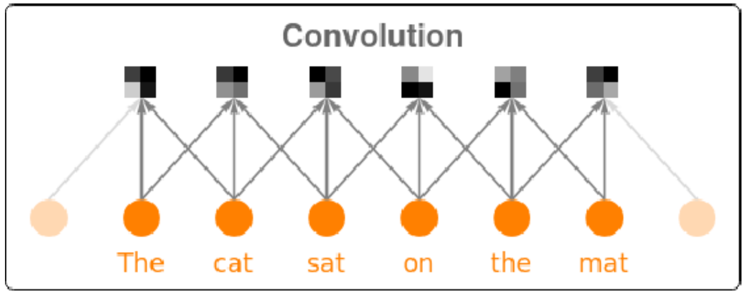

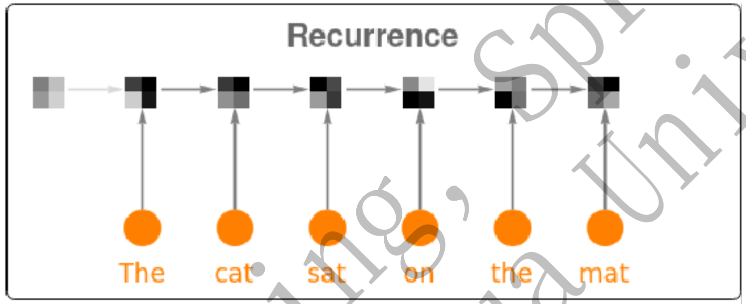

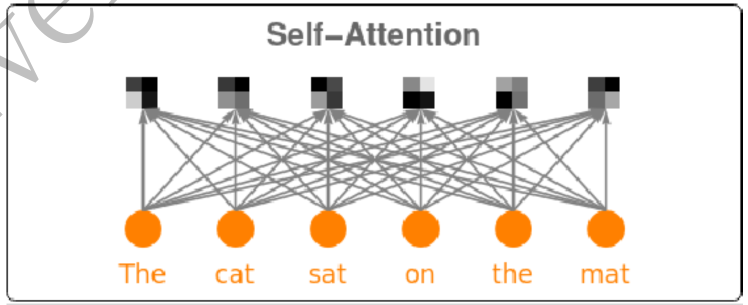

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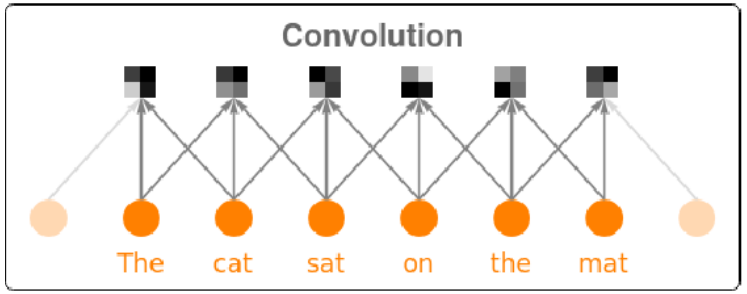

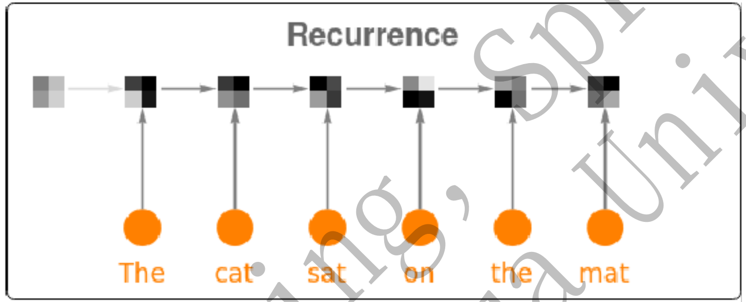

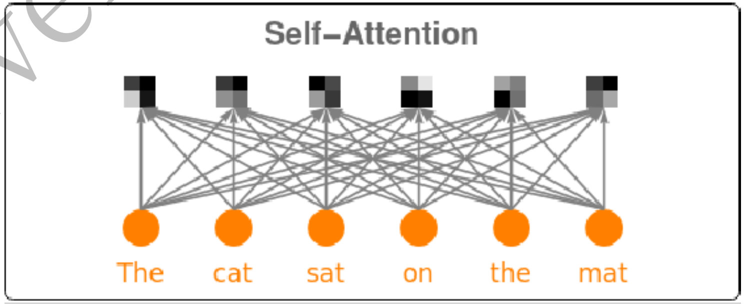

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Quadratic!!

Can we speedup transformer generation?

Speed up Transformers

- Quadratic generation cost
  - $O(L^2)$ for length L: sequential generation $O(L)$ × attention $O(L)$
    - What if we want to model sequence length of, say, $L > 10^4$

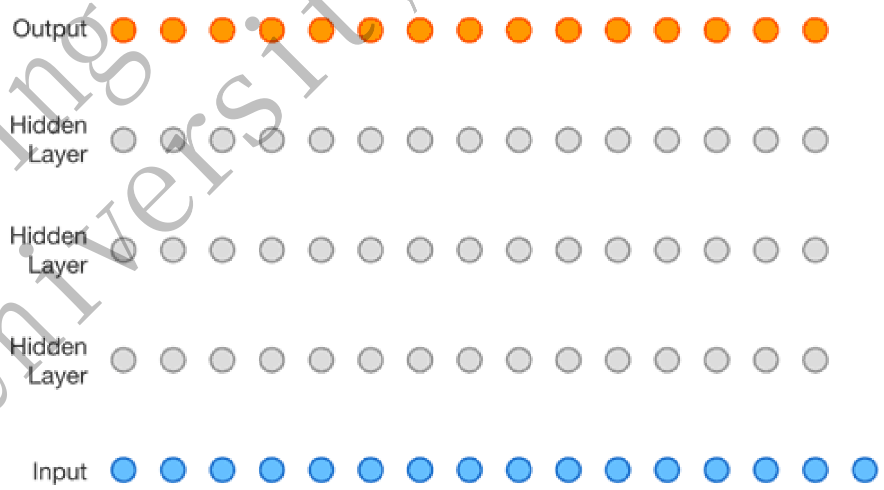
Speed up Transformers

- Quadratic generation cost
  - $O(L^2)$ for length L: sequential generation $O(L) \times$ attention $O(L)$
- Make attention faster/better
  - Large-scale training: transformer-XL; XL-net (Zhilin Yang, et al, Google, 2020)
  - Projection tricks: Linformer (Facebook AI, $O(n)$ computation, 2020)
  - Math tricks: Performer (Google, $O(n)$ computation, 2020)
  - Sparse interactions:
    - Big Bird (Google, 2020), Multi-head Latent Attention (DeepSeek, 2024) https://planetbanatt.net/articles/mla.html
  - Fast and memory-efficient attention:
    - Flash Attention (Tri Dao, et al, 2022) and Ring Attention (Hao Liu, et al, 2023)
    - System engines for fast generation: vLLM (Berkeley) and SGLang (xAI & UCLA)
  - Even Parallel/Contextualized RNN (make RNN great again):
    - RWKV RNN (Open-Source, 2023) & Mamba (Gu, Albert and Tri Dao, 2023)
  - Reduce attention flatten issue when length grows: Scalable-Softmax (2025)

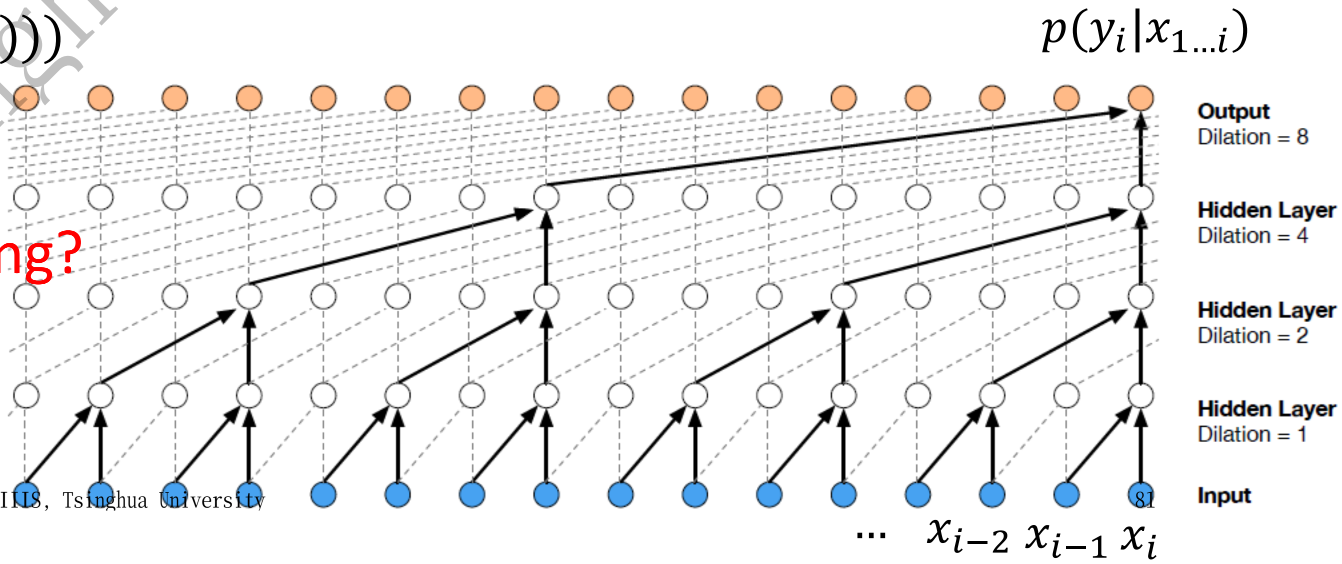
Speed up Transformers

- Quadratic generation cost
  - $O(L^2)$ for length L: sequential generation $O(L)$ × attention $O(L)$
- Remark:
  - Ideally, attention can be computed in parallel given unbounded computation and memory bandwidth
- Can we accelerate autoregressive generation?
  - This is the key bottleneck for language model generation, which cannot be accelerate by hardware improvement

Beyond Autoregressive Generation



- WaveNet (Recap)
  - Let's use the language model notations
    - Output $y_1 \dots y_i$
    - Input $x_1 \dots x_i$ $(x_i = y_{i-1})$
    - $p(y) = \prod_i p(y_i | x_{1 \dots i})$
  - y_i can only computed after y_{i-1}
    - $p(y_i) = N(\mu_\theta(x_{1\dots i}), \exp^2(\alpha_\theta(x_{1\dots i})))$
    - $x_i \leftarrow y_{i-1}$
    - y_{i-1} is part of input of y_i
  - Can we compute y_i without waiting?



Beyond Autoregressive Generation

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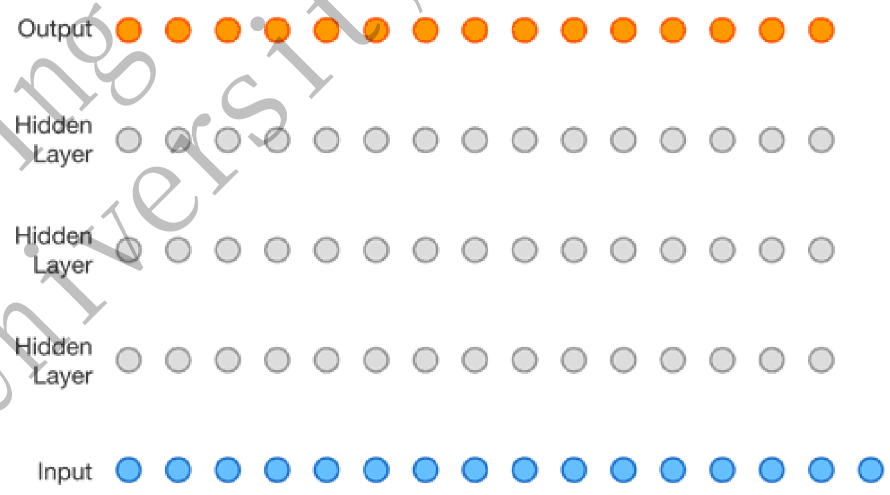
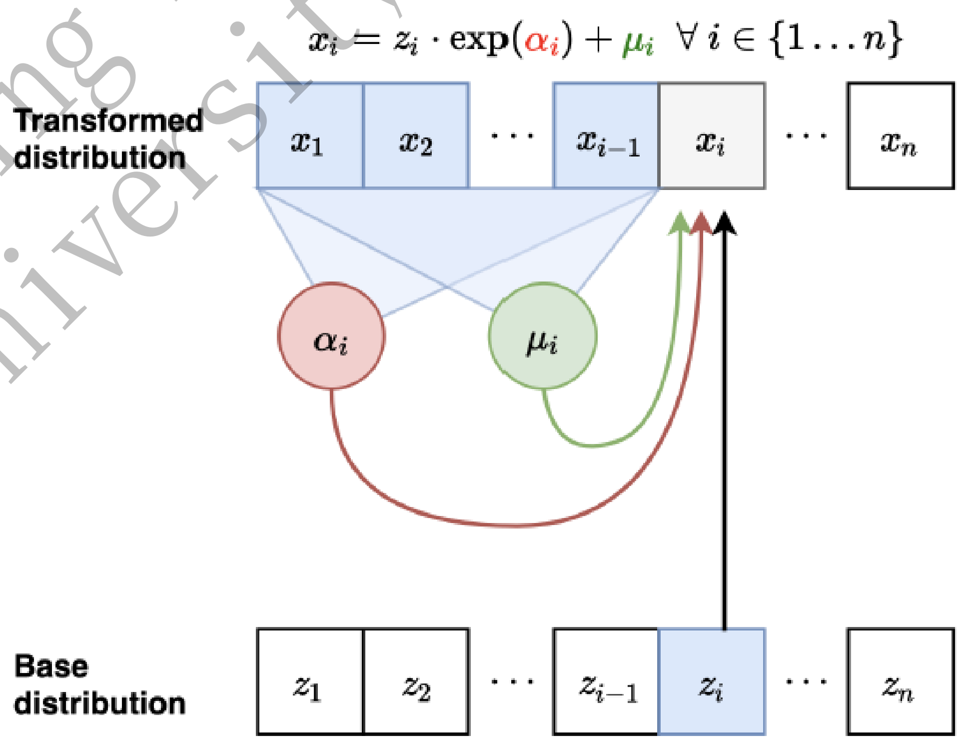
    - $p(y) = \prod_i p(y_i | x_{1\dots i})$
  - Reparameterization trick
    - $z_i \sim N(0,1)$
    - $y_i \leftarrow \mu_\theta(x_{1\dots i}) + z_i \cdot \exp(\alpha_\theta(x_{1\dots i}))$
    - $x_i \leftarrow y_{i-1}$



Beyond Autoregressive Generation



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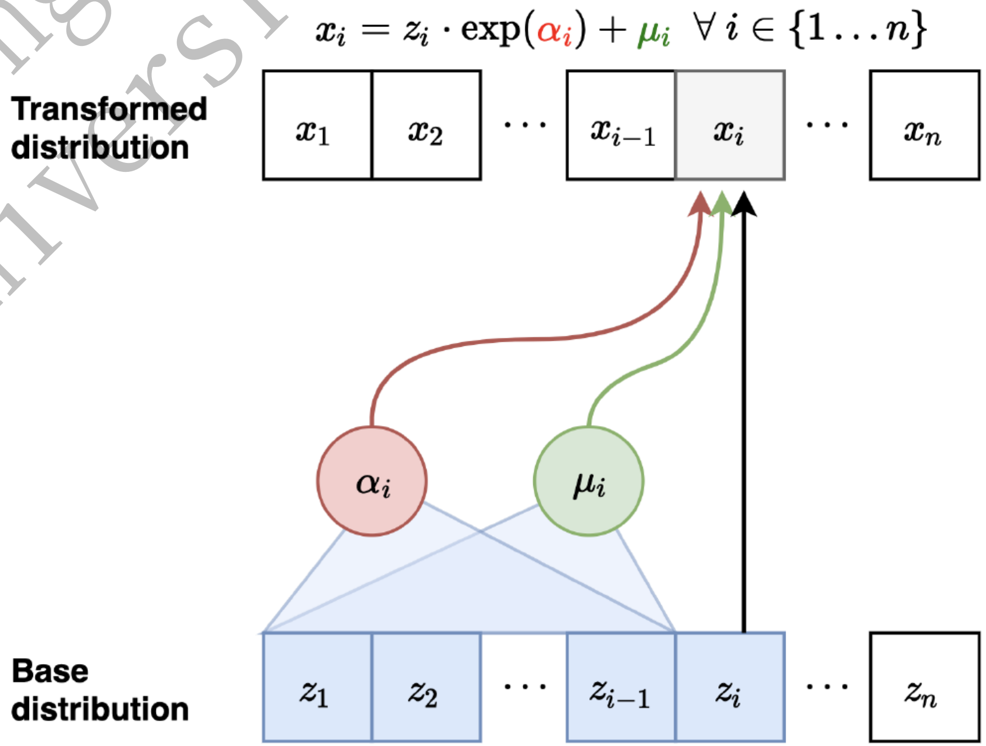
    - $x_i \leftarrow y_{i-1}$
- x_i can be written as a function of $z_{1\dots i}$ without compromising the representation power!
  - Each x is corresponding to a unique z! (your homework)

Beyond Autoregressive Generation

- Parallel WaveNet (DeepMind, ICML 2018)
  - Sequential modeling notation (ignore y)
    - Sequence tokens x & latent variable z
    - $p(x) = \prod_i p(x_i|x_{1\ldots i})$
  - Reparameterization trick
    - $z_i \sim N(0,1)$
    - $x_i \leftarrow \mu_\theta(z_{1\ldots i-1}) + z_i \cdot \exp(\alpha_\theta(z_{1\ldots i-1}))$
  - Parallel generation
    - First generate z and then x



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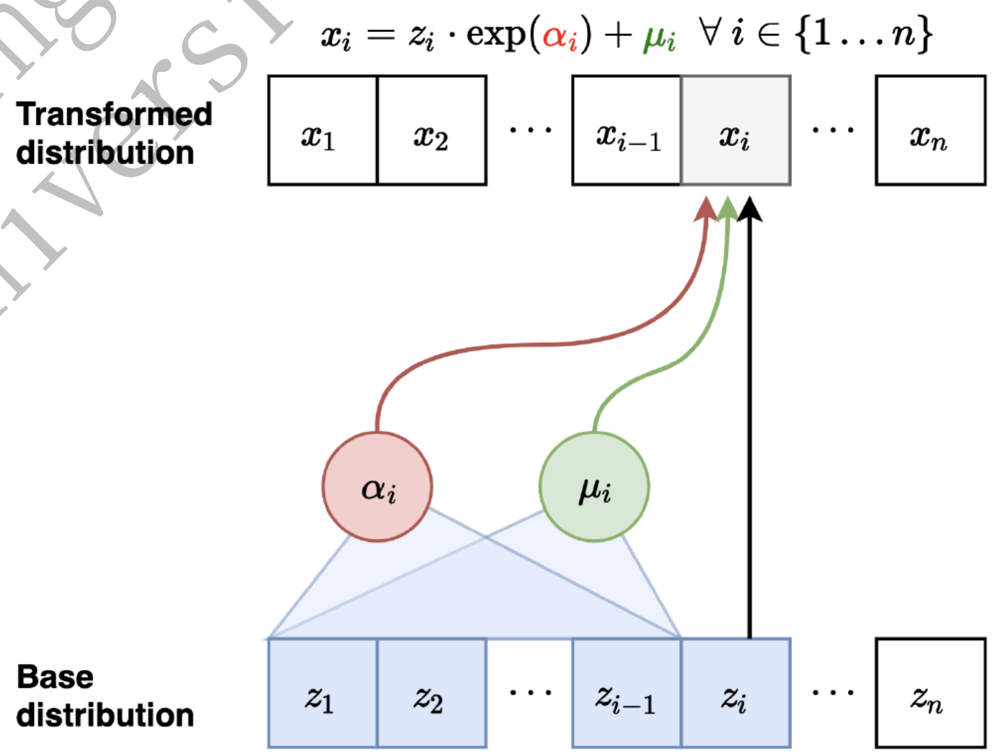
  - Parallel generation
    - First generate z and then x
  - What about inference?
    - Given x, how to compute $p(x)$ for MLE training?



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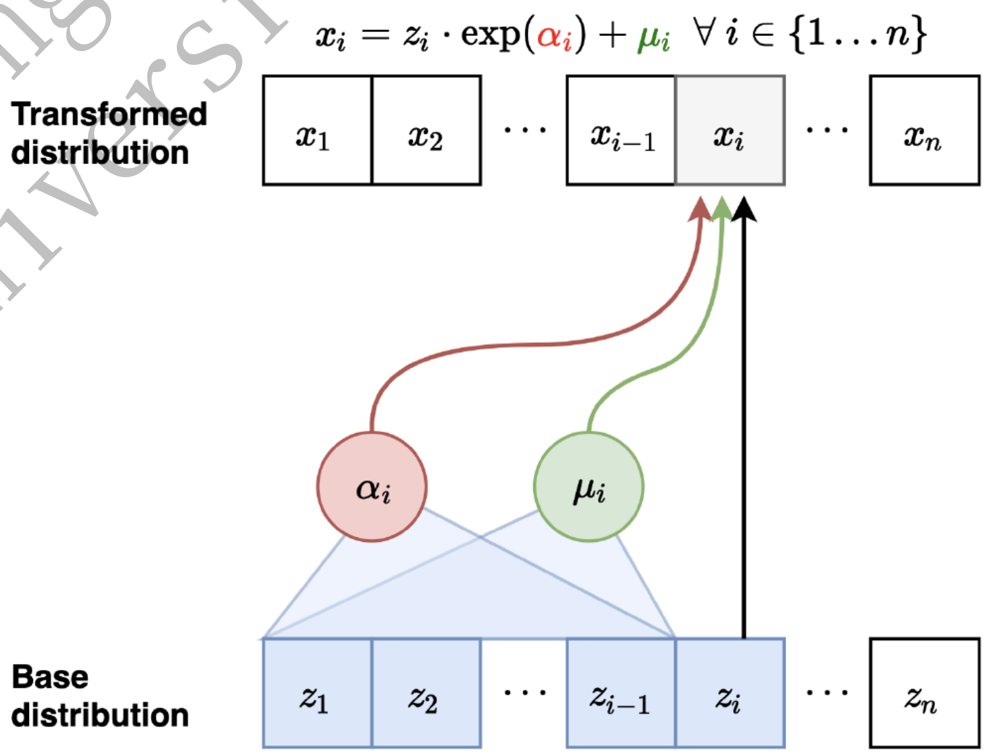
  - Parallel generation
    - First generate z and then x
  - Sequential inference $O(L)$
    - x_i is a function of $z_1 \ldots z_i$
    - $z_i \leftarrow (x_i - \mu_i)/\exp(\alpha_i)$
    - z_i can only be recovered after $z_1 \ldots z_{i-1}$ is computed



Beyond Autoregressive Generation

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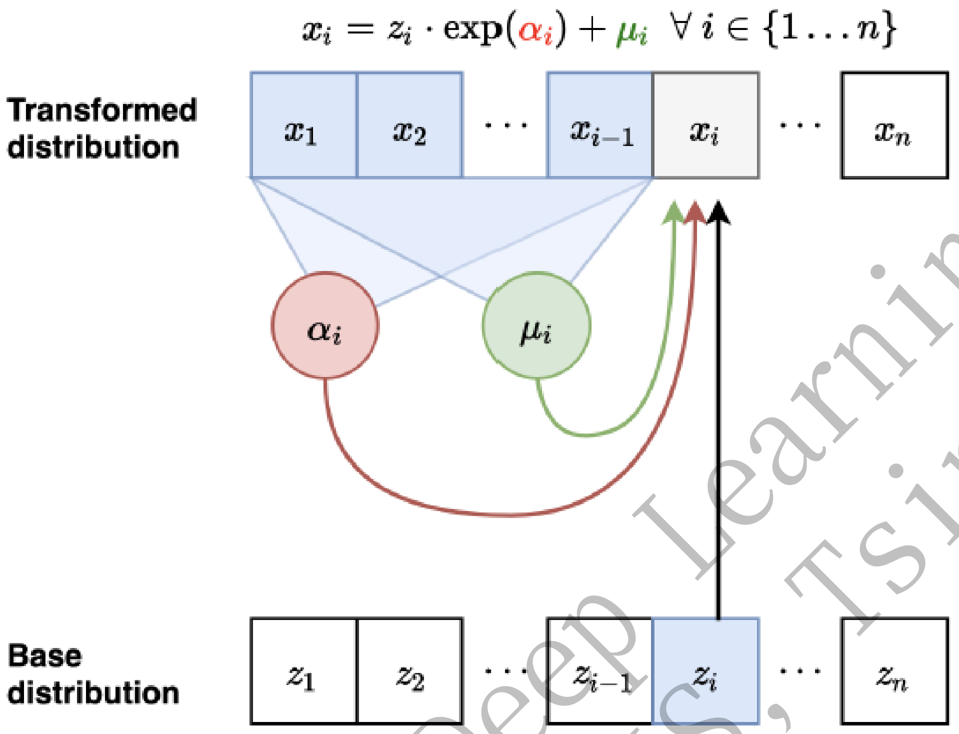
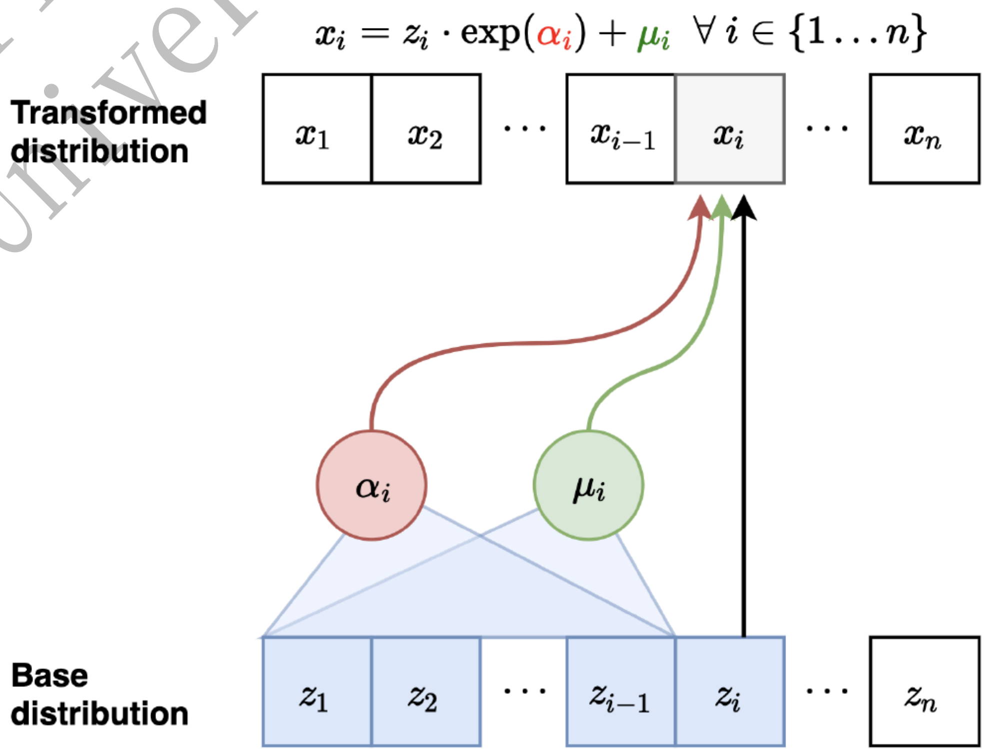


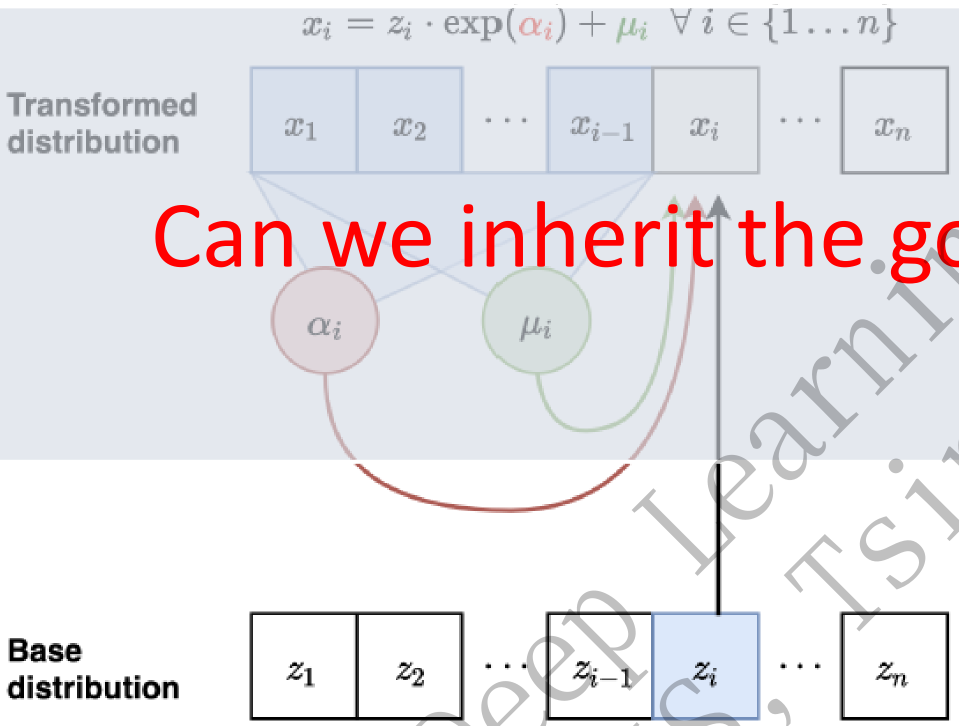
Standard WaveNet
- Autoregressive generation $O(L \log L)$
- Parallel inference $O(\log L)$

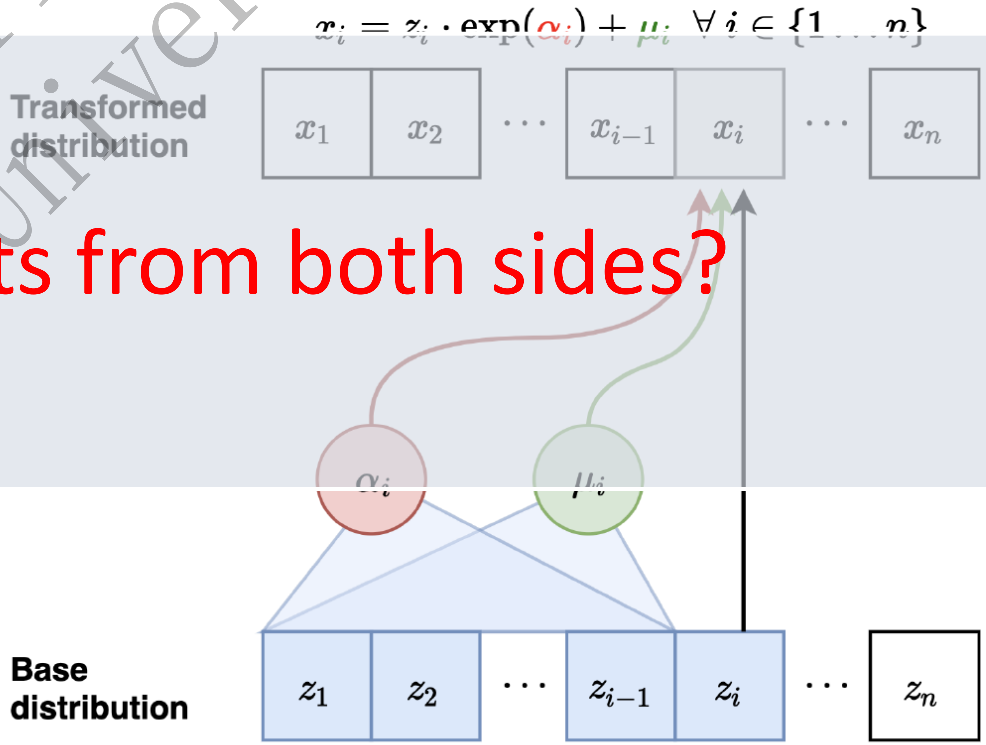


Parallel WaveNet
- Parallel generation $O(\log L)$
- Autoregressive inference $O(L \log L)$

Beyond Autoregressive Generation

- Parallel WaveNet (DeepMind, ICML 2018)





Can we inherit the good parts from both sides?

Standard WaveNet
- Autoregressive generation $O(L \log L)$
- Parallel inference $O(\log L)$

Parallel WaveNet
- Parallel generation $O(\log L)$
- Autoregressive inference $O(L \log L)$

Beyond Autoregressive Generation

- Parallel WaveNet (DeepMind, ICML 2018)
  - Key facts
    - Standard WaveNet is fast for training (inference is fast)
    - Parallel WaveNet is fast for serving (generation is fast)
  - Distillation by teacher-student framework!
    - Teacher: $p_T(x_i|x_{<i})$ a standard WaveNet for training on massive data
    - Student: $p_S(x_i|z_{<i})$ a parallel WaveNet for serving
      - p_S is trained by distillation from p_T
      - i.e., minimize the KL-difference between $p_S(x)$ and $p_T(x)$
  - Algorithm Sketch
    - Step 1: Train teacher $p_T(x_i|x_{<i})$ network and fix it
    - Step 2: Minimize the KL-difference $KL(p_S||p_T)$
    - Finally we use $p_S(x)$ for fast sampling

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    - Finally we use $p_S(x)$ for fast sampling

Pay attention to the order!

Beyond Autoregressive Generation

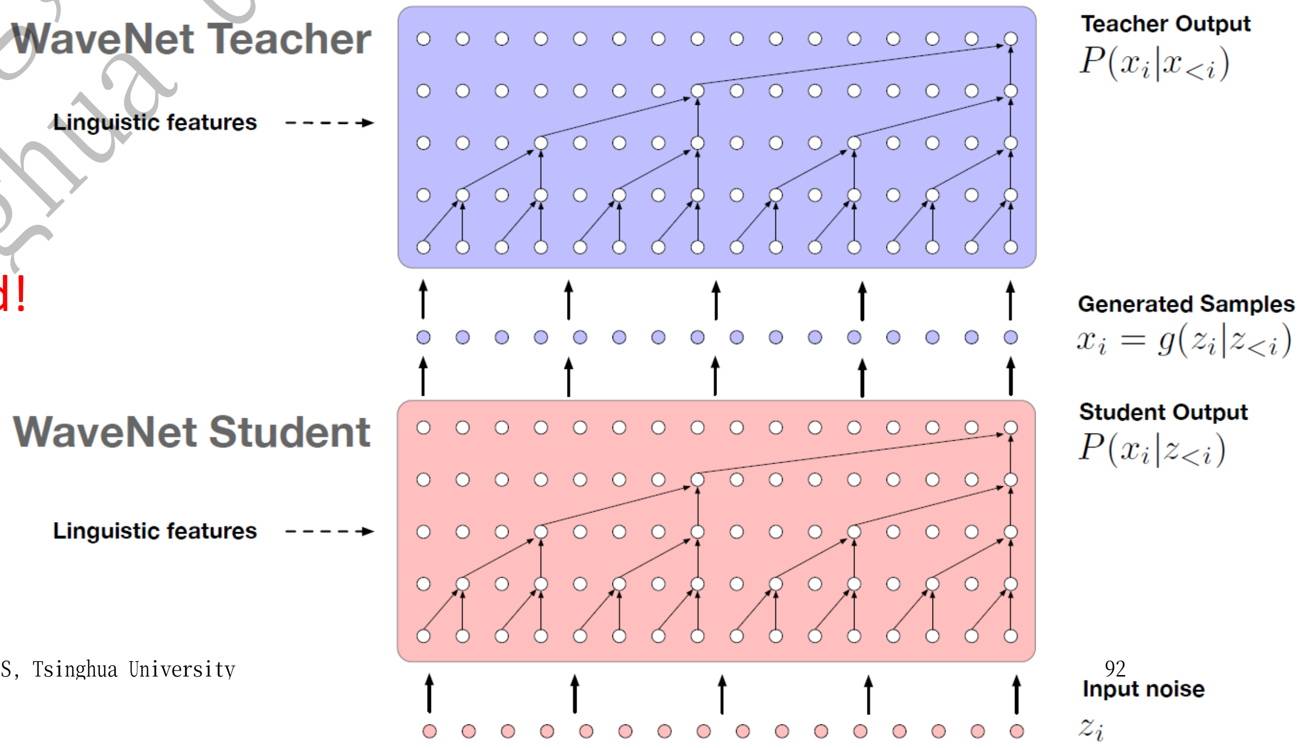
- Parallel WaveNet (DeepMind, ICML 2018)
  - Teacher-Student Learning
    - Pretrain $p_T(x)$ and then train $p_S(x)$ by imitation learning
  - Distance measure for two distributions
    - KL divergence: $KL(p||q) = \mathrm{E}_{x\sim p}\left[\log \frac{p(x)}{q(x)}\right]$
  - Distillation (Imitation learning)

$$L(\theta) = KL(p_S||p_T) = \mathrm{E}_{x\sim p_S}[\log p_S(x;\theta) - \log p_T(x)]$$

    - Monte Carlo estimates for the expectation
      - **Key: sample from the student network!**
    - Sample $z\sim N(0,I)$, generate $x\sim p_S(x|z)$ (parallel)
    - Evaluate $p_S(x|z)$ (parallel since z is known)
    - Evaluate $p_T(x)$ (parallel since $p_T(x)$ is a standard autoregressive model)

Beyond Autoregressive Generation

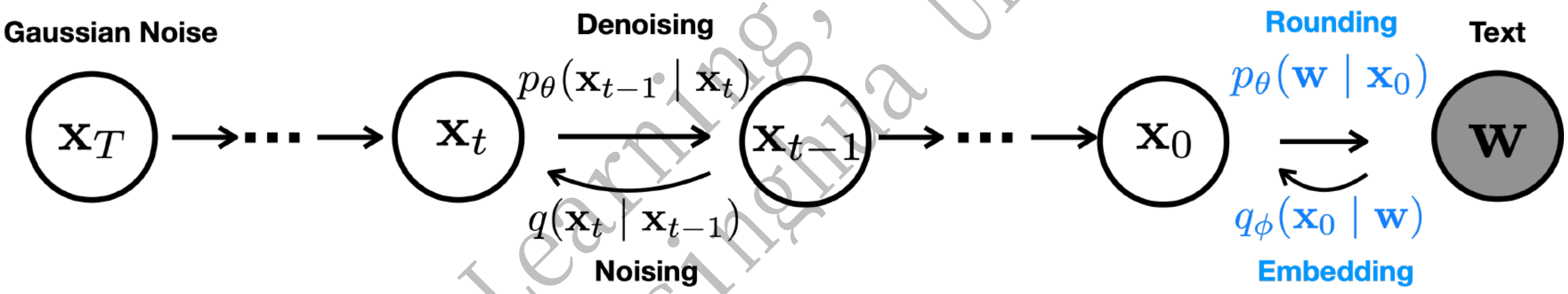
- Parallel WaveNet (DeepMind, ICML 2018)
  - Teacher-Student Learning
    - Pretrain $p_T(x)$ and then train $p_S(x)$ by imitation learning
  - Speedup
    - 20x faster than real-time
    - 1000x faster than WaveNet
    - Google production
  - Remark
    - A reparameterization trick is assumed!



- What about language model?
  - Output are discrete tokens
  - No parameterization available

Beyond Autoregressive Generation

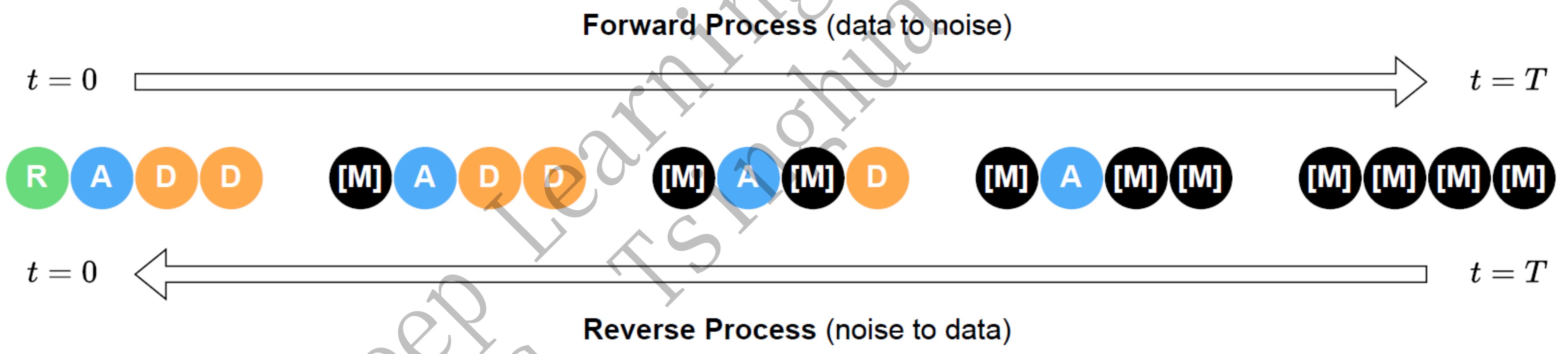
- Diffusion-based language model
  - Key idea: use a diffusion model to generate all tokens at once!
  - Idea#1: treat embeddings of tokens as images



  - Pros: we can directly apply all techniques from diffusion models
  - Cons: **length issue**, extremely high dimensions, poor generation quality

Beyond Autoregressive Generation

- Diffusion-based language model
  - Key idea: use a diffusion model to generate all tokens at once!
  - Idea#1: treat embeddings of tokens as images
  - Idea#2: define the denoising process over token masks

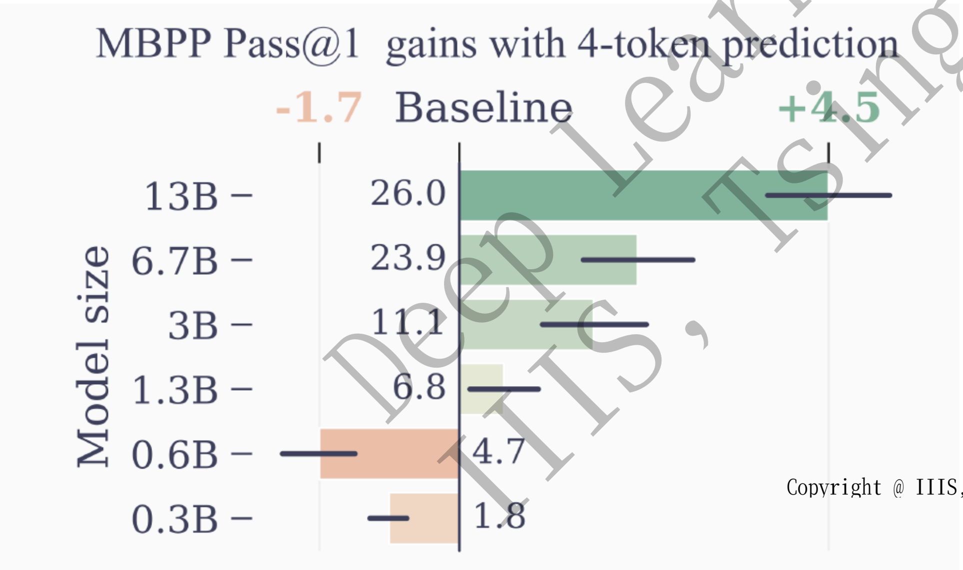


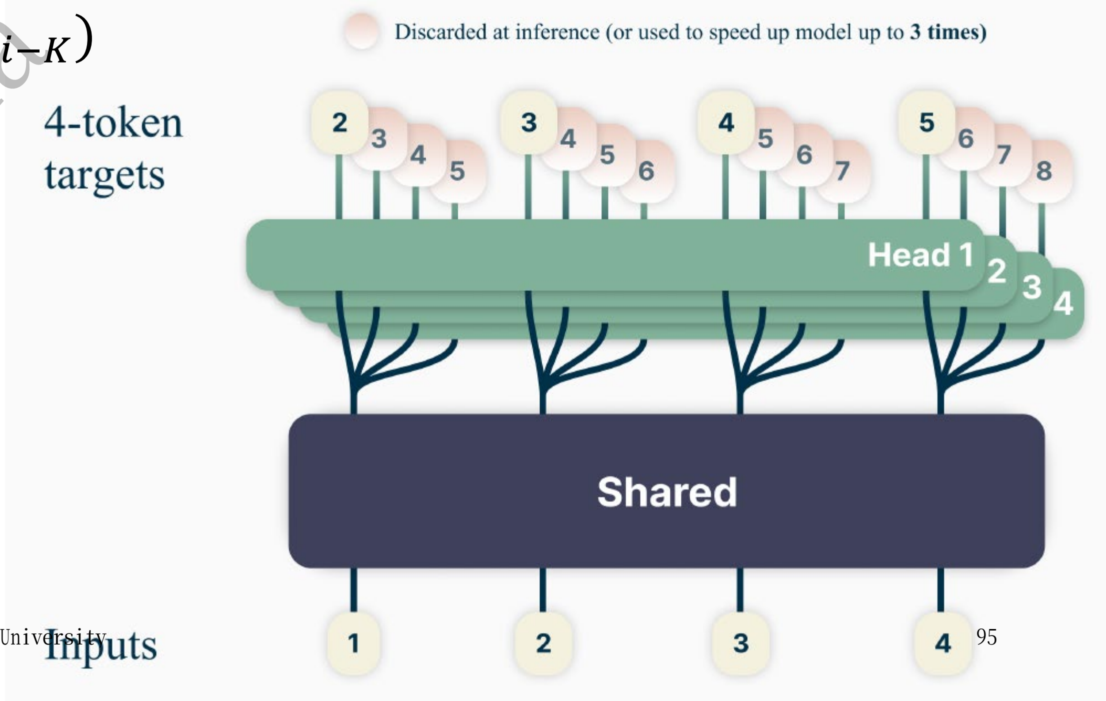
  - Pros: reduce denoising operator to standard token prediction, reasonable quality
  - Cons: **length issue**, no denoising acceleration anymore

- Any simpler method for joint token predictions?

Beyond Autoregressive Generation

- Multi-Token Prediction (ICML 2024)
  - Key insight $p(x_{1..L}) \approx \prod_i p(x_L)$
    - When the sequence length L is really short, we can break the sequential dependency
  - Predict K tokens jointly in parallel
    - $p(x_{i-K+1\ \dots i} | x_{1\dots i-K}) \approx \prod_{j=1}^{K} p(x_{i-j+1} | x_{1\dots i-K})$
    - Small K & larger models higher gains





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    - $p(x_{i-K+1\,\ldots i}|x_{1\ldots i-K}) \approx \prod_{j=1}^{K} p(x_{i-j+1}|x_{1\ldots i-K})$
  - Understanding multi-token prediction
    - Using a faster but worse model (independent model) to approximate the target distribution (full language model)
    - Other choice of fast sampling model?
      - E.g., an LSTM, or a just smaller model

Beyond Autoregressive Generation

- Speculative Decoding (ICML 2023)
  - Key facts
    - A general language model $p(x)$ is fast at evaluation but slow at generation
    - A sampling model $q(x)$ is fast at generation but at low quality
  - Goal: adaptively use $q(x)$ to generate at easy cases
    - How to define easy cases?

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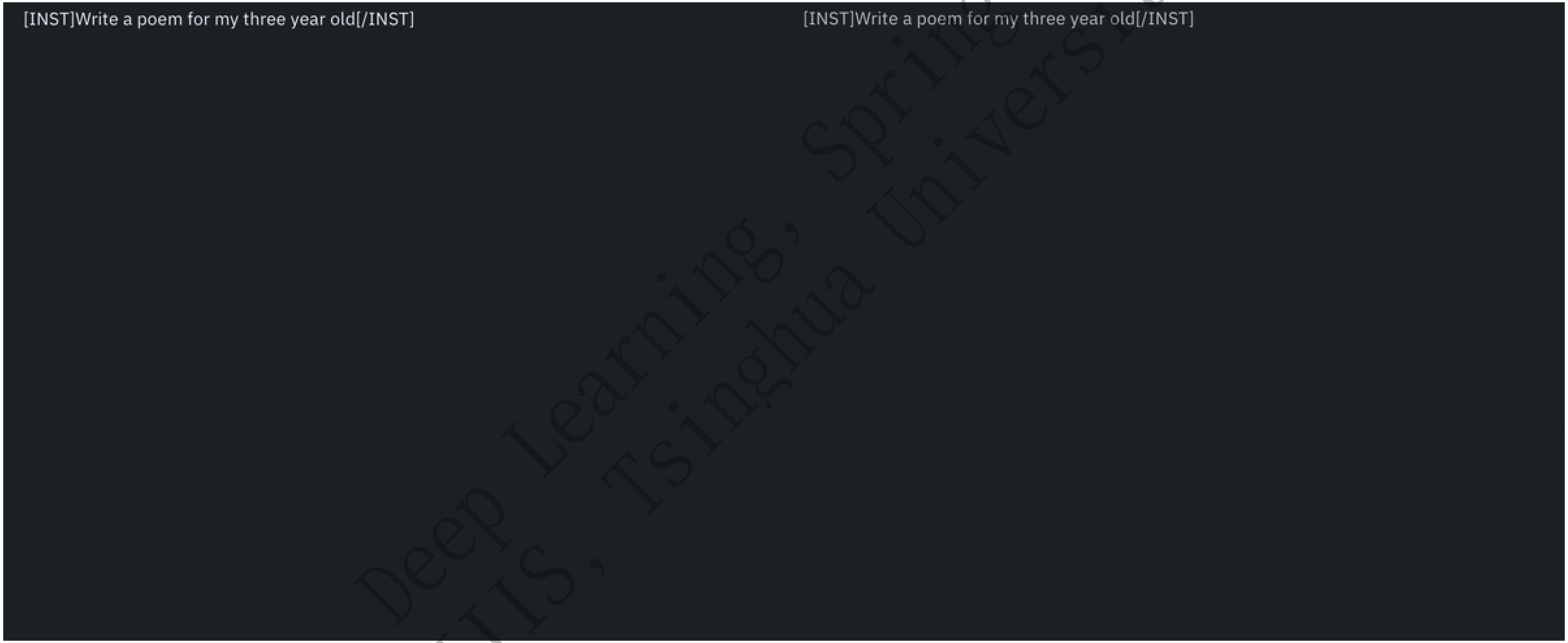
  - Goal: adaptively use $q(x)$ to generate at easy cases
  - MCMC Sampling!
    - We treat $q(x)$ as a proposal distribution
    - Given a partial prefix $x_{1\ldots i}$, run q to generate next K tokens x'
    - Evaluate $p(x'|x)$ and $q(x'|x)$, accept x' with prob. $\min\left(1, \frac{p(x'|x)}{q(x'|x)}\right)$ (parallel)
    - If rejection, re-sample $x' \propto \max\big(0, p(x'|x) - q(x'|x)\big)$ (autoregressive)
    - In practice, we can run speculative sampling for multiple K

Prove the correctness in your homework ☺

Beyond Autoregressive Generation



AR Generation of Llama 13B

Speculative decoding

Faster Transformer Generation

- Reparameterization and distillation
  - Pros: fast training and inference
  - Cons: only works for continuous values
- Diffusion-based language model
  - High complexity for generation and still low generation quality
- Multi-token prediction
  - Trade generation quality for speed
- Speculative decoding
  - Most general approach to speed up generation
  - Can be applied to any trained language model without modification

Summary

- Language Model & Sequence to Sequence Model
    - Fundamental ideas and methods for sequence modeling/tasks
- Attention Mechanism
    - So far the most successful idea for sequence data in deep learning
    - A scale/order-invariant representation
    - Transformer: a fully attention-based model for sequence data
- Speedup Transformers
    - Generation is the key bottleneck for transformer models
    - Acceleration by faster attention
    - Acceleration by non-autoregressive generation
        - Model changes: distillation, diffusion, multi-token prediction
        - Sampling methods: speculative decoding

Thanks