Sequence Modelling and Generation with Transformer

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Edstem for discussion

- Please check your email for invitation!

Paper Presentation Assignment

- https://docs.google.com/spreadsheets/d/1-d1NuvSyHQoE-ycmLNmNFSbxum-jvkYmwiS4CP7-7kk/edit?usp=sharing

- Please prepare slides and upload to canvas 7 days before your presentation day.

Can GenAI design molecules with desired functions?

Medicine

Vaccine

Enzyme - Biocatalysts

Biosensors (e.g. GFP)

New materials

Commonality and Distinction in Language and Molecule Generation

- Both are sequences of Discrete Tokens

- Both have discrete Structures

- Geometry (Unique for molecules)

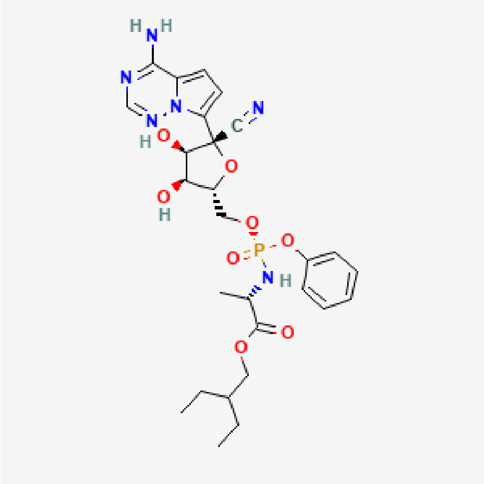
Discrete Sequences of Tokens

It was the best of times, it was the worst of times, it was the age of wisdom, it was the age of foolishness, it was the epoch of belief, it was the epoch of incredulity, it was the season of Light, it was the season of Darkness, …

Remdesivir: $C_{27}H_{35}N_6O_8P$

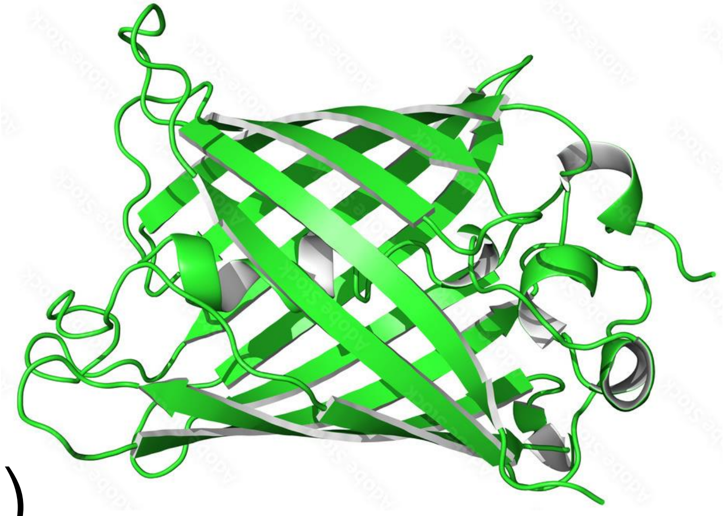
SMLES representation:

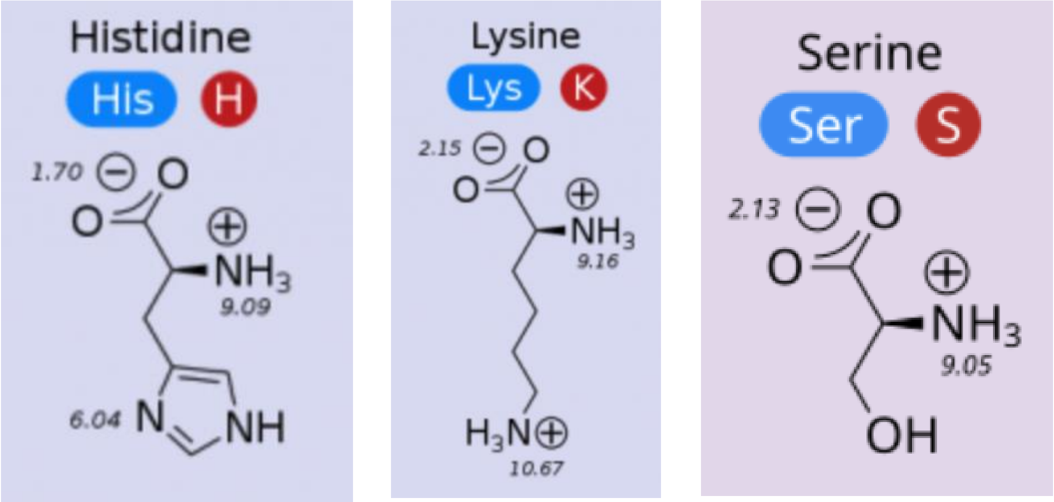
CCC(CC)COC(=O)C(C)NP(=O)(OCC1C(C(C(O1)(C#N)C2=CC=C3N2N=CN=C3N)O)O)OC4=CC=CC=C4



From Human Language to Protein Sequence

- Proteins are building blocks of life
- Important biological functions
- sequence of amino acid residues (20 types)





VLLPDNHYLSTQSALSKDPNE
KRDHMVLLEFVTAAGIT

Today's Topic

- Language Models

- Transformer Model
  - Embedding
  - Multihead Attention, Decoder Self-Attention
  - FFN
  - Layernorm

- Training Techniques and Performance of Transformer

- Code walkthrough

Language Model

- A probabilistic model of discrete sequences, including human languages and biological languages

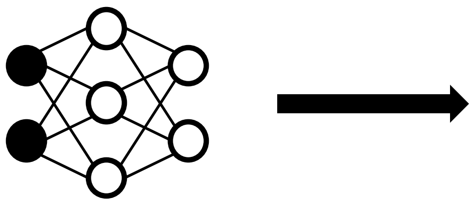
Probability(“Pittsburgh is a city of bridges”)

Probability(“VLLPDNHYLSTQSALSKDPN”)

Probability Model for Next Token

P(next word y_t | Prompt x, previous words $y_{1:t-1}$)

Santa Barbara has very nice ____



Pittsburgh is a city of ____

beach	0.5
weather	0.4
snow	0.01

bridges	0.6
corn	0.02

Mathematics of Language Model

Probability("Pittsburgh is a city of bridges")

$= P(\text{“}Pittsburgh\text{”}) \cdot P(\text{“}is\text{”}|\text{“}Pittsburgh\text{”})$

$\cdot P(\text{“}a\text{”}|\text{”}Pittsburgh\ is\text{”}) \cdot P(\text{“}city\text{”}|\ldots) \cdot P(\text{“}of\text{”}|\ldots)$

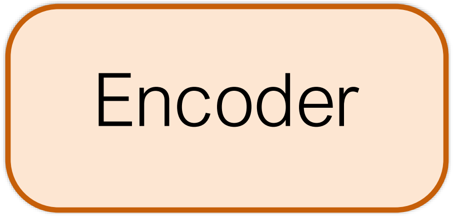
$\cdot P(\text{“}bridges\text{”}|\ldots)$

$$\text{Prob.}(x_{1..T}) = \prod_{t=1}^{T} \underline{\mathrm{P}(\mathrm{x}_{t+1}|\mathrm{x}_{1..t})}$$

Predicting using Neural Nets
(Transformer network, CNN, RNN)

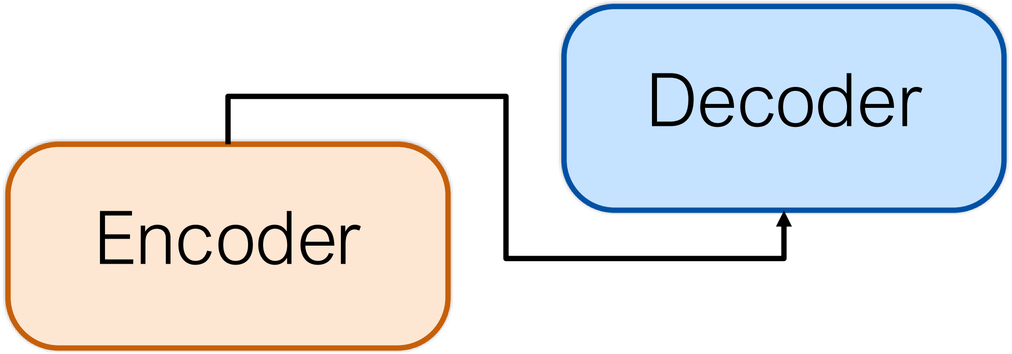
Type of Language Models

Encoder-only
Masked LM
Non-autoregressive



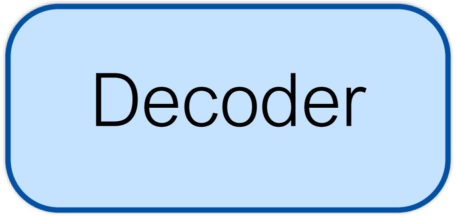
e.g. BERT
RoBERTa
ESM (for protein)

Encoder-decoder



e.g. T5

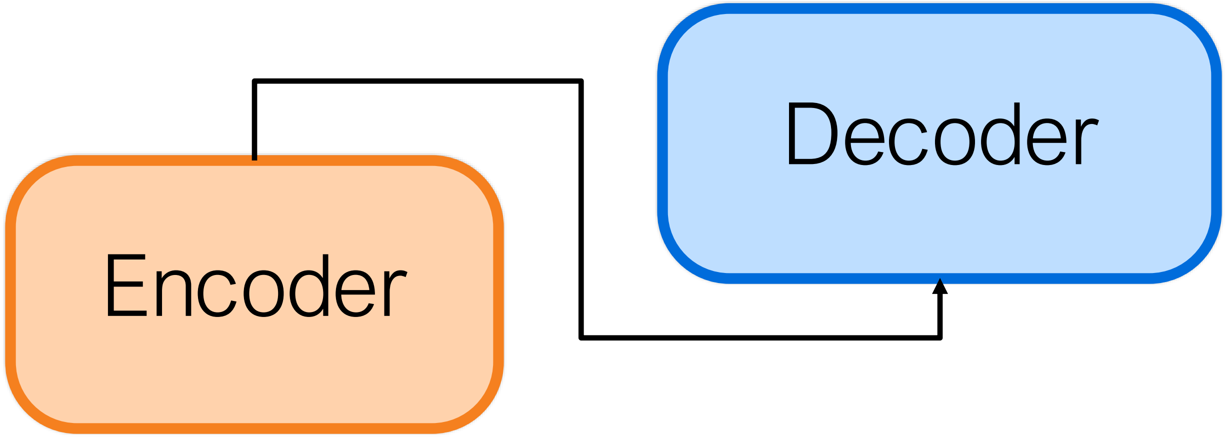
Decoder-only
Autoregressive



e.g. GPT
LLaMA
ProGen (for protein)

Encoder-Decoder Paradigm

target:
I like singing and dancing.



Source: 我喜欢唱歌和跳舞。

$$p_\theta(y|x) = \prod_i p(y_i|x, y_{1:i-1})$$

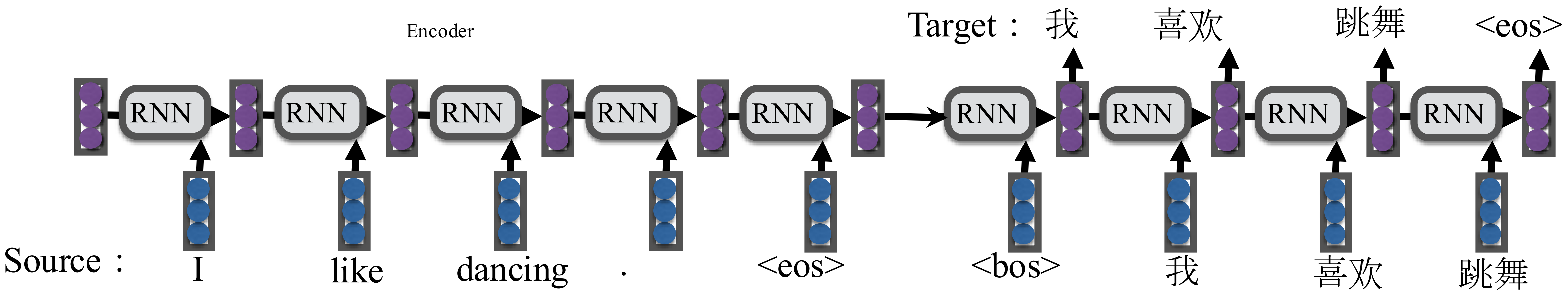
conditional prob. modeled by neural networks (Transformer)

Sequence to Sequence Learning

- Conditional text generation: directly learning a function mapping from source sequence to target sequence

$$p_\theta(y|x) = \prod_t p(y_t|x, y_{1:t-1}; \theta)$$

- Previous encoder/decoder: LSTM or GRU

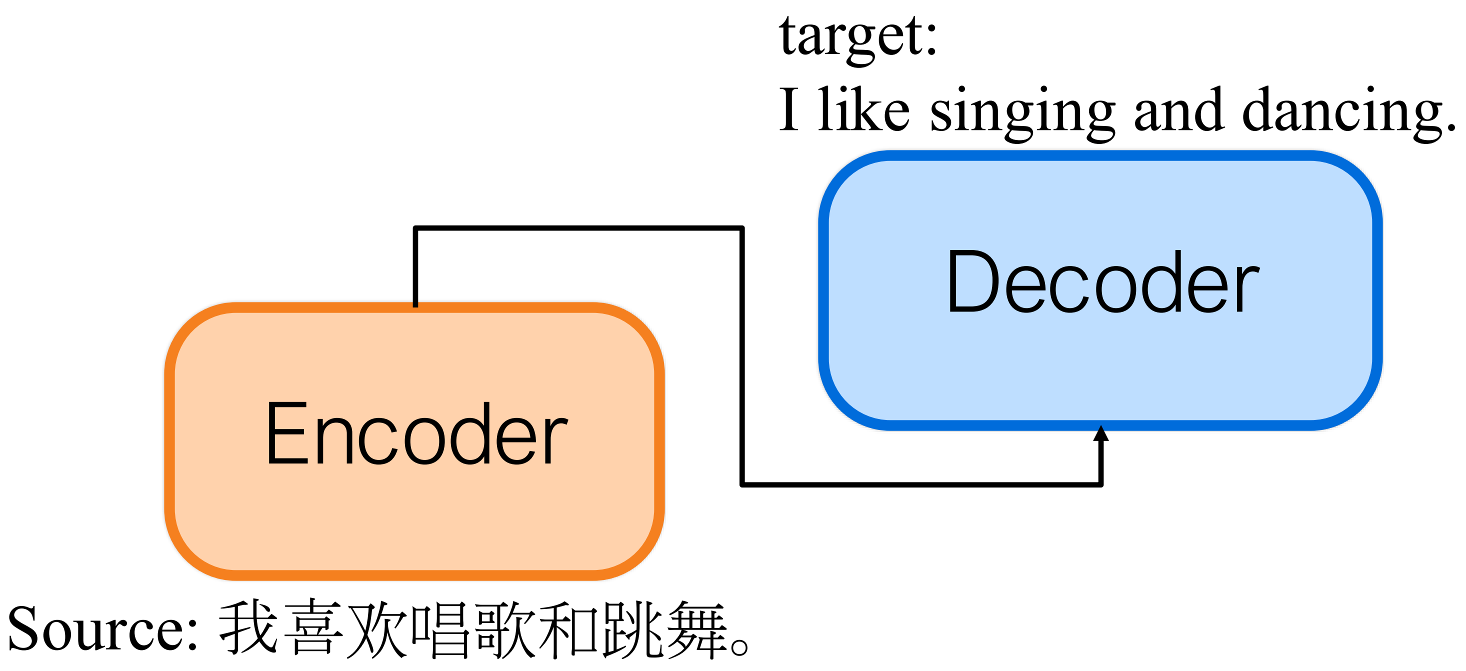


Sutskever et al. Sequence to Sequence Learning with Neural Networks. 2014

Motivation for a new Architecture

- Full context and parallel: use Attention in both encoder and decoder

- no recurrent ==> concurrent encoding



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- Encoder-decoder Architecture
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  - Multihead Attention, Decoder Self-Attention
  - FFN
  - Layernorm
- Training Techniques and Performance of Transformer
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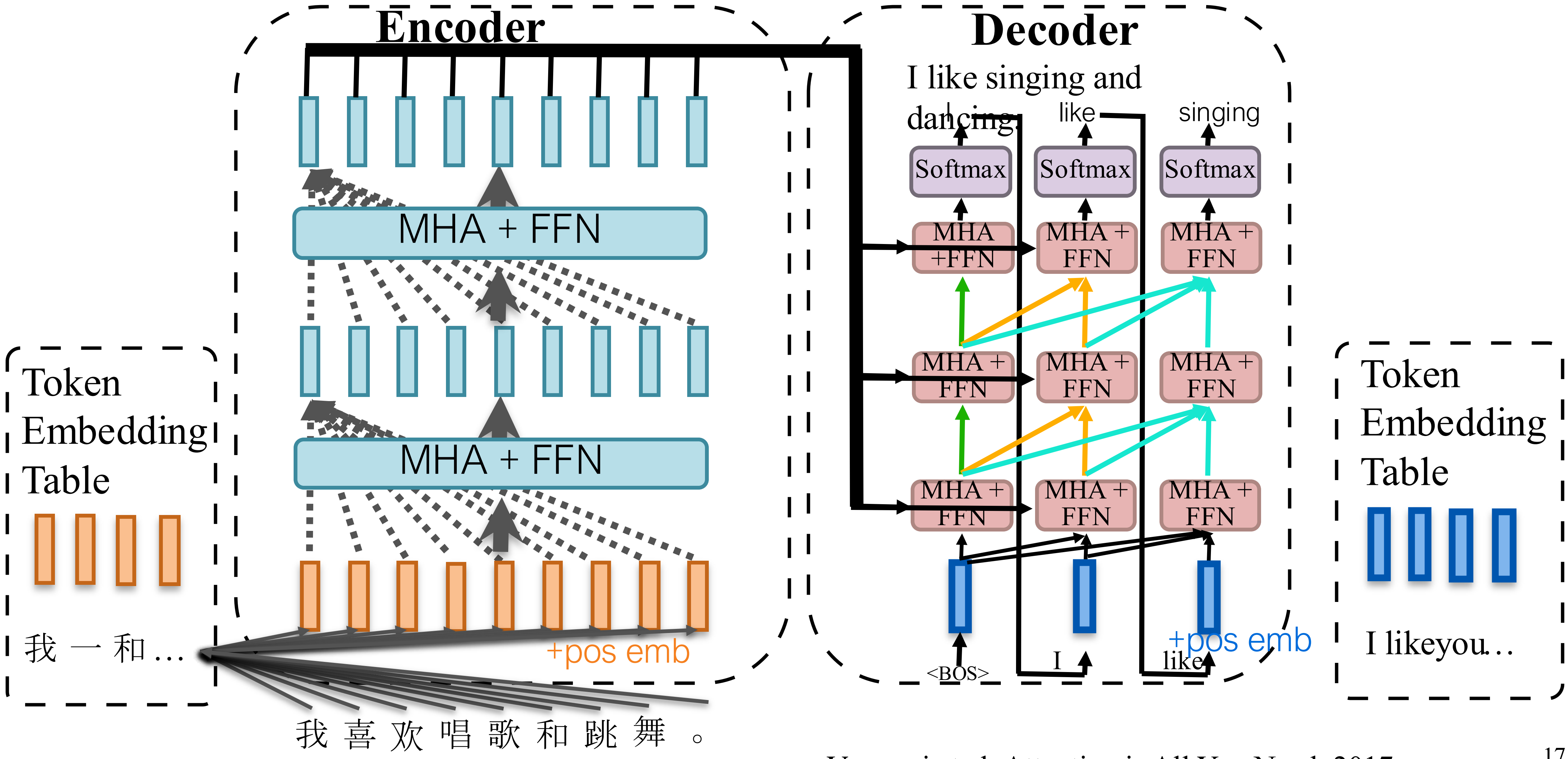
Transformer



Vaswani et al. Attention is All You Need. 2017

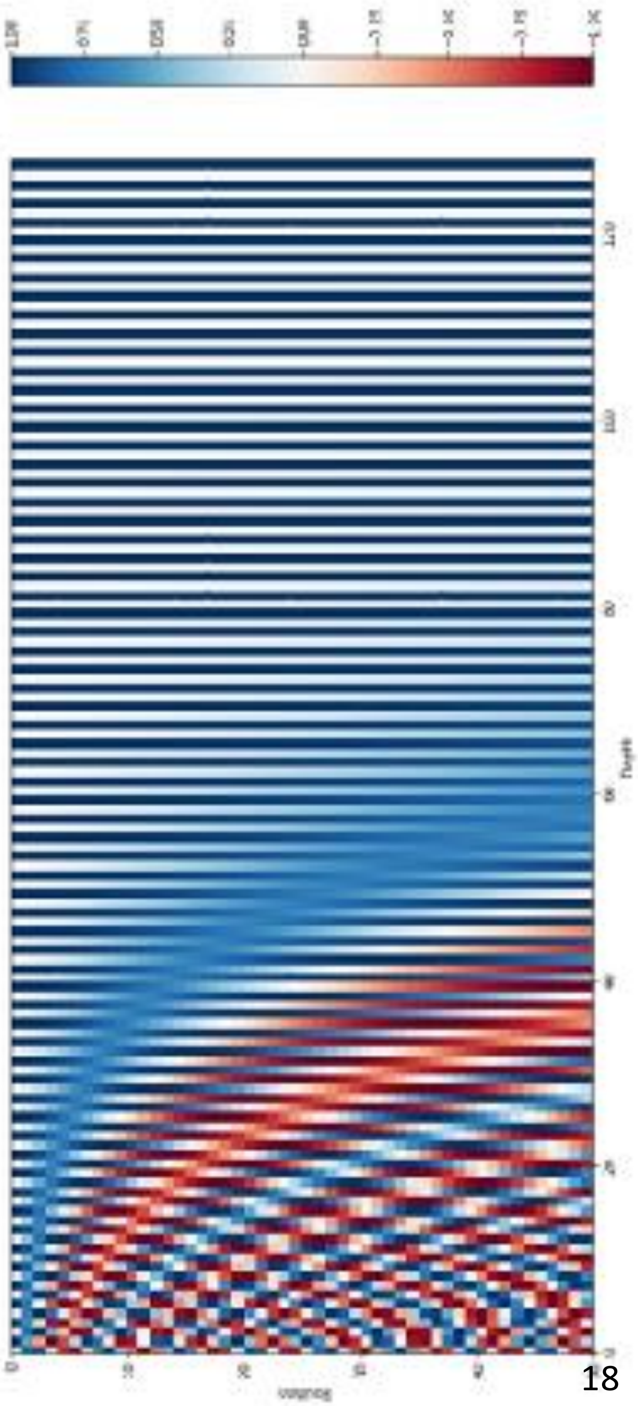
Embedding

- Token Embedding: (tokenization next lec.)
  - Shared (tied) input and output embedding from lookup table

- Positional Embedding:
  - to distinguish words in different position, Map position labels to embedding, dimension is same as Tok Emb, for t-th pos, i-th dim

$$PE_{\mathrm{t},2i} = \sin\left(\frac{t}{1000^{2i/d}}\right)$$

$$PE_{\mathrm{t},2i+1} = \cos\left(\frac{t}{1000^{2i/d}}\right)$$

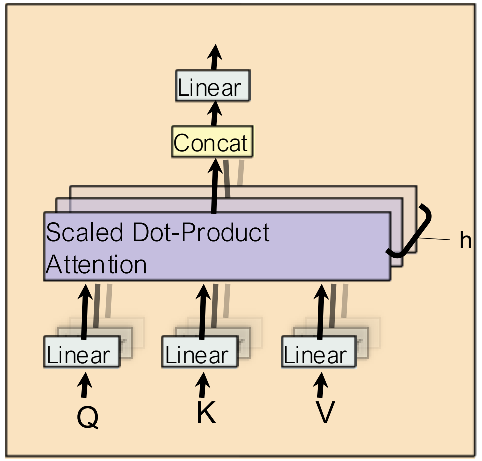


Multi-head Attention

- Instead of one vector for each token
- break into multiple heads
- each head perform attention

$$\text{Head}_i = \text{Attention}(QW_i^Q, KW_i^K, VW_i^V)$$

$$\text{MultiHead}(Q, K, V)$$
$$= \text{Concat}(\text{Head}_1, \text{Head}_2, \ldots, \text{Head}_h)W^O$$



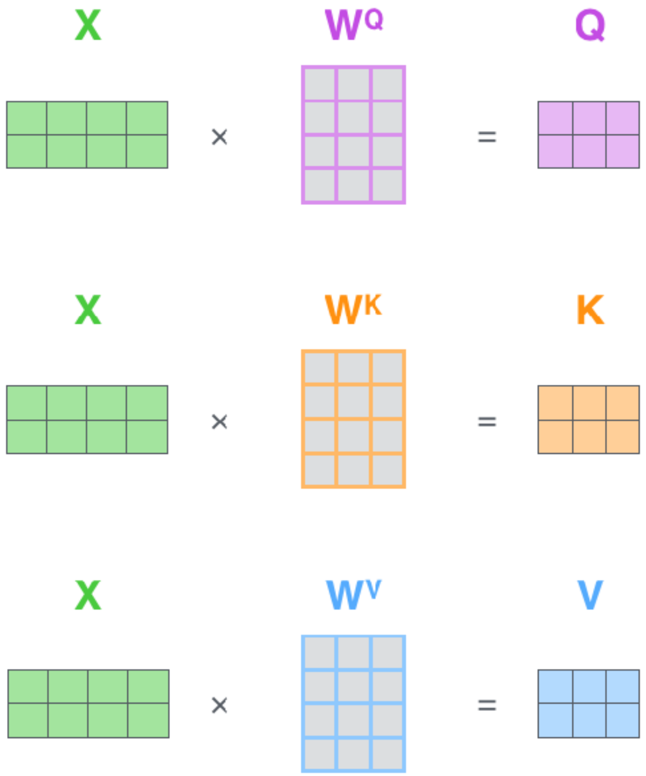
Multi-head Attention

X are input embeddings from previous layer (num of tok * dim)

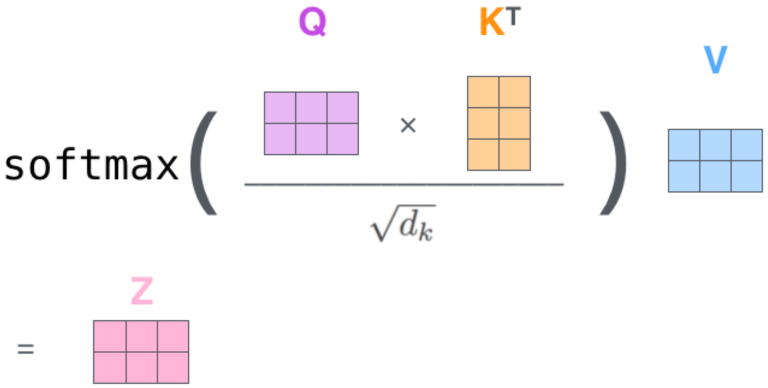
Query

Key

Value



sent len x sent len



len x dim

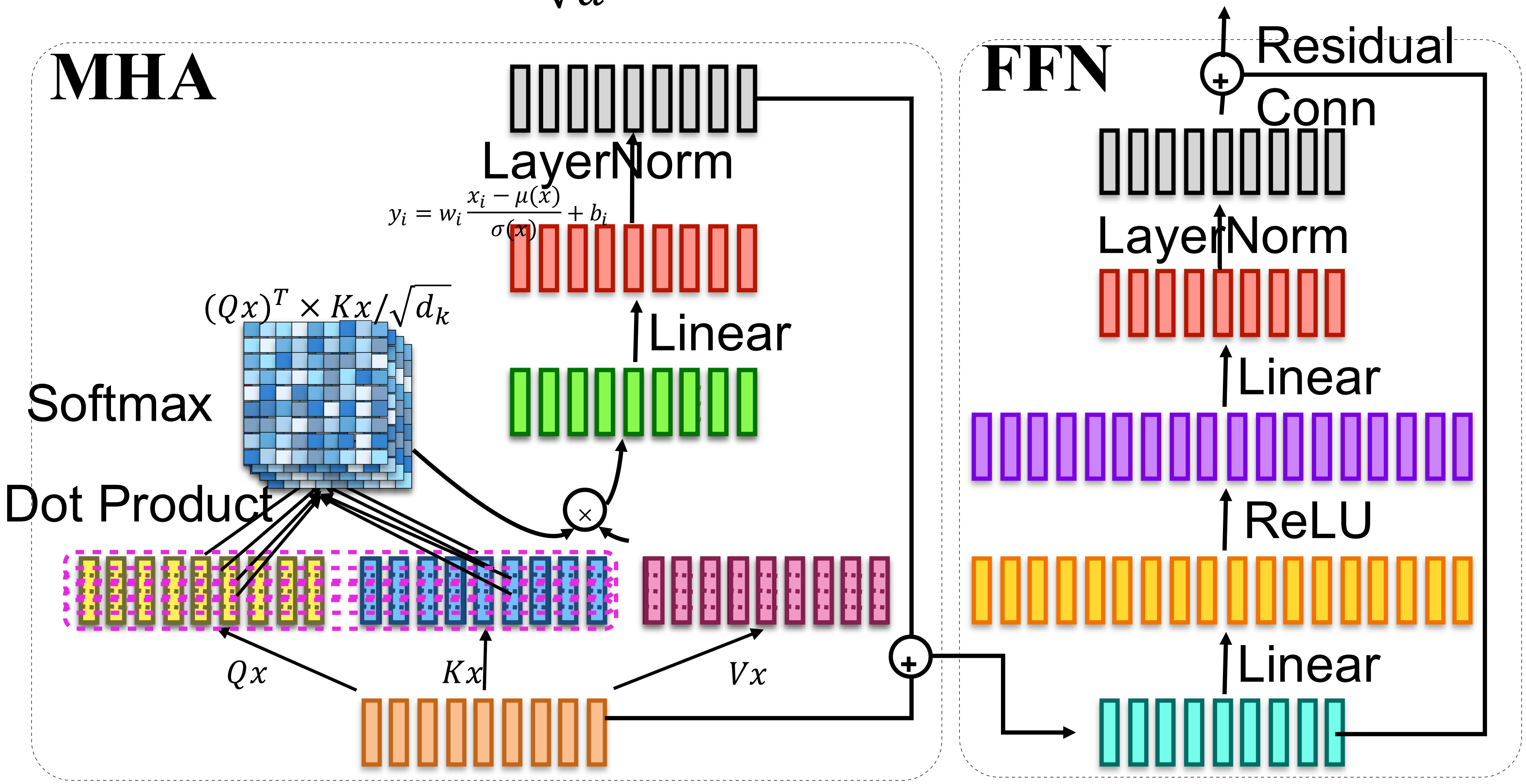
Q: why divided by sqrt(d)?

Alammar, The Illustrated Transformer

Multihead Attention and FFN

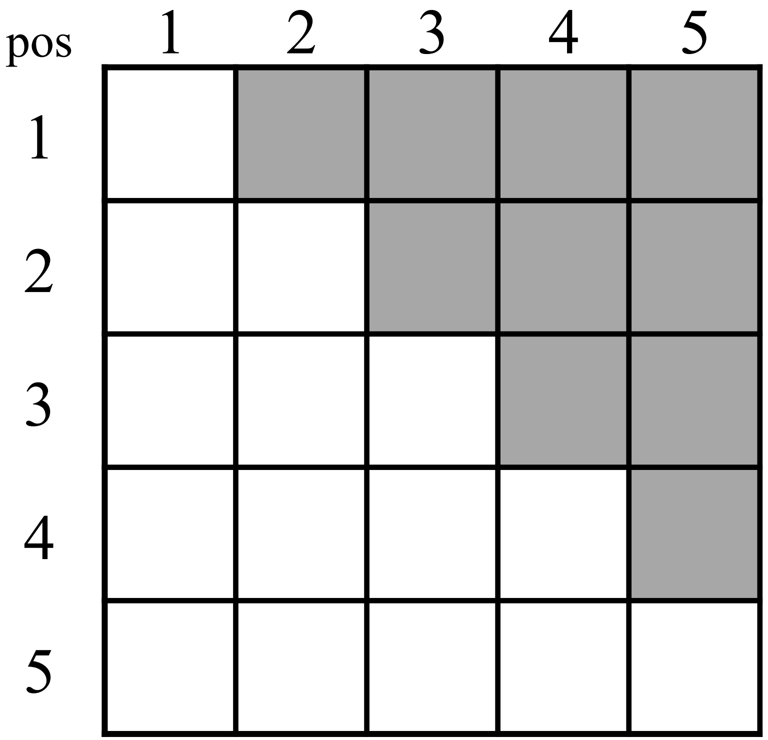
$$\text{Attention}(Q,K,V,x) = \text{Softmax}\left(\frac{(Qx)^T Kx}{\sqrt{d}}\right) \cdot (Vx)^T$$

$$\text{FFN}(x) = max(0, x \cdot W_1 + b_1) \cdot W_2 + b_2$$

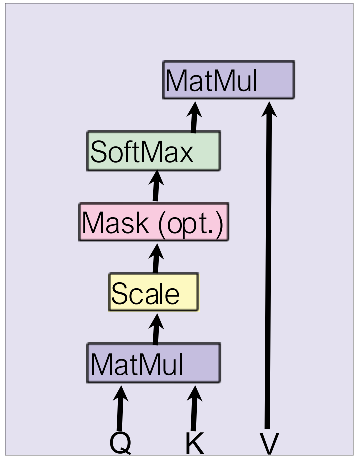


Decoder Self-Attention

- Maskout right side before softmax (-inf)

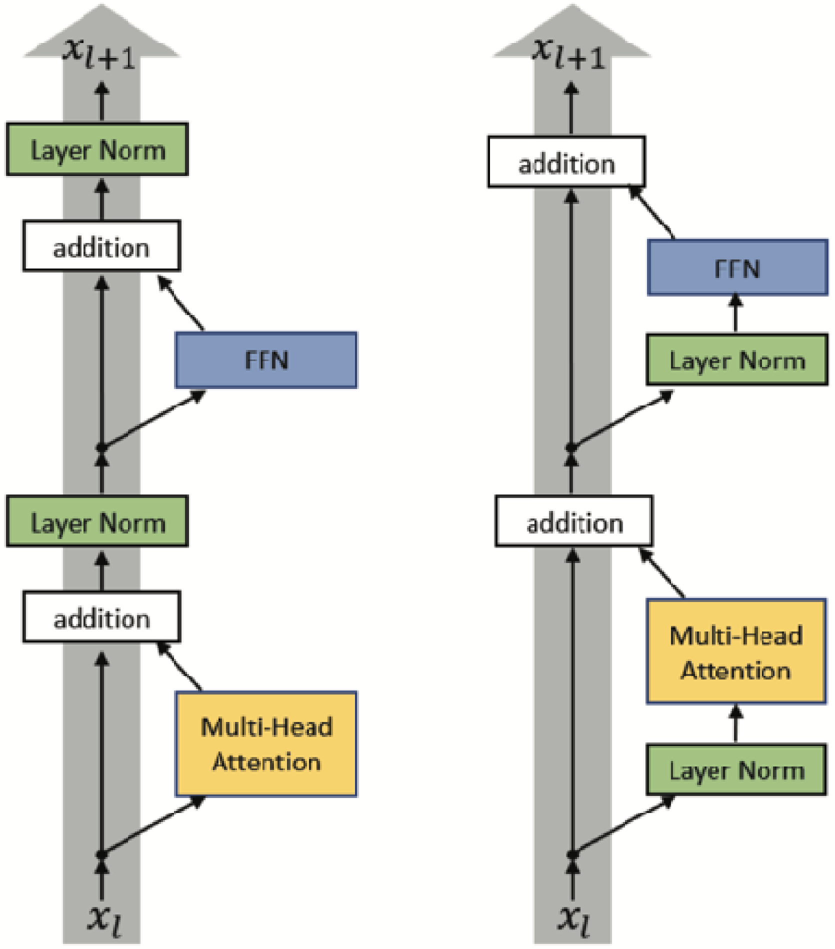


Scaled Dot-Product Attention



Residual Connection and Layer Normalization

- Residual Connection
- Make it zero mean and unit variance within layer
- Post-norm
- Pre-norm



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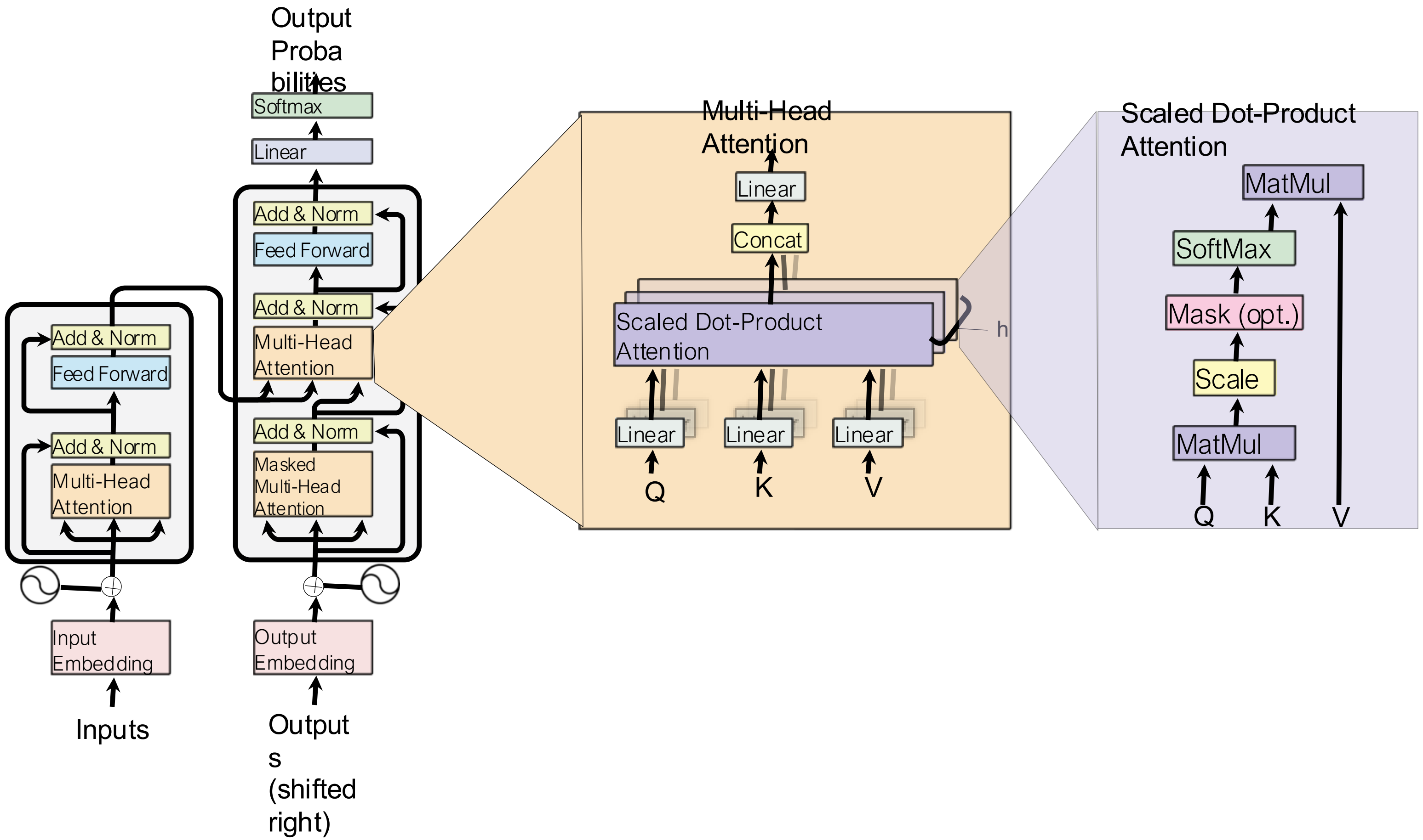
Transformer in Original Paper

- C layers of encoder (=6)
- D layers of decoder (=6)
- Token Embedding: 512 (base), 1024 (large)
- FFN dim=2048



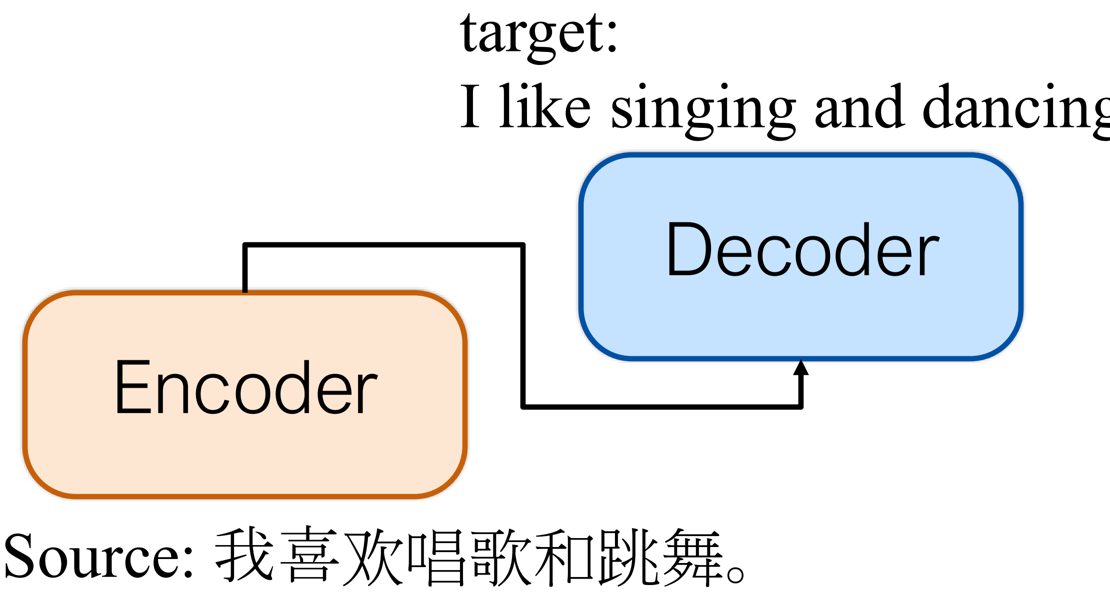
Training Transformer

$$P(Y|X) = \prod P(y_t|y_{<t}, x)$$

- Training loss: Cross-Entropy

$$l = -\sum_n \sum_t \log f_\theta(x_n, y_{n,1}, \ldots, y_{n,t-1})$$

- Teacher-forcing during training.
- pretend to know groundtruth for prefix



Training Transformer for MT

- Dropout
  - Applied to before residual
  - and to embedding, pos emb.
  - p=0.1 ~ 0.3
- Label smoothing
  - 0.1 probability assigned to non-truth
- Vocabulary:
  - En-De: 37K using BPE
  - En-Fr: 32k word-piece (similar to BPE)

Label Smoothing

- Assume $y \in R^n$ is the one-hot encoding of label

$$y_i = \begin{cases} 1 & \text{if belongs to class } i \\ 0 & \text{otherwise} \end{cases}$$

- Approximating 0/1 values with softmax is hard

- The smoothed version

$$y_i = \begin{cases} 1 - \epsilon & \text{if belongs to class } i \\ \epsilon/(n-1) & \text{otherwise} \end{cases}$$

  - Commonly use $\epsilon = 0.1$

Training

- Batch
  - group by approximate sentence length
  - still need shufflingHardware
  - one machine with 8 GPUs (in 2017 paper)
  - base model: 100k steps (12 hours)
  - large model: 300k steps (3.5 days)

- Adam Optimizer
  - increase learning rate during warmup, then decrease
  - $\eta = \frac{1}{\sqrt{d}} min(\frac{1}{\sqrt{t}}, \frac{t}{\sqrt{t_0^3}})$

ADAM

$$m_{t+1} = \beta_1 m_t - (1 - \beta_1)\nabla \ell(x_t)$$

$$v_{t+1} = \beta_2 v_t + (1 - \beta_2)(\nabla \ell(x_t))^2$$

$$\hat{m}_{t+1} = \frac{m_{t+1}}{1 - \beta_1^{t+1}}$$ momentum

$$\hat{v}_{t+1} = \frac{v_{t+1}}{1 - \beta_2^{t+1}}$$ variance

$$x_{t+1} = x_t - \frac{\eta}{\sqrt{\hat{v}_{t+1}} + \epsilon} \hat{m}_{t+1}$$ parameter

Model Average

- A single model obtained by averaging the last 5 checkpoints, which were written at 10-minute interval (base)

- decoding length: within source length + 50
  - more on decoding in next lecture

Summary

- Sequence-to-sequence encoder-decoder framework for conditional generation, including Machine Translation
- Key components in Transformer (why each?)
  - Positional Embedding (to distinguish tokens at different pos)
  - Multihead attention
  - Residual connection
  - layer norm
  - FFN

In-class Quiz 1 on Canvas

- https://canvas.cmu.edu/courses/49548/quizzes/150414

Code Go-through

https://nlp.seas.harvard.edu/annotated-transformer/