Autoregressive models and attention

Instructor: Seunghoon Hong

Course logistics

- Claim session for midterm
  - Time: 1-3pm, Friday (Nov. 3rd)
  - Location: E3-1, 3428

Recap: objective of deep generative models

- Learning a model that its outputs follow the true data distribution

$$G_\theta \sim P(X)$$

Generated images from G

True Images X

Recap: objective of deep generative models

- Maximum Likelihood Estimation (MLE)

$$\hat{\theta} = \arg\max_{\theta \in \Theta} \sum_{x_i \in \mathcal{X}} \boxed{\log p_\theta(x_i)}$$ Log Likelihood

$$\leftrightarrow \arg\max_{\theta \in \Theta} \prod_{x_i \in \mathcal{X}} \boxed{p_\theta(x_i)}$$ Likelihood

Find model parameters that maximize the probability of sampling training data (likelihood)

$$\leftrightarrow \arg\min_{\theta \in \Theta} \sum_{x_i \in \mathcal{X}} -\log p_\theta(x_i)$$

In practice, we minimize the negative log likelihood for gradient descent

Recap: Challenges in evaluating likelihood

$$\hat{\theta} = \arg\min_{\theta \in \Theta} \sum_{x_i \in \mathcal{X}} -\log \boxed{p_\theta(x_i)}$$

- For high-dimensional data, it is difficult to optimize the joint distribution at once

$$x_i = [x_i^1, x_i^2, x_i^3, \ldots, x_1^d] \in \mathbb{R}^d$$
$$p(x_i) = p(x_i^1, x_i^2, x_i^3, \ldots, x_1^d)$$

- Examples of high-dimensional data
  - Image (d = number of pixels)
  - Sentence (d = length of sentence)

Recap: Auto-Regressive Model (AR)

- Factorizing the likelihood via **chain rule**

$$p(a, b) = p(a|b)p(b)$$

Recap: Auto-Regressive Model (AR)

- Factorizing the likelihood via chain rule

$$
\begin{aligned}
p_\theta(x) &= p_\theta(x_1, x_2, x_3, ..., x_T) \\
&= p_\theta(x_T | x_1, x_2, ..., x_{T-1}) \boxed{p_\theta(x_1, x_2, ..., x_{T-1})} \\
&= \prod_{t=1}^{T} p_\theta(x_t | x_1, ..., x_{t-1})
\end{aligned}
$$

apply recursively

Auto-Regressive Model (AR)

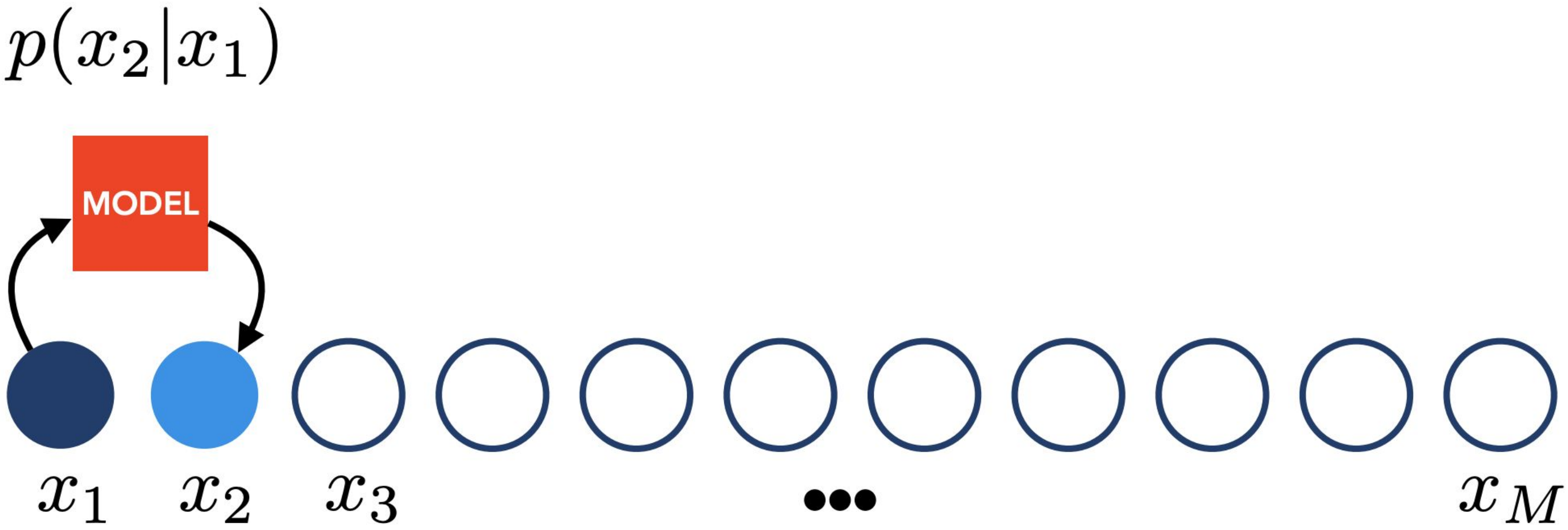
$$p_\theta(x) = \prod_{t=1}^{T} p_\theta(x_t | x_1, ..., x_{t-1})$$

$$p(x_1)$$

Slide credit: http://www.yisongyue.com/courses/cs155/2018_winter/lectures/Lecture_17.pdf

Auto-Regressive Model (AR)

$$p_\theta(x) = \prod_{t=1}^{T} p_\theta(x_t | x_1, ..., x_{t-1})$$



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Auto-Regressive Model (AR)

$$p_\theta(x) = \prod_{t=1}^{T} p_\theta(x_t | x_1, ..., x_{t-1})$$

$$p(x_3 | x_2, x_1)$$

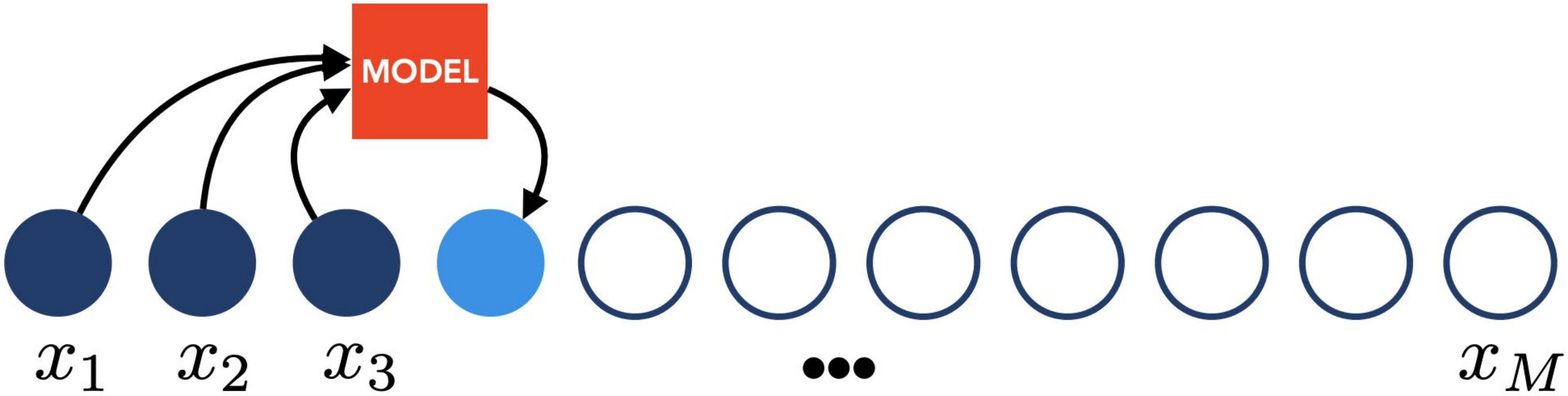
x_1 x_2 x_3 ••• x_M

Slide credit: http://www.yisongyue.com/courses/cs155/2018_winter/lectures/Lecture_17.pdf

Auto-Regressive Model (AR)

$$p_\theta(x) = \prod_{t=1}^{T} p_\theta(x_t | x_1, ..., x_{t-1})$$

$$p(x_4 | x_3, x_2, x_1)$$



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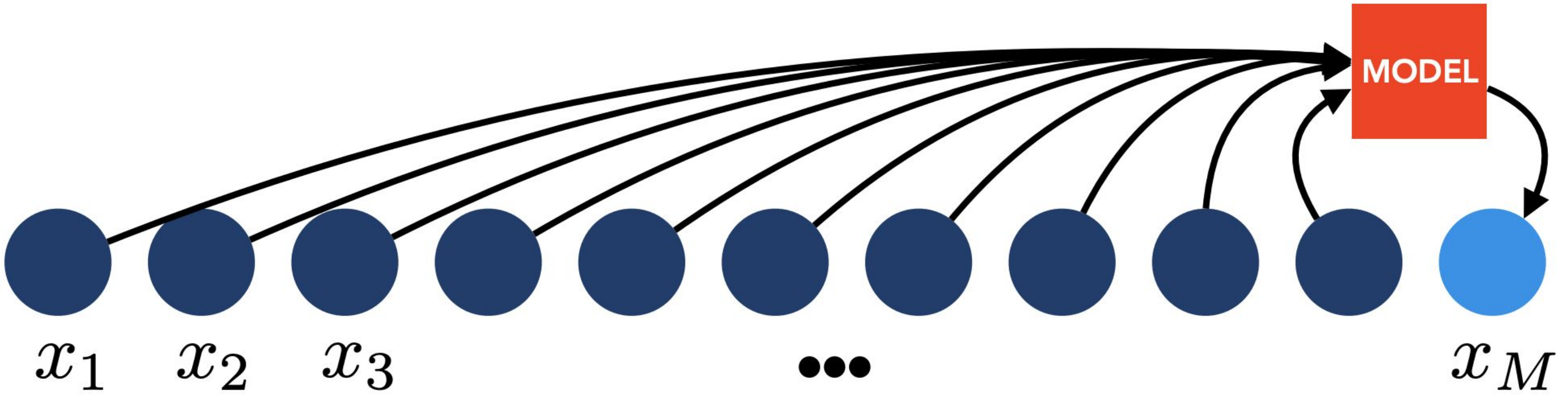
Auto-Regressive Model (AR)

$$p_\theta(x) = \prod_{t=1}^{T} p_\theta(x_t | x_1, ..., x_{t-1})$$

$$p(x_M | x_{M-1}, \ldots, x_1)$$



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Recap: autoregressive model

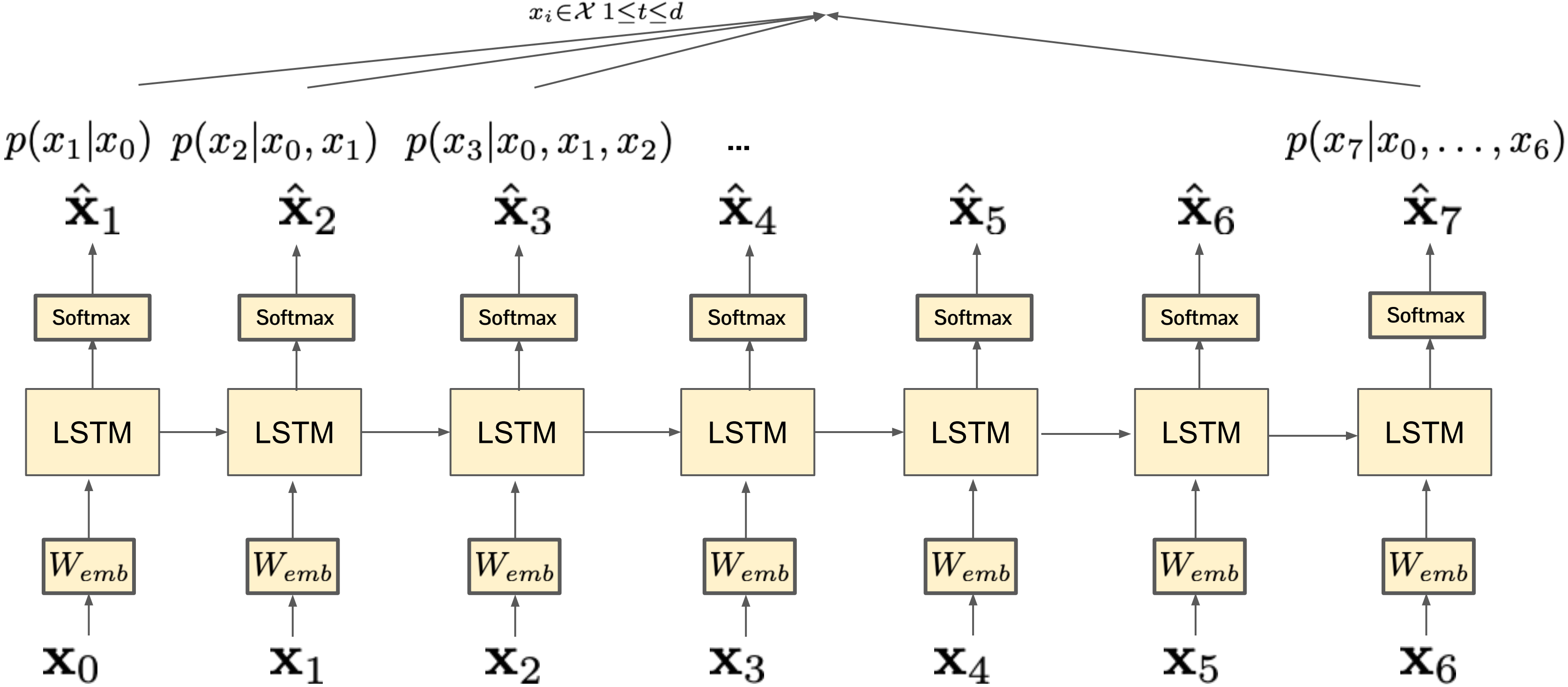
- Factorized objective function

$$\hat{\theta} = \arg\min_{\theta \in \Theta} \sum_{x_i \in \mathcal{X}} -\log p_\theta(x_i)$$

$$= \arg\min_{\theta \in \Theta} \sum_{x_i \in \mathcal{X}} \sum_{1 \leq t \leq d} -\log p_\theta(x_i^t | x_i^1, \ldots, x_i^{t-1})$$

Recap: RNN as autoregressive model

$$\sum_{x_i \in \mathcal{X}} \sum_{1 \le t \le d} - \log p_\theta(\hat{x}_i^t = x_i^t | x_i^1, \ldots, x_i^{t-1})$$

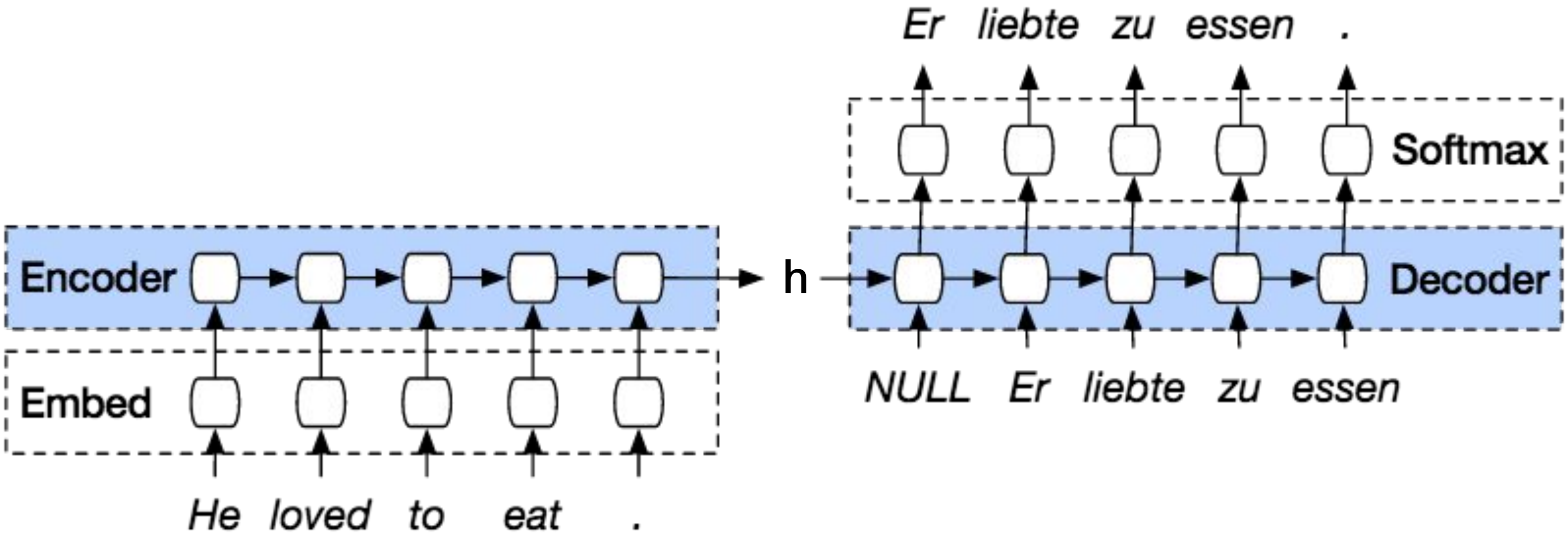


Today's agenda

- AR for machine translation
- AR with attention

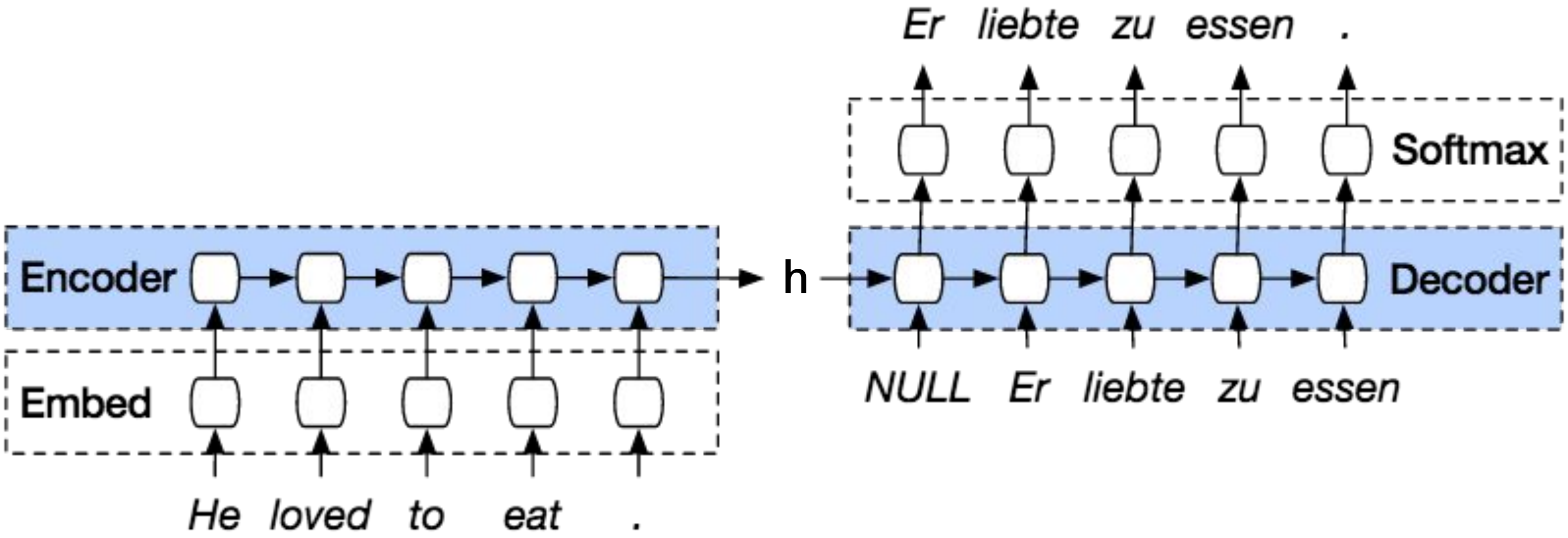
Task: machine translation

- Translating a sentence in one language to another
  - Example: English to French
- Generally, this problem is also referred to **sequence-to-sequence** generation



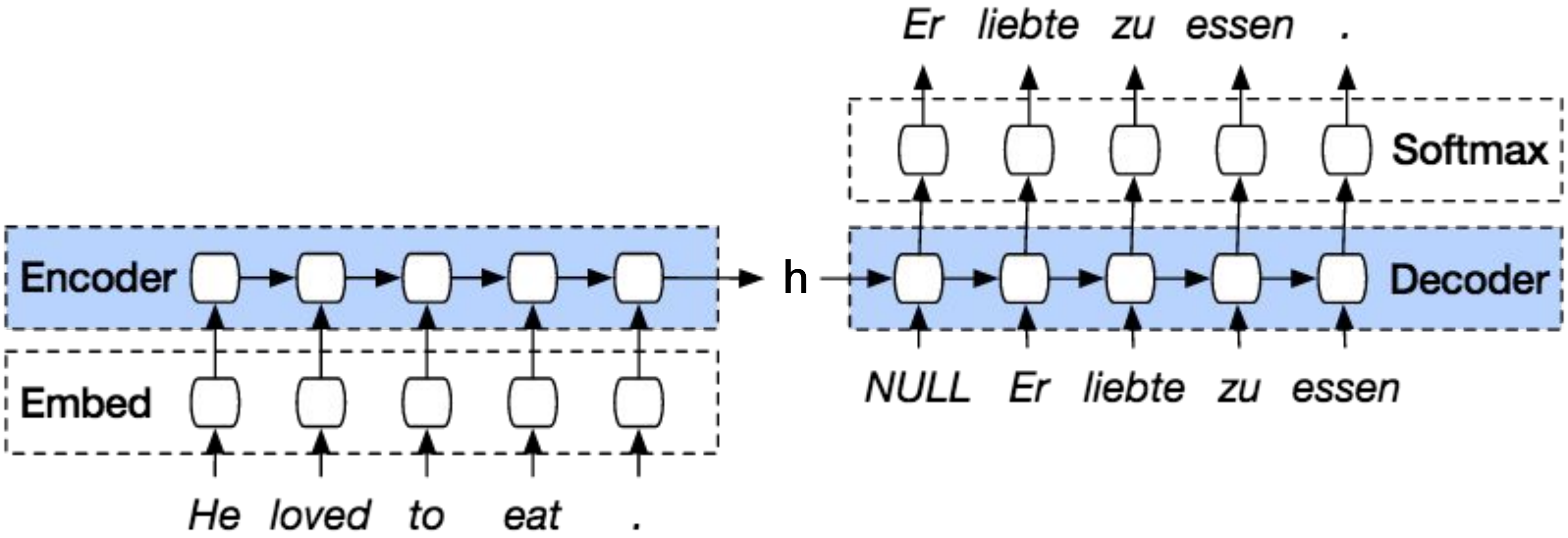
Sequence-to-sequence model

- Sequence-to-sequence model is a **conditional** autoregressive model
  - Conditioning variable: $\mathbf{x} = \{x_1, x_2, \ldots, x_M\}$
  - Decoding variable: $\mathbf{y} = \{y_1, y_2, \ldots, y_N\}$
  - Learning objective: $\theta^* = \arg\min_\theta - \sum_i \log p(\mathbf{y}_i | \mathbf{x}_{\cancel{i}})$



Sequence-to-sequence model

- A recurrent neural network with encoder-decoder architecture
  - **Encoder:** encode information of source sentence
  - **Decoder:** decode the encoded source sentence into another sequence (e.g. machine translation)



AR as Sequence-to-Sequence model

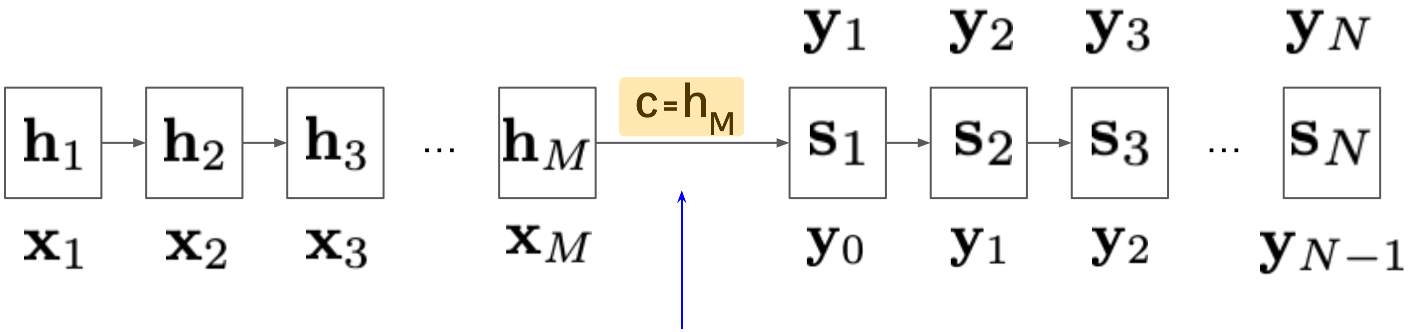
- Plain sequence-to-sequence model

Encoder

$$h_t = f\left(x_t, h_{t-1}\right)$$

Decoder

$$p(y_t \mid \{y_1, \cdots, y_{t-1}\}, c) = g(y_{t-1}, s_t, c)$$

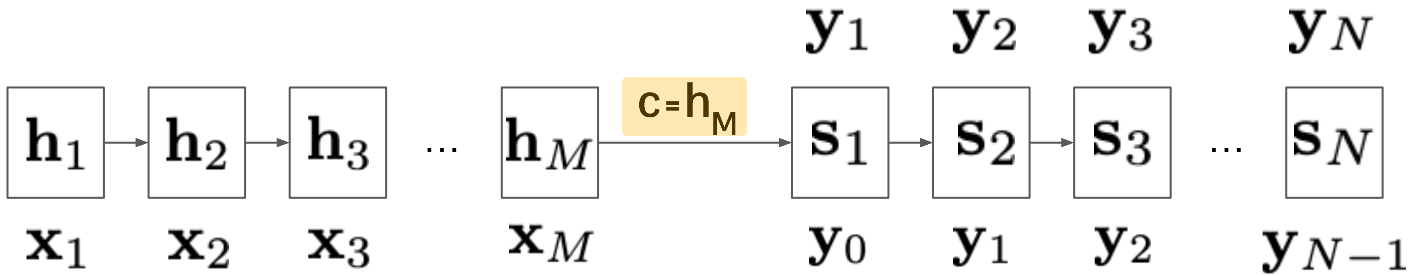


The entire source sentence is
encoded by a fixed length vector

즉, bottleneck이 되어 info. loss가 있을수도

Challenges in Sequence-to-sequence model

- Modeling long-term dependency
  - Encoder network should squash all source sentence information into a single vector **c**
  - This may lead to lossy compression, and not be appropriate to model long-term dependency



Encoder

$$h_t = f\left(x_t, h_{t-1}\right)$$

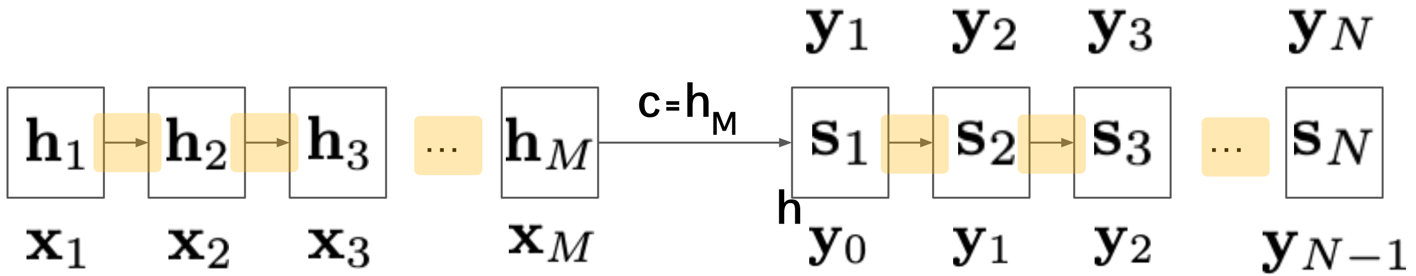
Decoder

$$p(y_t \mid \{y_1, \cdots, y_{t-1}\}, c) = g(y_{t-1}, s_t, c)$$

Challenges in Sequence-to-sequence model

- Limited to serial processing (cannot be parallelized)
  - Can be a bottleneck for efficient training

cannot parallalize



Encoder

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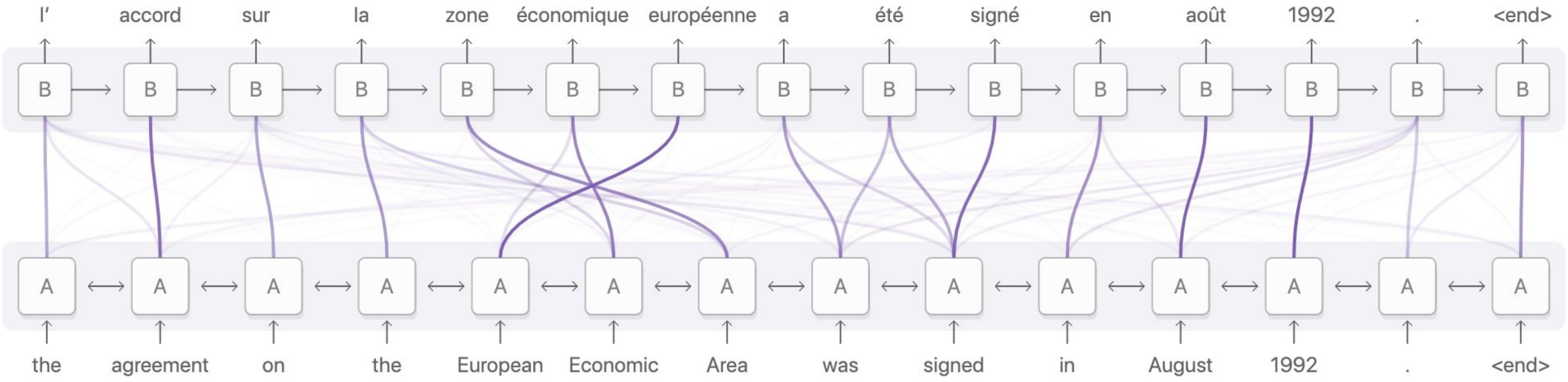
Today’s agenda

- AR for machine translation
- **AR with attention**

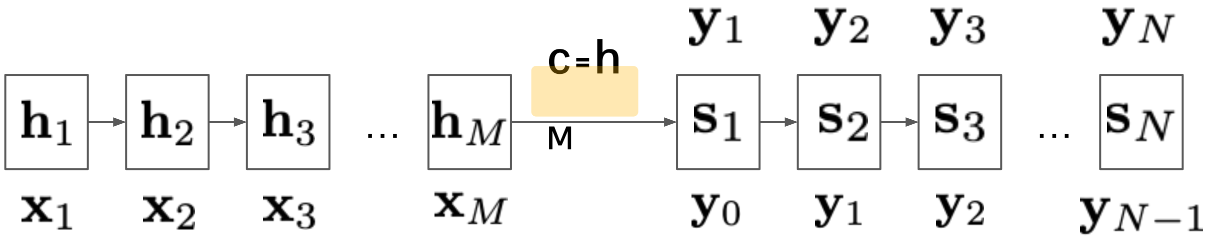
Sequence-to-sequence with attention

- Let the decoder to directly access the words in the input sentence



Sequence-to-sequence with attention

- Let the decoder to directly access the words in the input sentence



Encoder

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Decoder

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Sequence-to-sequence with attention

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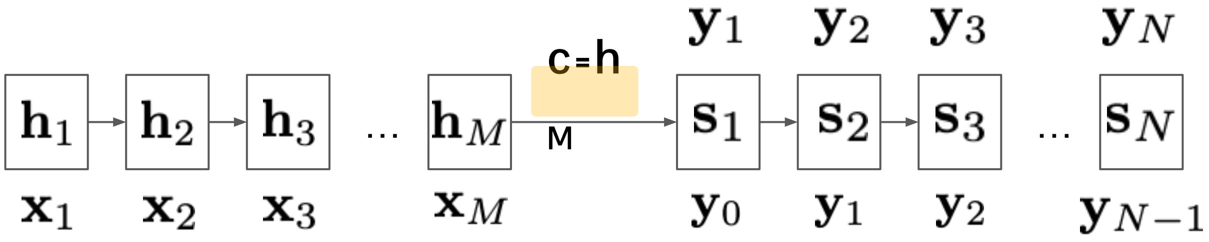
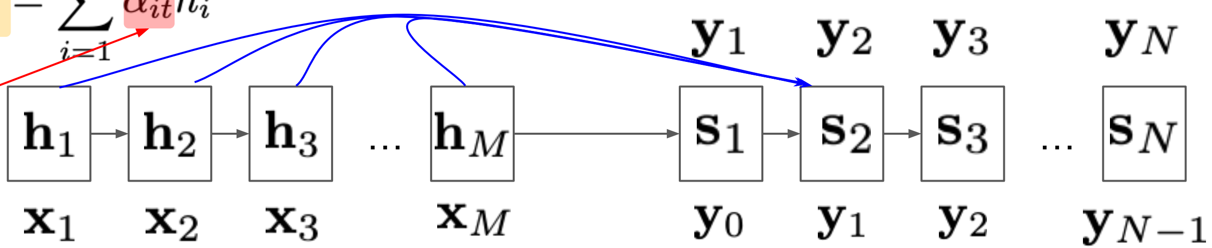


t: decoding step

$$c_t = \sum_{i=1}^{M} \alpha_{it} h_i$$

Weighted average
= attention



Encoder

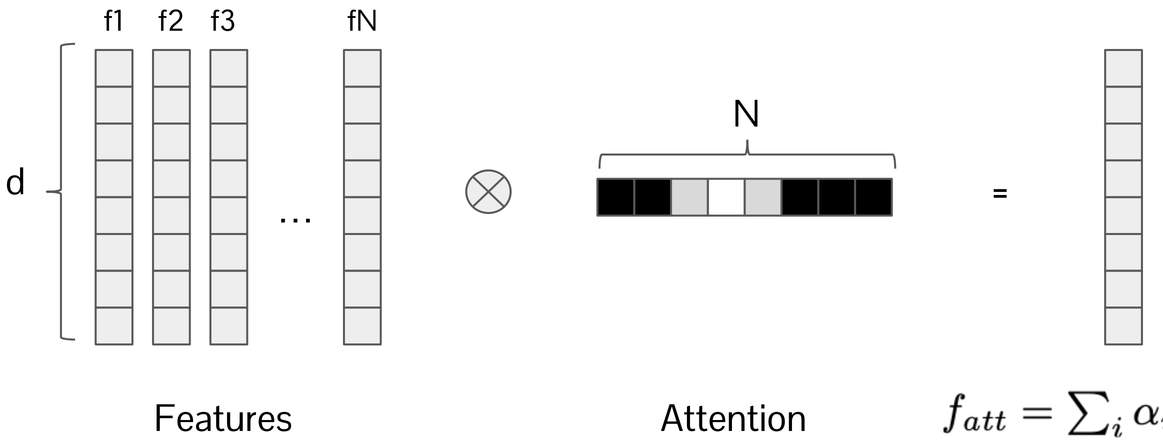
$$h_t = f\left(x_t, h_{t-1}\right)$$

Decoder

$$p(y_t | \{y_1, \dots, y_{t-1}\}, \{x_1, \dots, x_M\}) = g(y_{t-1}, s_t, c_t)$$

Recap: attention

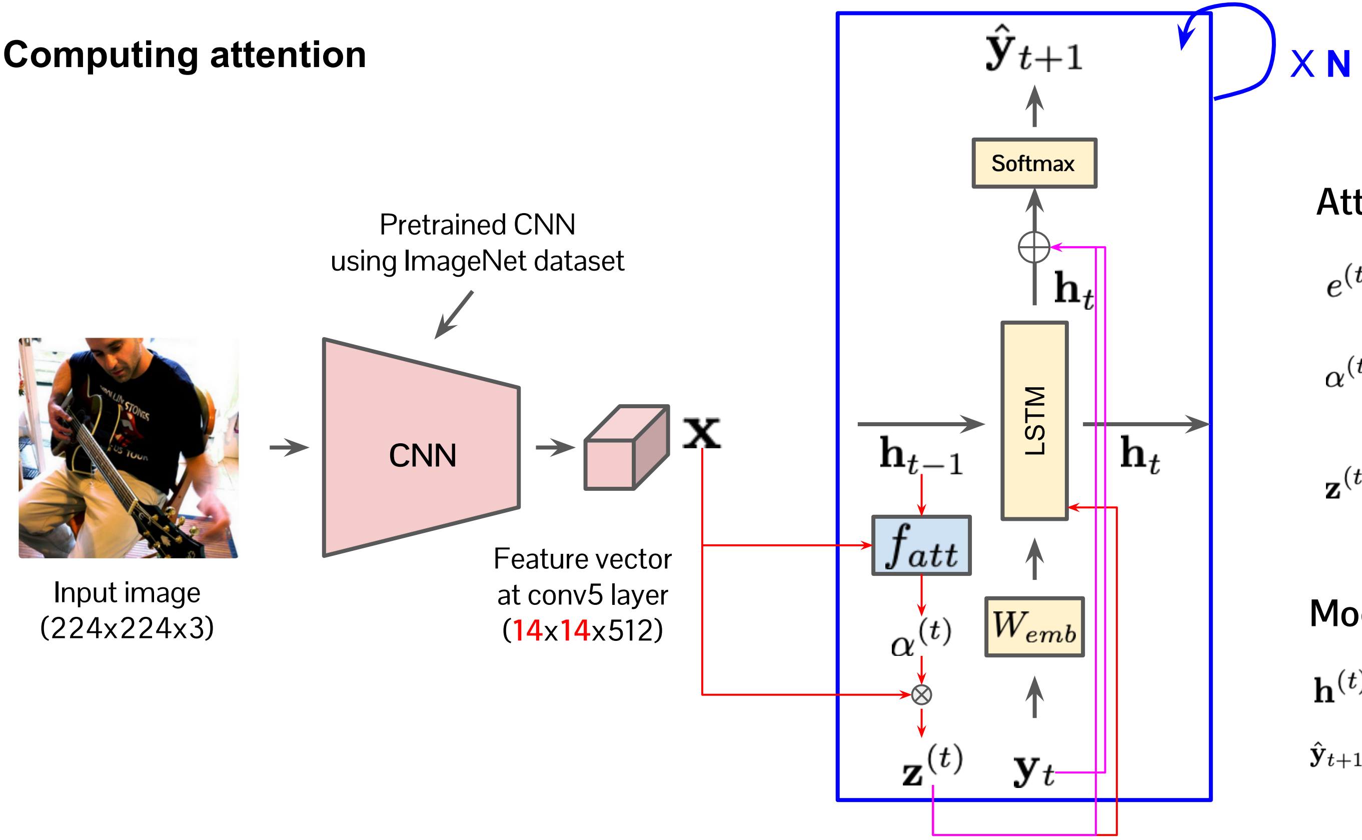
- Attention
  - A non-negative vector that summed to one $\alpha \in \mathbb{R}^N, \quad \sum_i \alpha_i = 1$
  - The size of attention vector is same as the feature that we want to apply the attention to
  - Larger value in attention means that the corresponding feature is more important than the others



$$f_{att} = \sum_i \alpha_i \mathbf{f}_i \in \mathbb{R}^d$$

Recap: attention in image captioning

Computing attention



Attention module

$$e^{(t)} = f_{att}(\mathbf{x}, \mathbf{h}_{t-1})$$

$$\alpha^{(t)} = \frac{\exp(e^{(t)})}{\sum_{i,j} \exp(e^{(t)}_{i,j})}$$

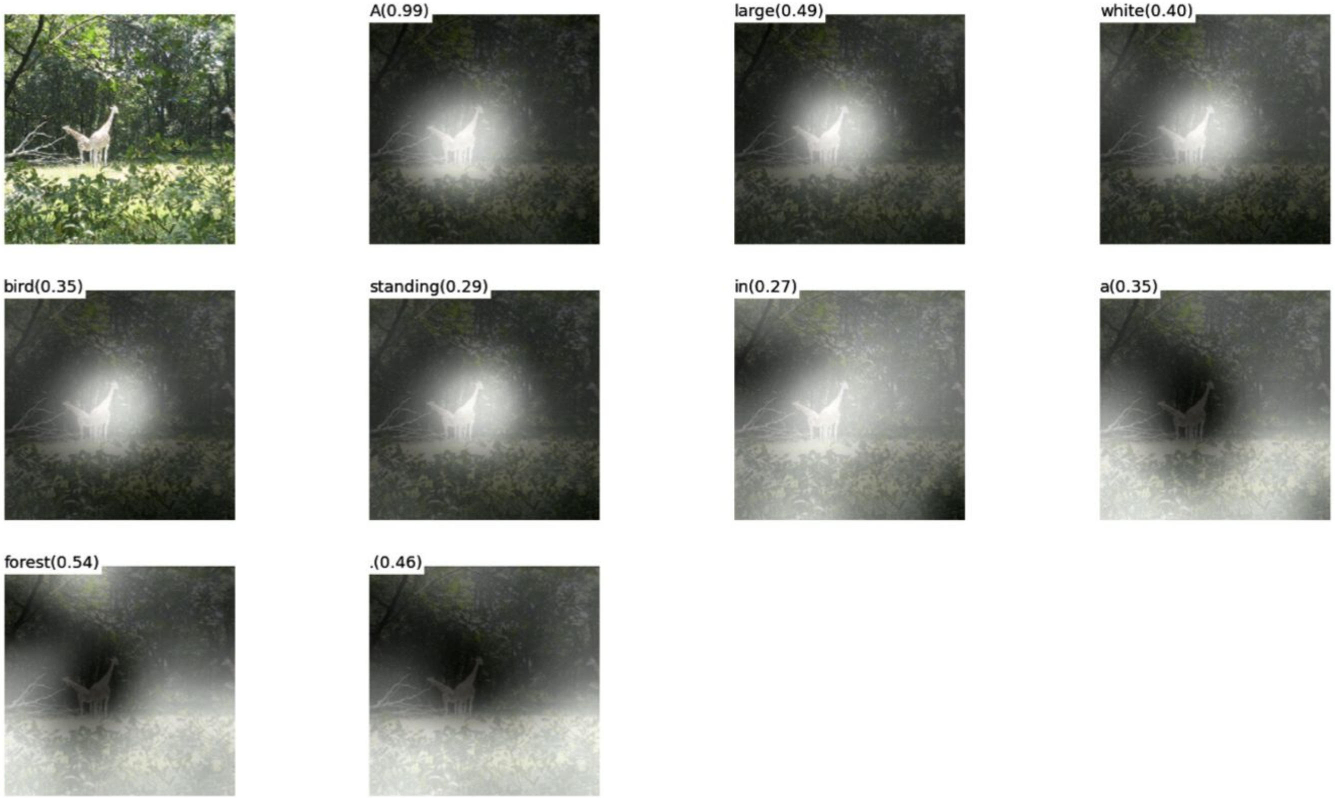
$$\mathbf{z}^{(t)} = \sum_{i,j} \alpha^{(t)}_{i,j} \mathbf{x}_{i,j}$$

Modified LSTM

$$\mathbf{h}^{(t)} = LSTM(\mathbf{h}_{t-1}, W_{emb}\mathbf{y}_t, \mathbf{z}^{(t)})$$

$$\hat{\mathbf{y}}_{t+1} = \exp(W^o(W_{emb}\mathbf{y}_t + W^h\mathbf{h}_t + W^z\mathbf{z}_t))$$

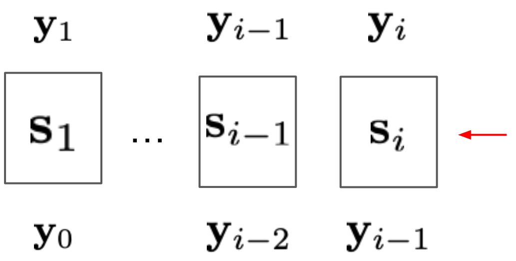
Recap: attention in image captioning



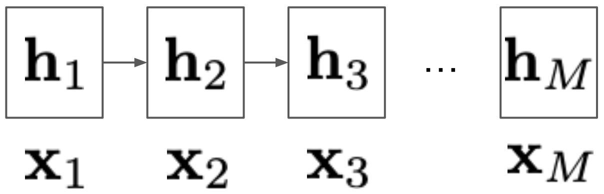
AR with attention

Decoder

$$p(y_i|y_1,\ldots,y_{i-1},\mathbf{x}) = g(y_{i-1},s_i,c_i)$$



We will compute the attention at ith step



Encoder

$$h_t = f\left(x_t, h_{t-1}\right)$$

AR with attention

Decoder

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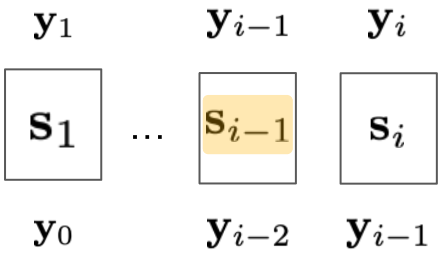
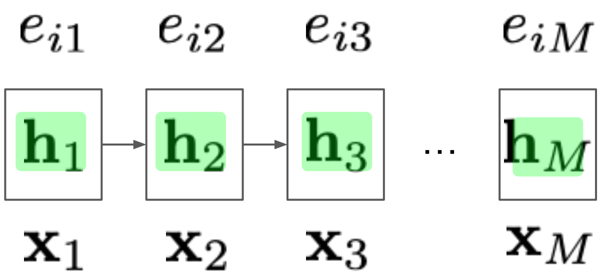


Attention

$$e_{ij} = a(s_{i-1}, h_j)$$



Encoder

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AR with attention

Decoder

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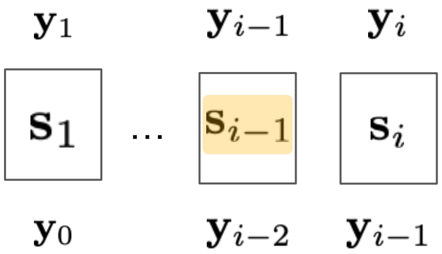
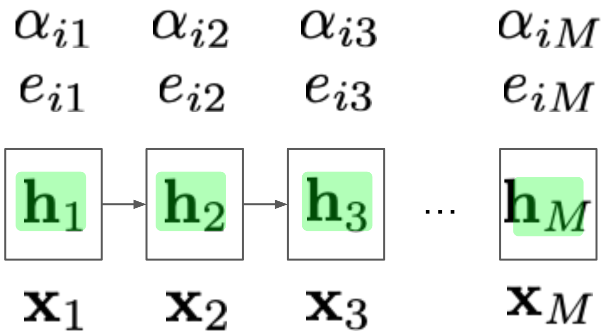


Attention

$$e_{ij} = a(s_{i-1}, h_j)$$

$$\alpha_{ij} = \frac{\exp(e_{ij})}{\sum_{k=1}^{M}\exp(e_{ik})}$$



Encoder

$$h_t = f(x_t, h_{t-1})$$

AR with attention

Decoder

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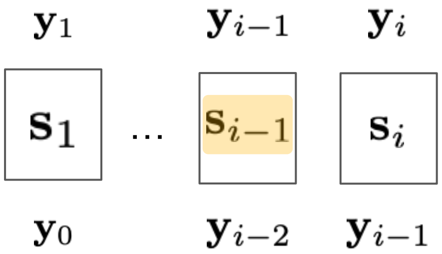
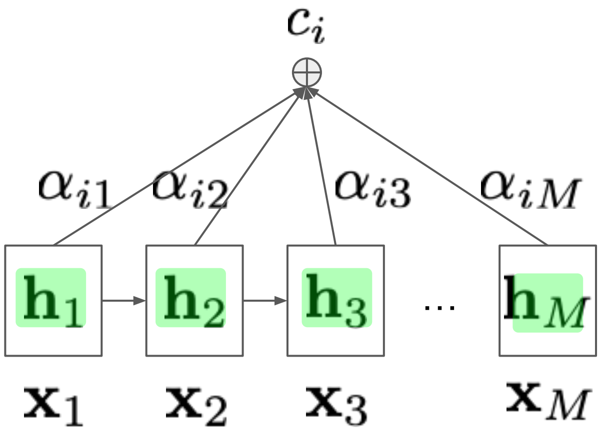


Attention

$$e_{ij} = a(s_{i-1}, h_j)$$

$$\alpha_{ij} = \frac{\exp(e_{ij})}{\sum_{k=1}^{M} \exp(e_{ik})}$$

$$c_i = \sum_{j=1}^{M} \alpha_{ij} h_j$$



Encoder

$$h_t = f(x_t, h_{t-1})$$

AR with attention

Decoder

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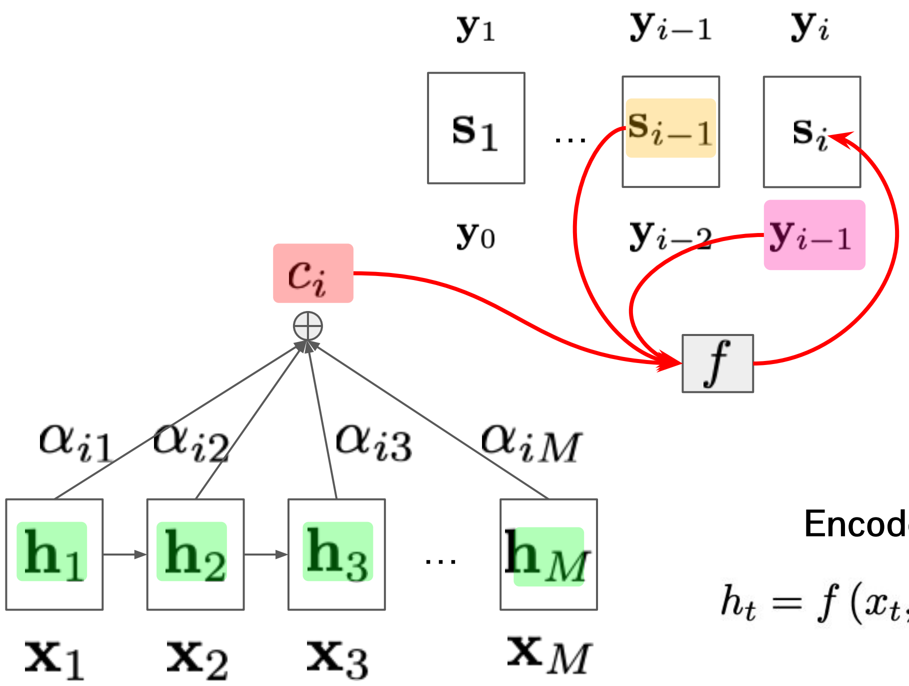


Encoder

$$h_t = f\left(x_t, h_{t-1}\right)$$

Attention

$$e_{ij} = a(s_{i-1}, h_j)$$

$$\alpha_{ij} = \frac{\exp(e_{ij})}{\sum_{k=1}^{M} \exp(e_{ik})}$$

$$c_i = \sum_{j=1}^{M} \alpha_{ij} h_j$$

$$s_i = f(s_{i-1}, y_{i-1}, c_i)$$

AR with attention

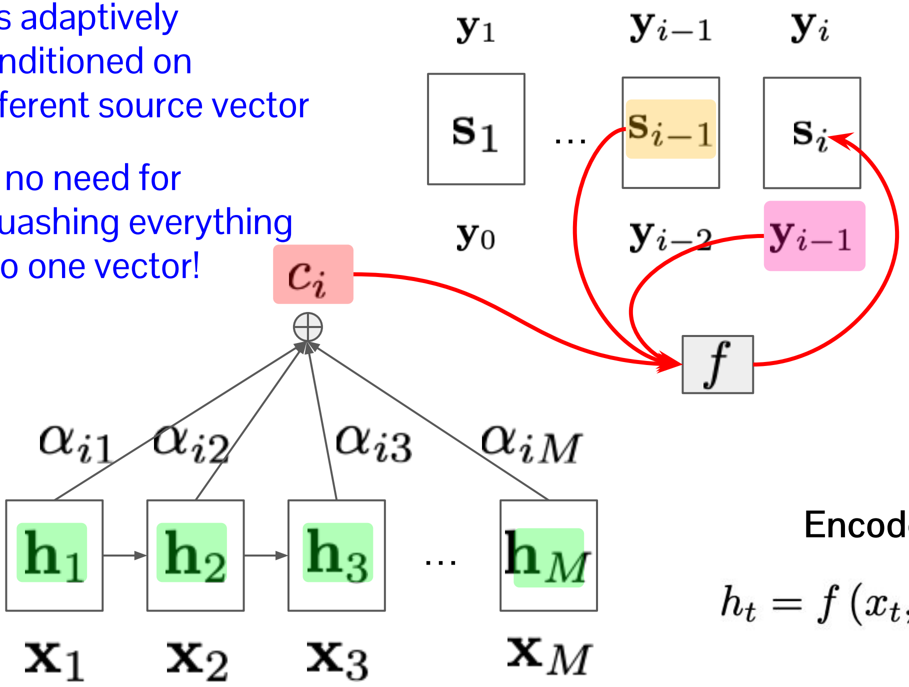
decoding step인 i가 뭐든
input과의 distance가 똑같다
-> long term dependency easy

Each step in decoder, it is adaptively conditioned on different source vector

→ no need for squashing everything into one vector!

Decoder

$$p(y_i | y_1, \ldots, y_{i-1}, \mathbf{x}) = g(y_{i-1}, s_i, c_i)$$



Encoder

$$h_t = f(x_t, h_{t-1})$$

Attention

$$e_{ij} = a(s_{i-1}, h_j)$$

Arbitrary long sentence에 a 적용 가능

$$\alpha_{ij} = \frac{\exp(e_{ij})}{\sum_{k=1}^{M} \exp(e_{ik})}$$

$$c_i = \sum_{j=1}^{M} \alpha_{ij} h_j$$

$$s_i = f(s_{i-1}, y_{i-1}, c_i)$$

Results

- Visualization of attention
  - English → French
  - The attention aligns the target and source words
  - Some target words are conditioned more than one source words
  - The attention is (roughly) sequentially aligned

NOTE: 언어 문법 구조에 따라 저렇게 대각선으로 안나올수도

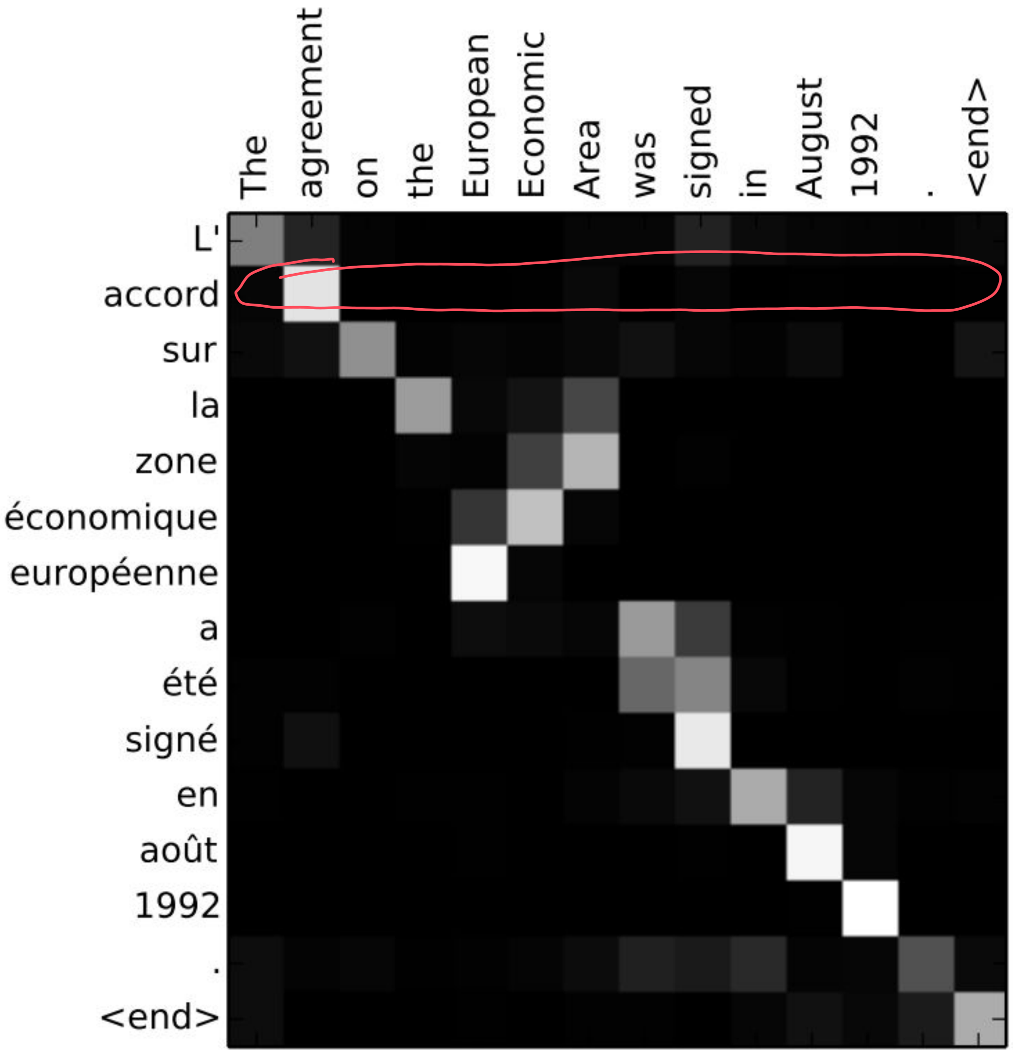
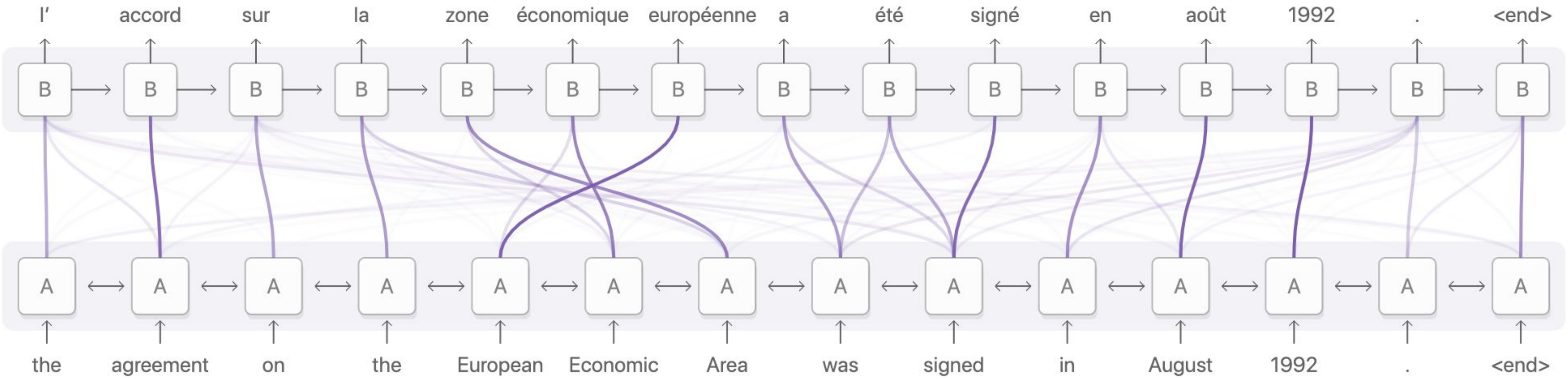


Image source: Bahdanau et al., NEURAL MACHINE TRANSLATION BY JOINTLY LEARNING TO ALIGN AND TRANSLATE, In ICLR, 2015

Results

- Attention allows us to align the source and target sentence



Discussions: AR with attention

- Attention is turned out to be very useful in modeling long-term dependency
- Interesting observations
  - In naive AR, we used recursive connection for modeling temporal dependencies
  - Attention itself can carry the information of source during decoding (without recurrent encoder)
  - Attention is also adaptive; we can dynamically update the attention during decoding
  - Can we replace recursive connection by attention?

What is the benefit of it? → **it removes necessary for serial processing!**

Fully attention-based autoregressive model

- Transformer

Vaswani et al., Attention Is All You Need, In NIPS, 2017

Self-attention

X: input seq.

$$\text{Attn}(\mathbf{x}W_q, \mathbf{x}W_k, \mathbf{x}W_v) = \text{softmax}\left(\frac{\mathbf{x}W_q(\mathbf{x}W_k)^T}{\sqrt{d}}\right)\mathbf{x}W_v$$

Self-attention

$$\mathrm{Attn}(\mathbf{x}W_q, \mathbf{x}W_k, \mathbf{x}W_v) = \mathrm{softmax}\left(\frac{\mathbf{x}W_q(\mathbf{x}W_k)^T}{\sqrt{d}}\right)\mathbf{x}W_v$$

We have three linear projection matrices

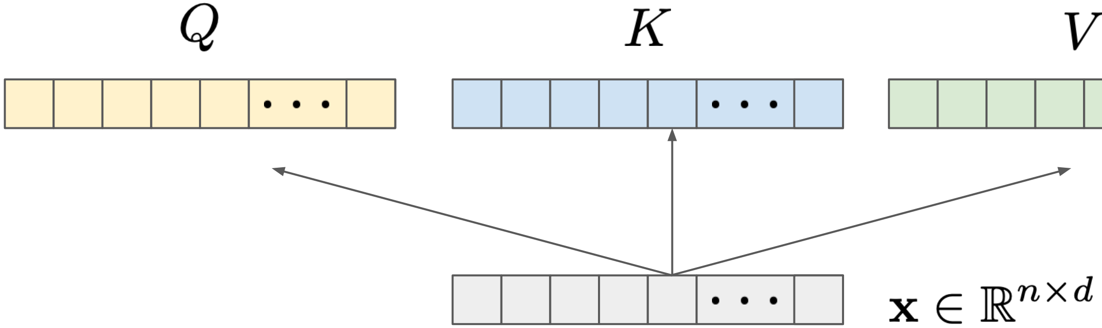
$$W_q, W_k, W_v \in \mathbb{R}^{d \times d'}$$

Self-attention

$$\mathrm{Attn}(\underbrace{\mathbf{x}W_q}_{Q}, \underbrace{\mathbf{x}W_k}_{K}, \underbrace{\mathbf{x}W_v}_{V}) = \mathrm{softmax}\left(\frac{\mathbf{x}W_q(\mathbf{x}W_k)^T}{\sqrt{d}}\right)\mathbf{x}W_v$$

We project inputs into query, key, and value

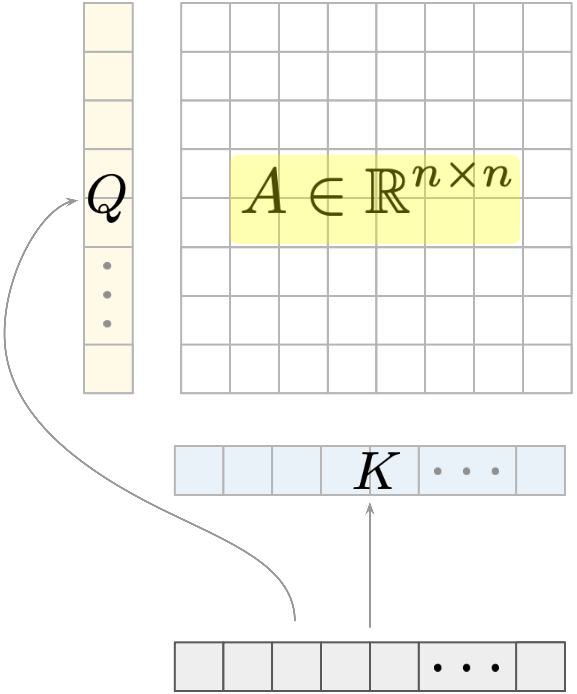
$$Q = \mathbf{x}W_q \in \mathbb{R}^{n\times d'}$$
$$K = \mathbf{x}W_k \in \mathbb{R}^{n\times d'}$$
$$V = \mathbf{x}W_v \in \mathbb{R}^{n\times d'}$$



Self-attention

Q K V

$$\mathrm{Attn}(\mathbf{x}W_q, \mathbf{x}W_k, \mathbf{x}W_v) = \mathrm{softmax}\left(\frac{\mathbf{x}W_q(\mathbf{x}W_k)^T}{\sqrt{d}}\right)\mathbf{x}W_v$$



$\mathbf{x} \in \mathbb{R}^{n \times d}$

$A = QK^T$

where

$Q \in \mathbb{R}^{n \times d'}$

$K \in \mathbb{R}^{n \times d'}$

Query and key matrices are used to compute the pairwise attention

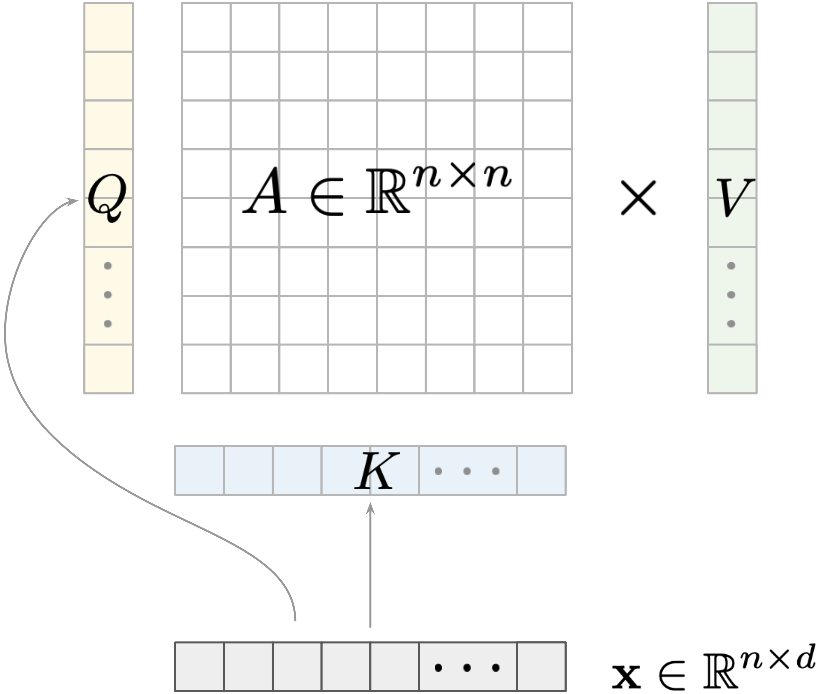
Each (i,j)th entry of attention indicates how i-th query is relevant to j-th key

The attention is row-wise sum-to-one due to softmax normalization

$\Rightarrow A_{ij} = \langle Q_i, K_j \rangle$, 즉, similarity 측정.

Self-attention

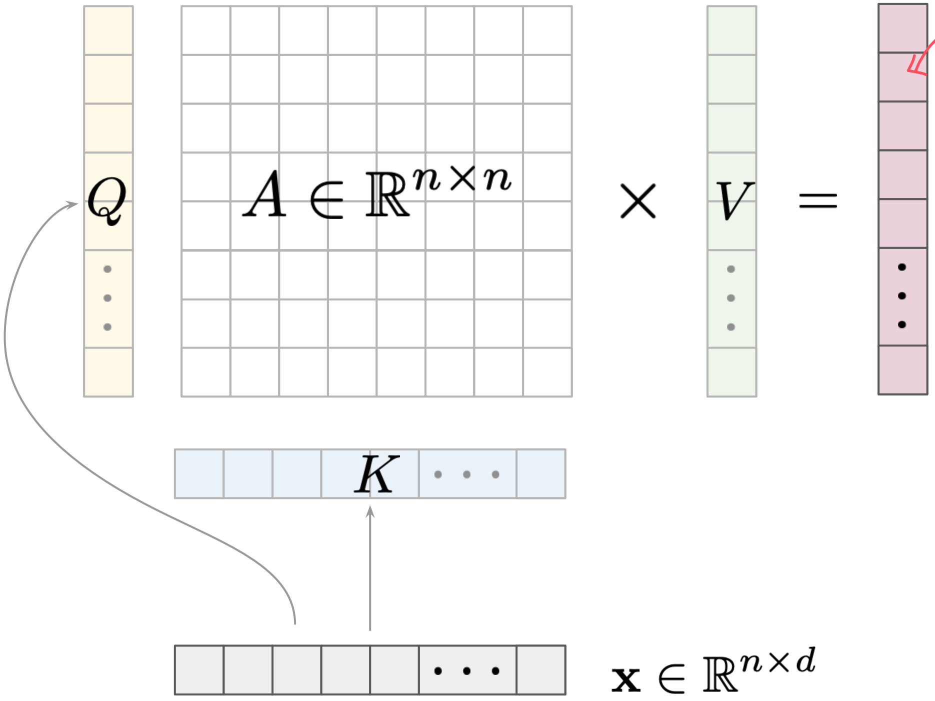
$$\mathrm{Attn}(\mathbf{x}W_q, \mathbf{x}W_k, \mathbf{x}W_v) = \mathrm{softmax}\left(\frac{\mathbf{x}W_q(\mathbf{x}W_k)^T}{\sqrt{d}}\right)\mathbf{x}W_v$$



Attention is used to take weighted average of the value matrix (matrix multiplication)

Self-attention

$$\mathrm{Attn}(\mathbf{x}W_q, \mathbf{x}W_k, \mathbf{x}W_v) = \mathrm{softmax}\left(\frac{\mathbf{x}W_q(\mathbf{x}W_k)^T}{\sqrt{d}}\right)\mathbf{x}W_v$$



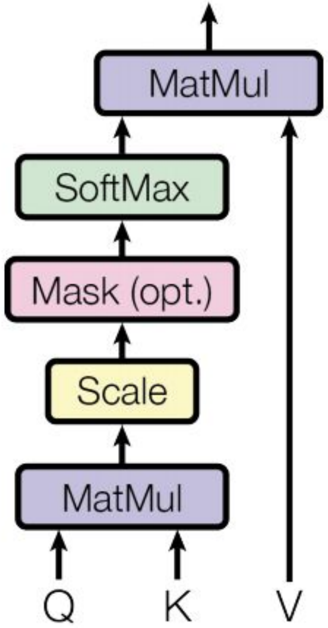
$O_i = \sum A_{i\alpha} V_\alpha$

The output is contexture encoding of input (receptive field=the whole)

$$V = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}$$

Scaled Dot-Product Attention

Scaled Dot-Product Attention



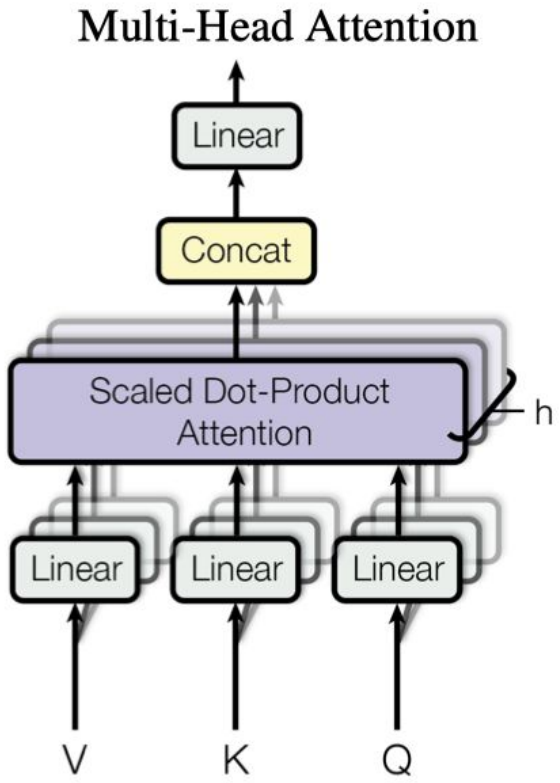
- Query, key, value attention with scaling factor

$$\mathrm{Attention}(Q, K, V) = \mathrm{softmax}(\frac{QK^T}{\sqrt{d_k}})V$$

We normalize the logits for the softmax with the size of query and key.

It prevents the softmax function produces too sharp attention thus makes gradient stronger

Multi-head attention



- Each head corresponds to query, key, value attention (=scaled dot product attention)

$$\mathrm{MultiHead}(Q,K,V) = \mathrm{Concat}(\mathrm{head_1}, \ldots, \mathrm{head_h})W^O$$
$$\text{where } \mathrm{head_i} = \mathrm{Attention}(QW_i^Q, KW_i^K, VW_i^V)$$

- Multi-head attention computes multiple attentions using (Q_i,K_i,V_i) and aggregates them
- Note that the multi-head attention can be computed not only within the encoder and decoder features, but features between encoder and decoder as well.

Overview of Transformer architecture

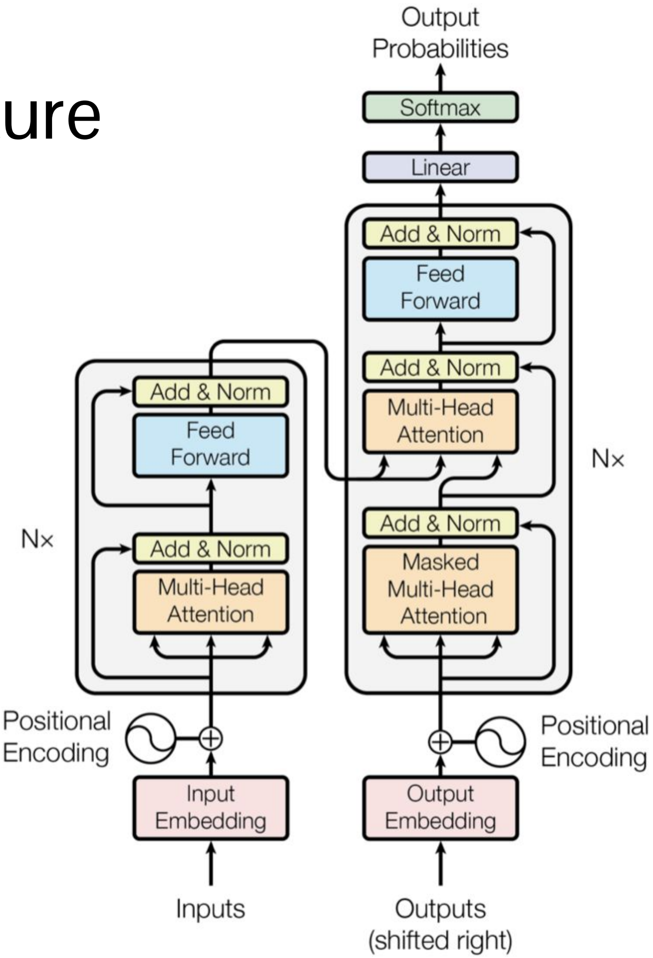


Figure 1: The Transformer - model architecture.

Transformer - Encoder

- Each word is encoded into continuous embedding

$$\mathbf{h}_i = \mathrm{FF}(\mathbf{x}_i)$$

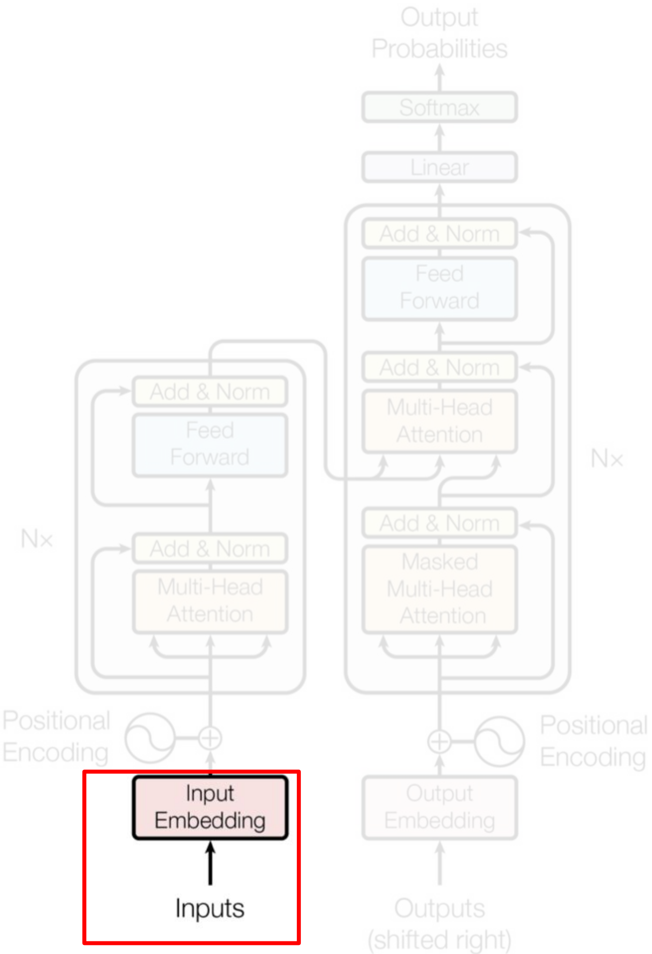
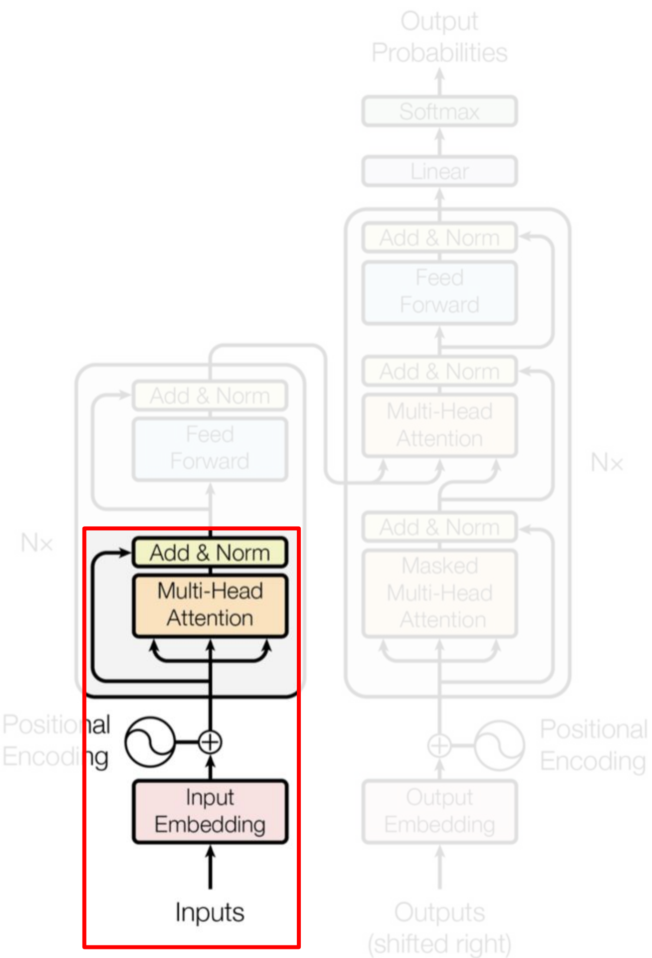


Figure 1: The Transformer - model architecture.

Transformer - Encoder

- Each word is encoded into continuous embedding
  $\mathbf{h}_i = \mathrm{FF}(\mathbf{x}_i)$
- Each word is then encoded by aggregating context within the entire source sentence
  via multi-head attention (a.k.a. **self-attention**)
  $\mathbf{h}_i = \mathrm{LayerNorm}(\mathbf{h}_i + \mathrm{Attn}(\mathbf{h}_i, \{\mathbf{h}_j\}_{\forall j \neq i}))$



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- We further encode the word with residual connection
$$\mathbf{h}_i = \mathrm{LayerNorm}(\mathbf{h}_i + \mathrm{FF}(\mathbf{h}_i))$$

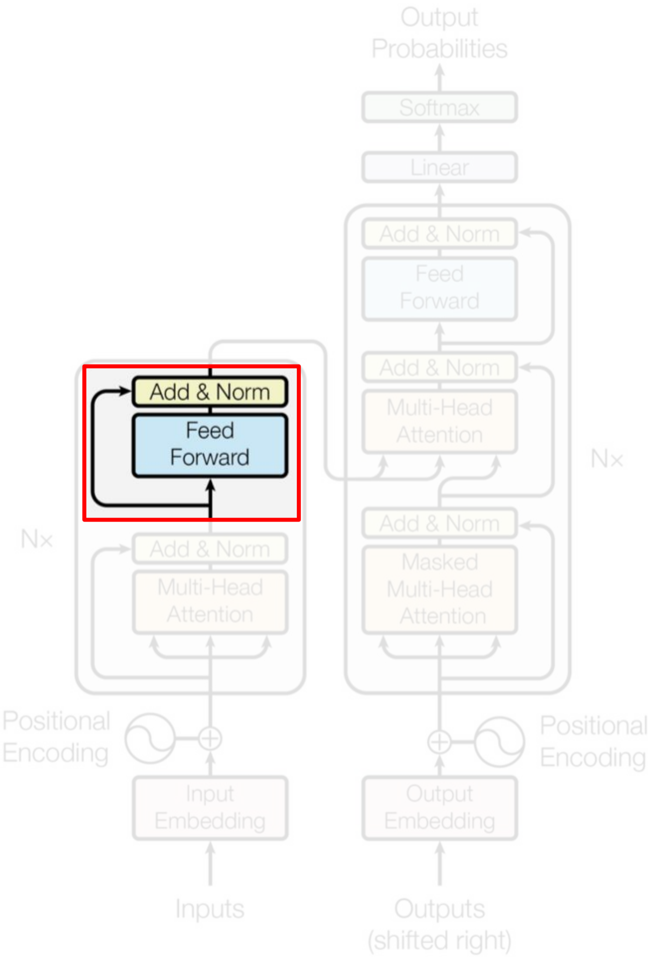


Figure 1: The Transformer - model architecture.

Transformer - Decoder

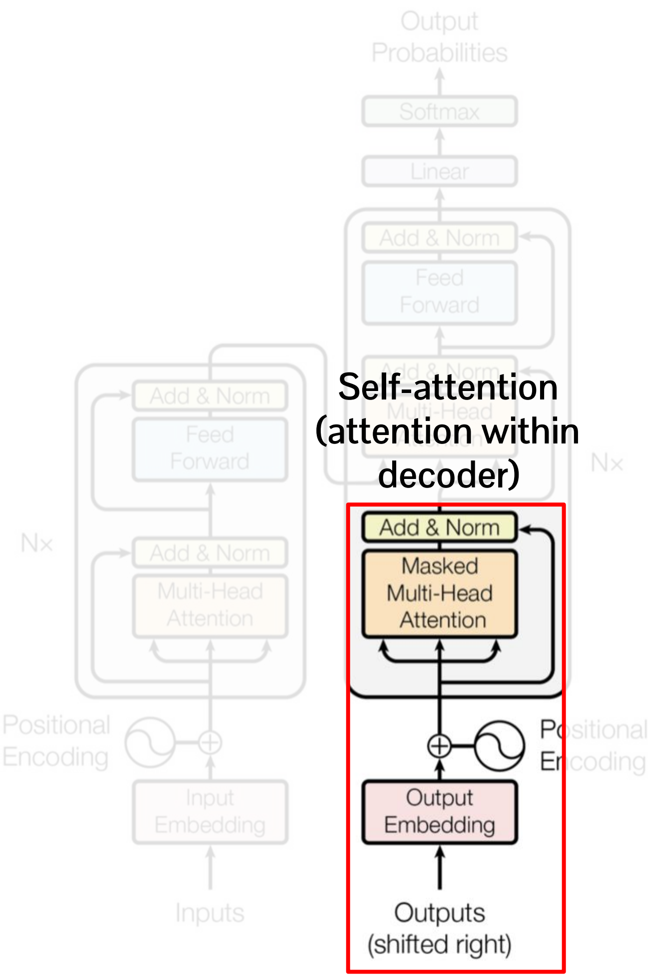
- We apply the self-attention for each target word

$$\mathbf{s}_i = \mathrm{FF}(\mathbf{y}_i)$$

$$\mathbf{s}_i = \mathrm{LayerNorm}(\mathbf{s}_i + \mathrm{Attn}(\mathbf{s}_i, \{\mathbf{s}_j\}_{\forall j<i}))$$

In decoder, we apply the attention only up to the current word (i.e., not the next words)

This is implemented via applying attention with the mask (masking the future time steps with 0)



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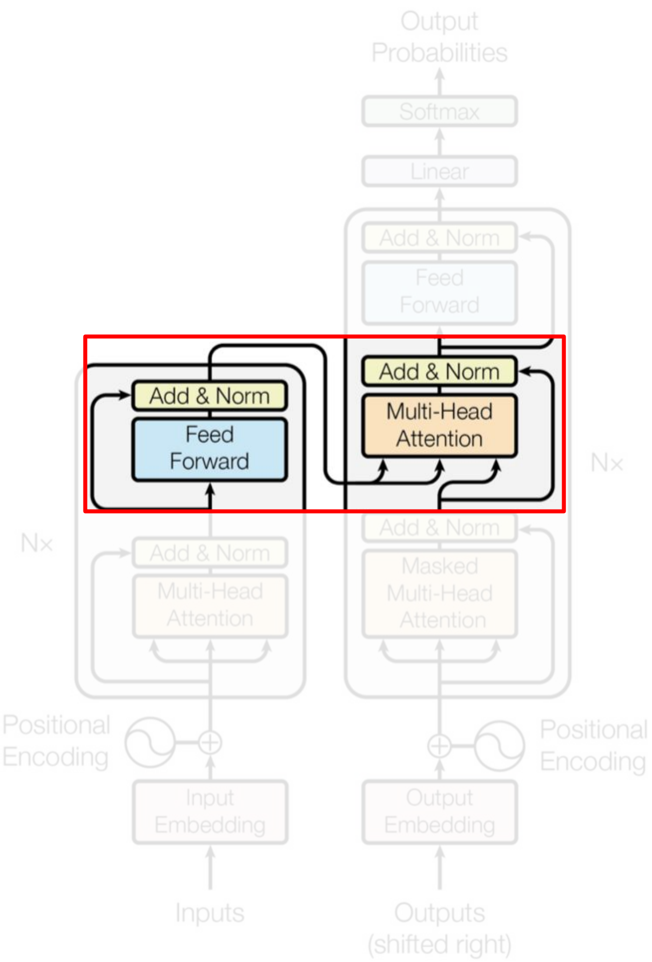
- The target word is encoded with source sentence via attention (a.k.a. **cross-attention**)

$$\mathbf{s}_i = \mathrm{LayerNorm}(\mathbf{s}_i + \mathrm{Attn}(\mathbf{s}_i, \{\mathbf{h}_j\}_{\forall j}))$$

All encoded words in the **source** sentence



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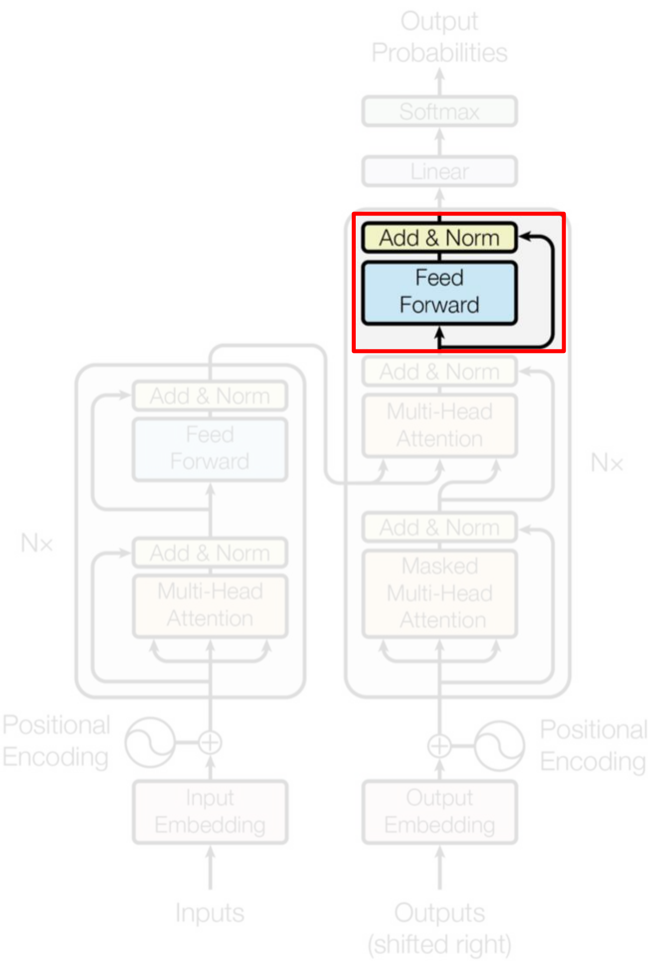


Figure 1: The Transformer - model architecture.

Transformer - Encoder & Decoder

- We stack this encoding layers multiple time for both encoder and decoder

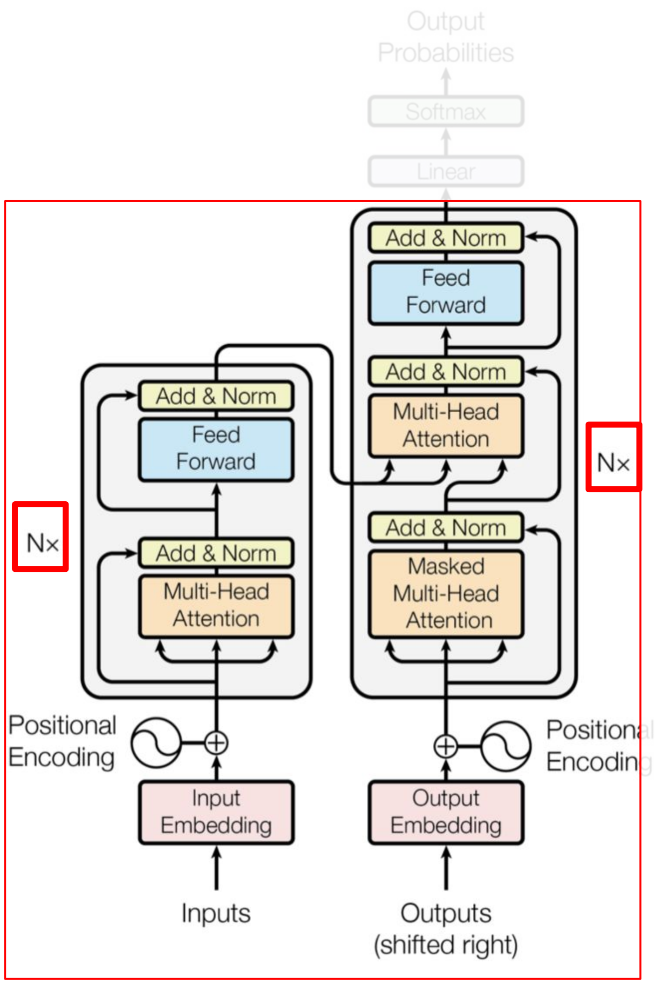


Figure 1: The Transformer - model architecture.

Transformer - Output

- The translated word is produced at each step of the decoder

$$\hat{\mathbf{y}}_{i+1} = \mathrm{Softmax}(\mathrm{FF}(\mathbf{s}_i))$$

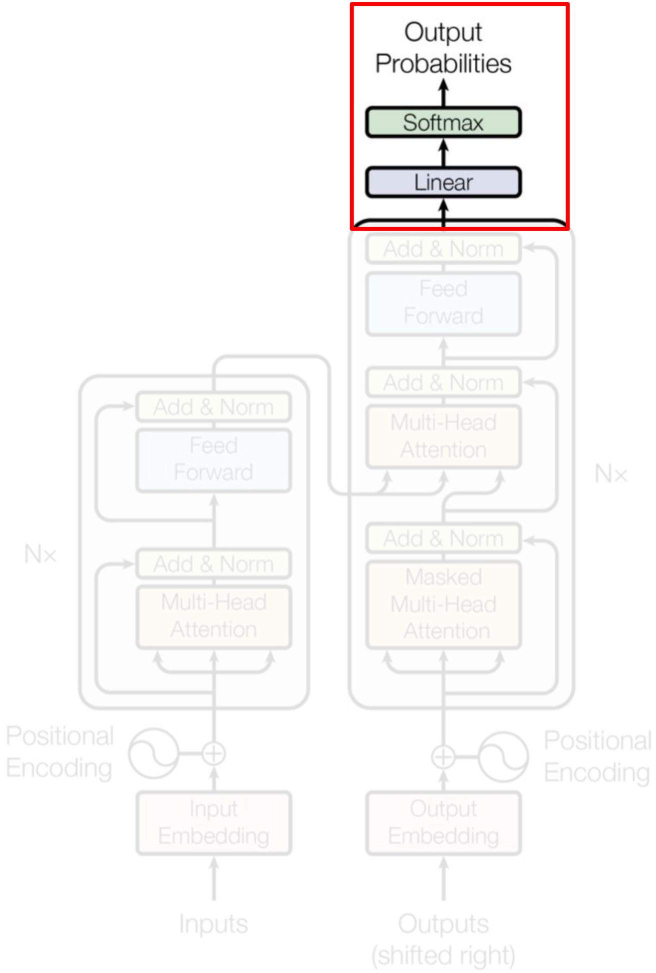


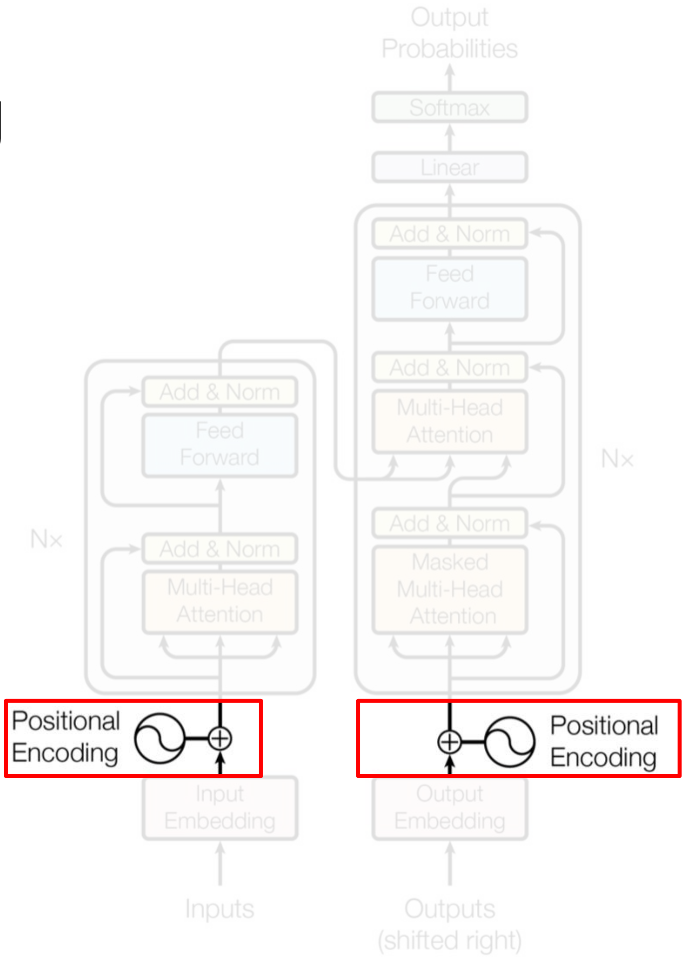
Figure 1: The Transformer - model architecture.

Transformer - Positional encoding

- When encoding both source and target words, we add extra embedding that encodes **position** of the word.

- We can use any periodic function for positional embedding, or even learn how to encode position

$$PE_{(pos,2i)} = sin(pos/10000^{2i/d_{\text{model}}})$$
$$PE_{(pos,2i+1)} = cos(pos/10000^{2i/d_{\text{model}}})$$



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Overview of Transformer architecture

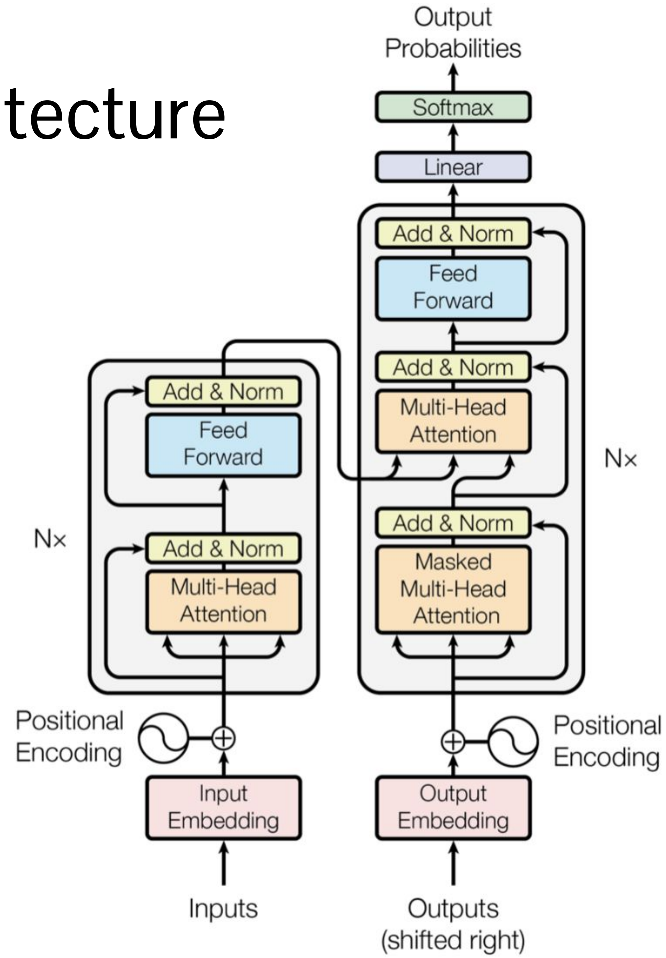

Figure 1: The Transformer - model architecture.

Applications

- Machine translation

Applications

- Text generation

SYSTEM PROMPT (HUMAN-WRITTEN)

Miley Cyrus was caught shoplifting from Abercrombie and Fitch on Hollywood Boulevard today.

MODEL COMPLETION (MACHINE-WRITTEN, SECOND TRY)

The 19-year-old singer was caught on camera being escorted out of the store by security guards.

The singer was wearing a black hoodie with the label ‘Blurred Lines’ on the front and ‘Fashion Police’ on the back.

Scroll down for video

Shoplifting: Miley Cyrus was caught shoplifting from Abercrombie and Fitch on Hollywood Boulevard today (pictured)

The singer was wearing a black hoodie with the label ‘Blurred Lines’ on the front and ‘Fashion Police’ on the back

The singer was also wearing a pair of black-rimmed glasses, a black jacket, black jeans and black sandals.

She was carrying a pair of black and white striped gloves and a small black bag.

https://openai.com/blog/better-language-models/

Applications

- Music sequence generation

https://openai.com/blog/musenet/

Next

- Variational Autoencoder