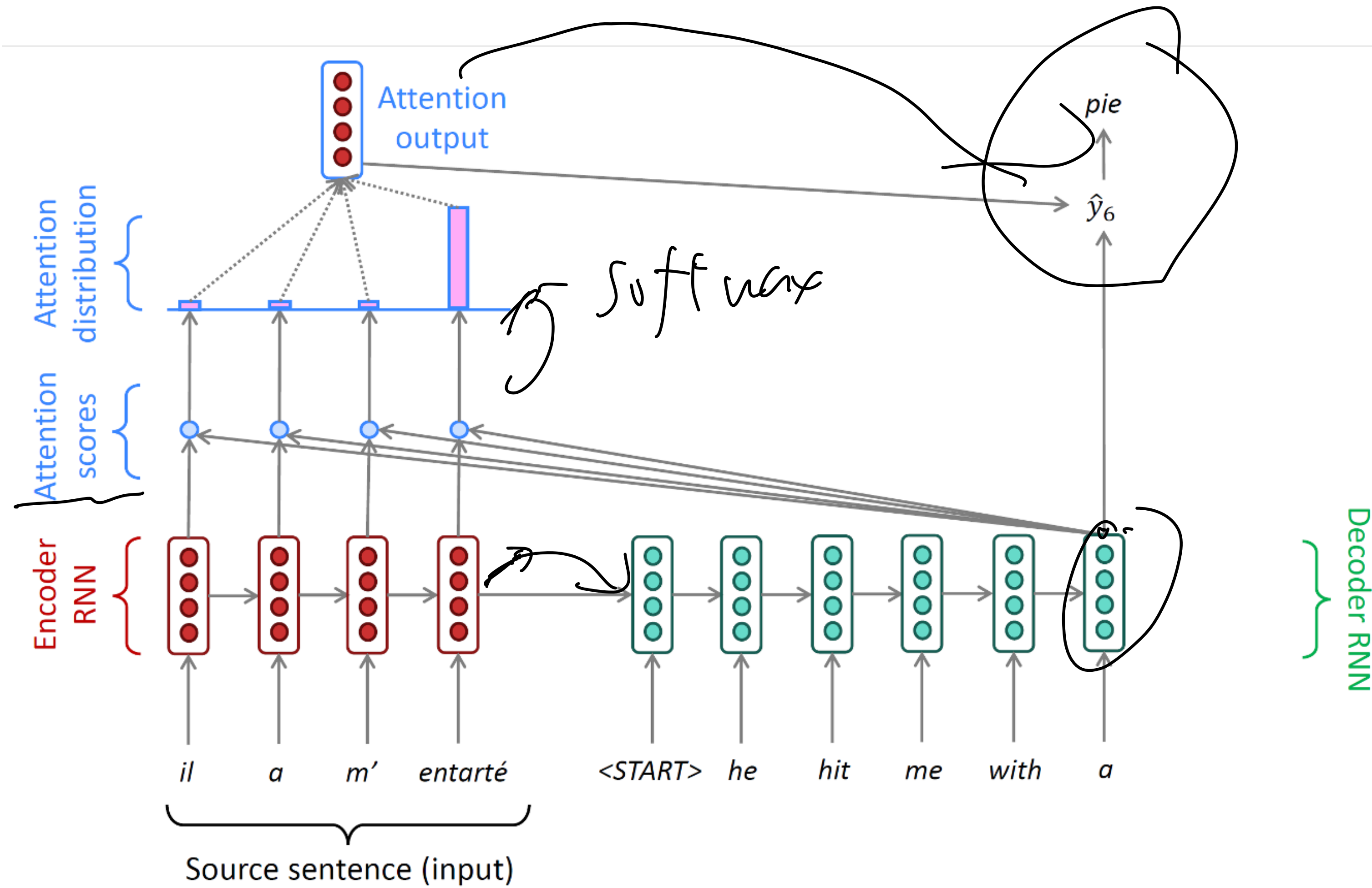
Attention Mechanism

Seq2Seq with Attention



Seq2Seq with Attention

Summary

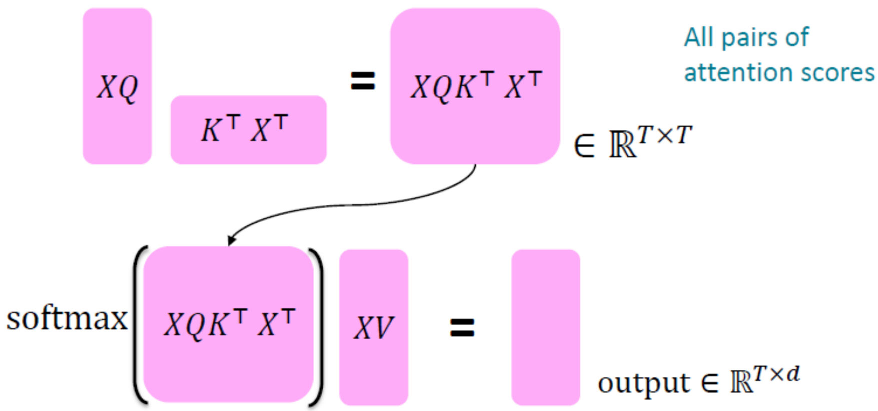
- Input sequence X, encoder f_{enc}, and decoder f_{dec}
- $f_{enc}(X)$ produces hidden states $h_1^{enc}, h_2^{enc}, \ldots, h_N^{enc}$

$X_1 \ldots X_N$

- 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}

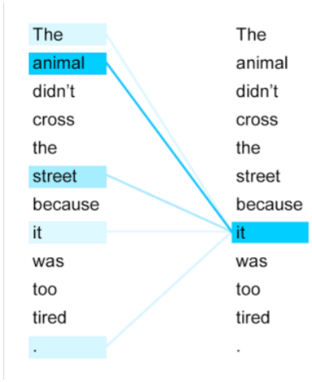
Key-query-value attention

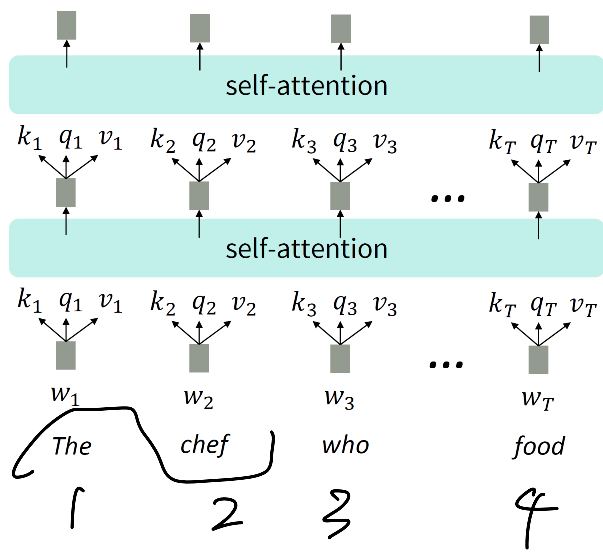
- Obtain q_t, v_t, k_t from X_t
- $q_t = W^q X_t$; $v_t = W^v X_t$; $k_t = W^k X_t$
  - W^q, W^v, W^k are learnable weight matrices
- $\alpha_{i,j} = \text{softmax}(q_i^\top k_j)$; $out_i = \sum_k \alpha_{i,j} v_j$
- Intuition: key, query, and value can focus on different parts of input



Attention is all you need (Vsawani '17)

- A pure attention-based architecture for sequence modeling
  - No RNN at all!
- Basic component: self-attention, $Y = f_{SA}(X; \theta)$
  - X_t uses attention on entire X sequence
  - Y_t computed from X_t and the attention output
- Computing Y_t
  - Key k_t, value v_t, query q_t from X_t
    - $(k_t, v_t, q_t) = g_1(X_t; \theta)$
  - Attention distribution $\alpha_{t,j} = \text{softmax}(q_t^\top k_j)$
    - Attention output $out_t = \sum_j \alpha_{t,j} v_j$
    - $Y_t = g_2(out_t; \theta)$





Issues of Vanilla Self-Attention

- Attention is order-invariant

- Lack of non-linearities
  - All the weights are simple weighted average

$Y_1, Y_2, \ldots Y_N$

- Capability of autoregressive modeling
  - In generation tasks, the model cannot “look at the future”
  - e.g. Text generation:
    - Y_t can only depend on $X_{i<t}$
    - But vanilla self-attention requires the entire sequence

Position Encoding

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

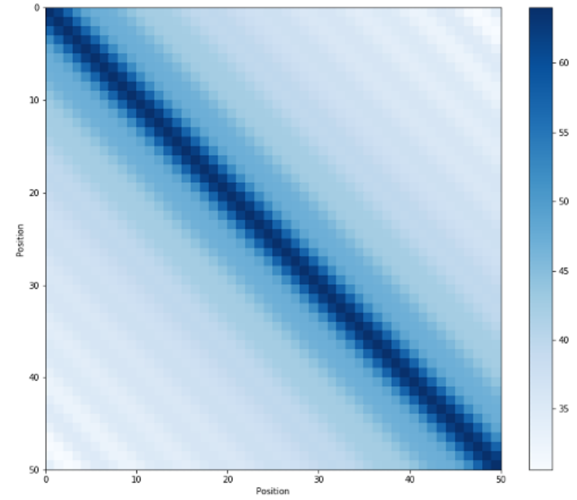
$p_t, \ k, v, q \in \mathbb{R}^d$

- 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

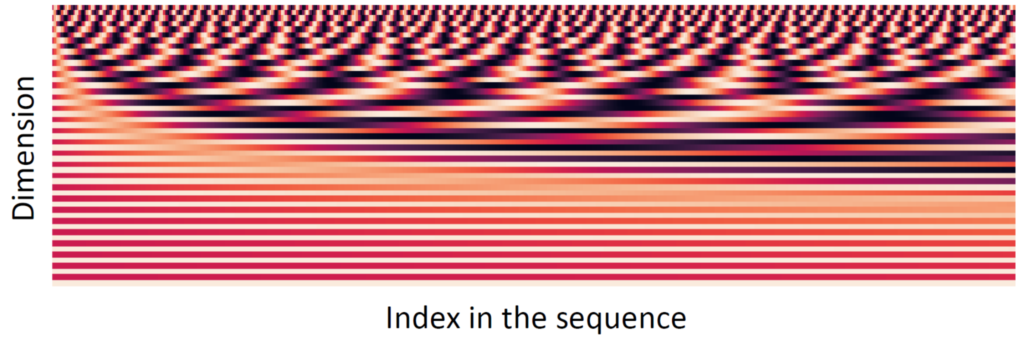
p_t design 1: **Sinusoidal position representation**

- 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

p_t design 2: **Learned representation**

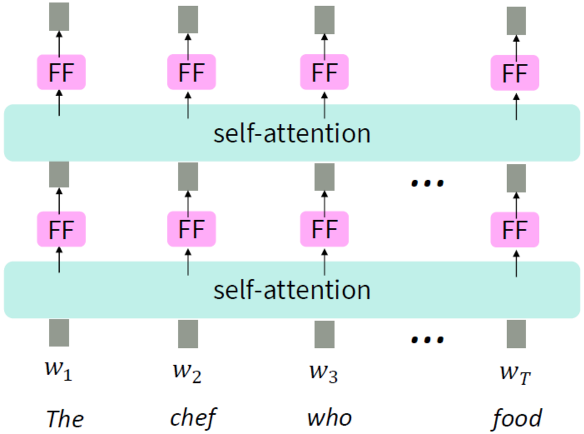
- Assume maximum length L, learn a matrix $p \in \mathbb{R}^{d \times T}$, p_t is a column of p
- Pros:
  - Flexible
  - Learnable and more powerful
- Cons:
  - Need to assume a fixed maximum length L
  - Does not work at all for length above L

- p_t design 3: **Relative position representation** (Shaw, Uszkoreit, Vaswani '18)

Combine Self-Attention with Nonlinearity

- Vanilla self-attention
  - No element-wise activation (e.g., ReLU, tanh)
  - Only weighted average and softmax operator

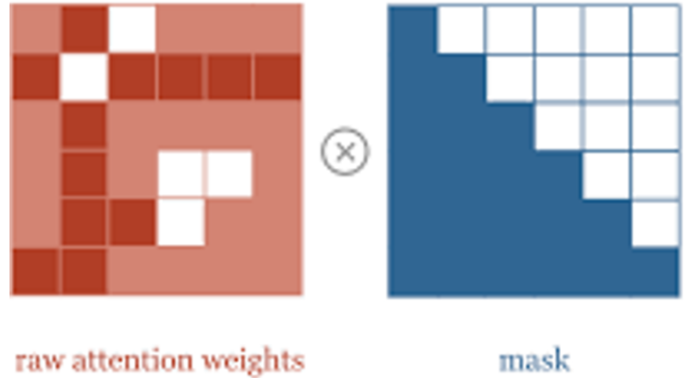
- Fix:
  - Add an MLP to process out_i
  - $m_i = MLP(out_i) = W_2 \text{ReLU}(W_1 out_i + b_1) + b_2$
  - Usually do not put activation layer before softmaax

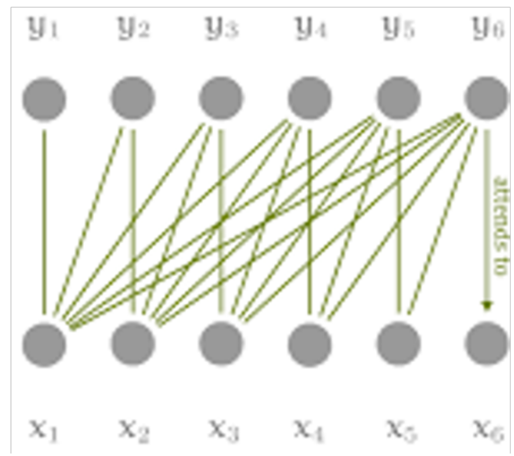


Masked Attention

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

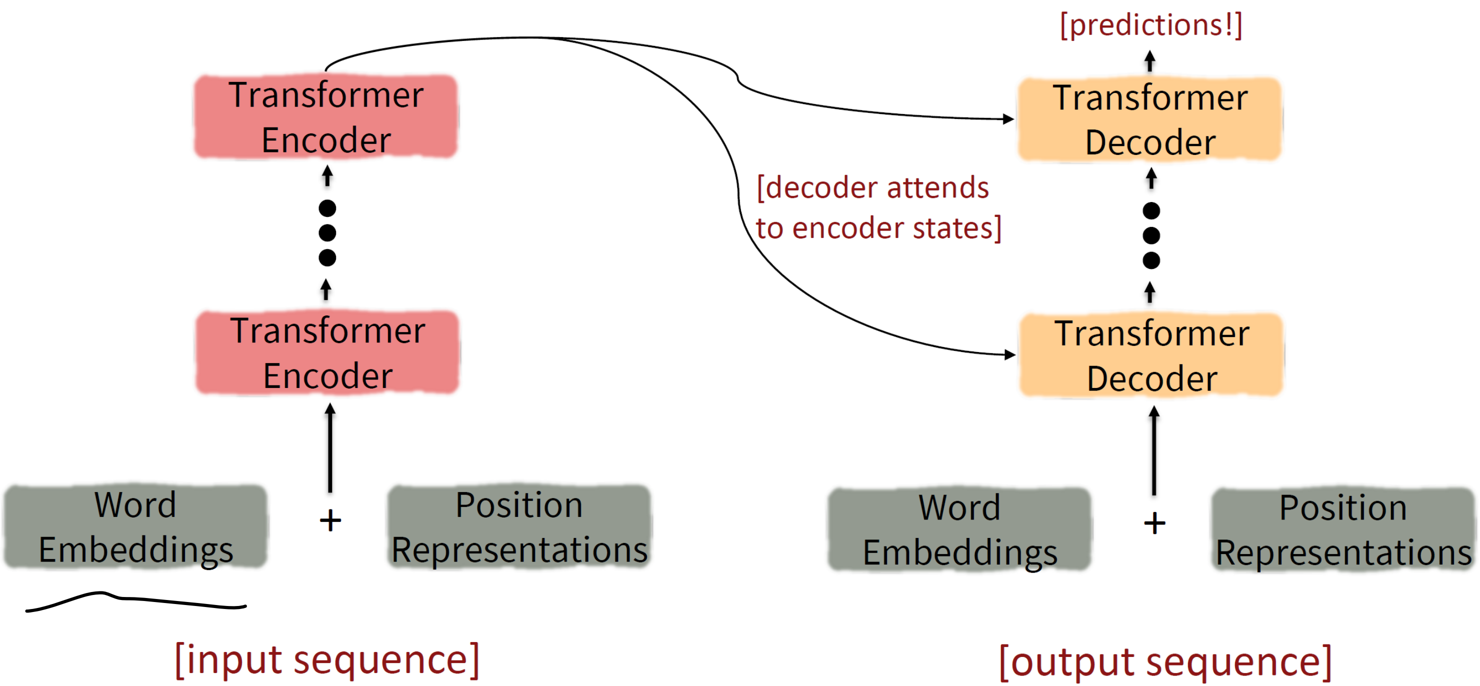
- Masked attention attention score
  - Compute $e_{i,j} = q_i^\top k_j$ as usuall
  - Mask out $e_{i>j}$ by setting $e_{i>j} = -\infty$
    - $e \odot (1-M) \leftarrow -\infty$
    - M is a fixed 0/1 mask matrix
  - Then compute $\alpha_i = \mathrm{softmax}(e_i)$
  - Remarks:
    - $M = 1$ for full self-attention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





Transformer

Transformer-based sequence-to-sequence modeling



word → vector

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
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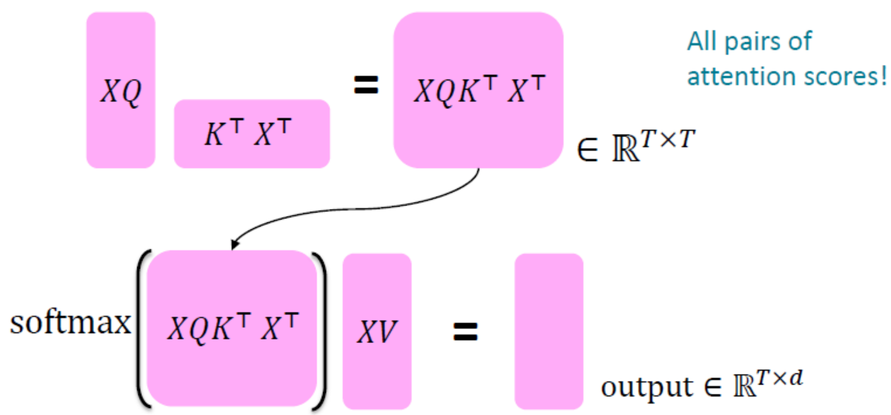
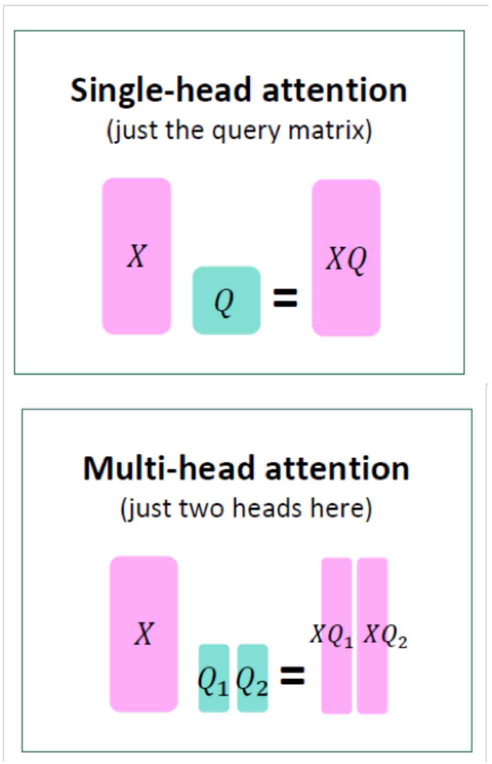


Multi-headed attention

- 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!



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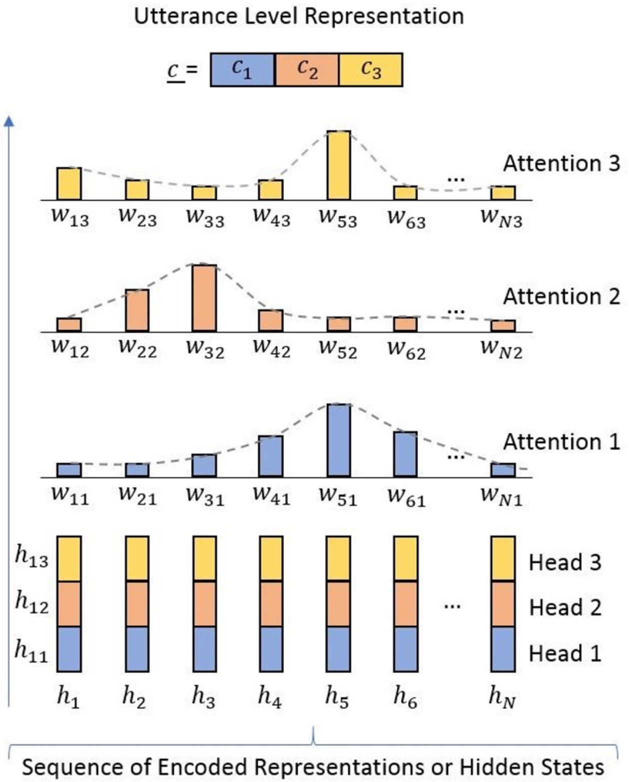
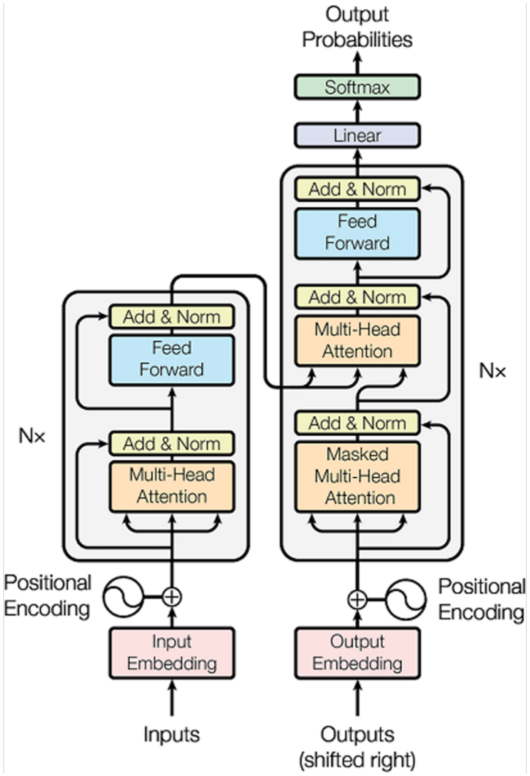


Transformer

Transformer-based sequence-to-sequence model

- Basic building blocks: self-attention
  - Position encoding
  - Post-processing MLP
  - Attention mask

- Enhancements:
  - Key-query-value attention
  - Multi-headed attention
  - Architecture modifications:
    - Residual connection
    - Layer normalization



Transformer

Machine translation with transformer

Model	BLEU		Training Cost (FLOPs)	
	EN-DE	EN-FR	EN-DE	EN-FR
ByteNet [18]	23.75			
Deep-Att + PosUnk [39]		39.2		$1.0 \cdot 10^{20}$
GNMT + RL [38]	24.6	39.92	$2.3 \cdot 10^{19}$	$1.4 \cdot 10^{20}$
ConvS2S [9]	25.16	40.46	$9.6 \cdot 10^{18}$	$1.5 \cdot 10^{20}$
MoE [32]	26.03	40.56	$2.0 \cdot 10^{19}$	$1.2 \cdot 10^{20}$
Deep-Att + PosUnk Ensemble [39]		40.4		$8.0 \cdot 10^{20}$
GNMT + RL Ensemble [38]	26.30	41.16	$1.8 \cdot 10^{20}$	$1.1 \cdot 10^{21}$
ConvS2S Ensemble [9]	26.36	**41.29**	$7.7 \cdot 10^{19}$	$1.2 \cdot 10^{21}$
Transformer (base model)	27.3	38.1	$\mathbf{3.3 \cdot 10^{18}}$	
Transformer (big)	**28.4**	**41.8**	$2.3 \cdot 10^{19}$	

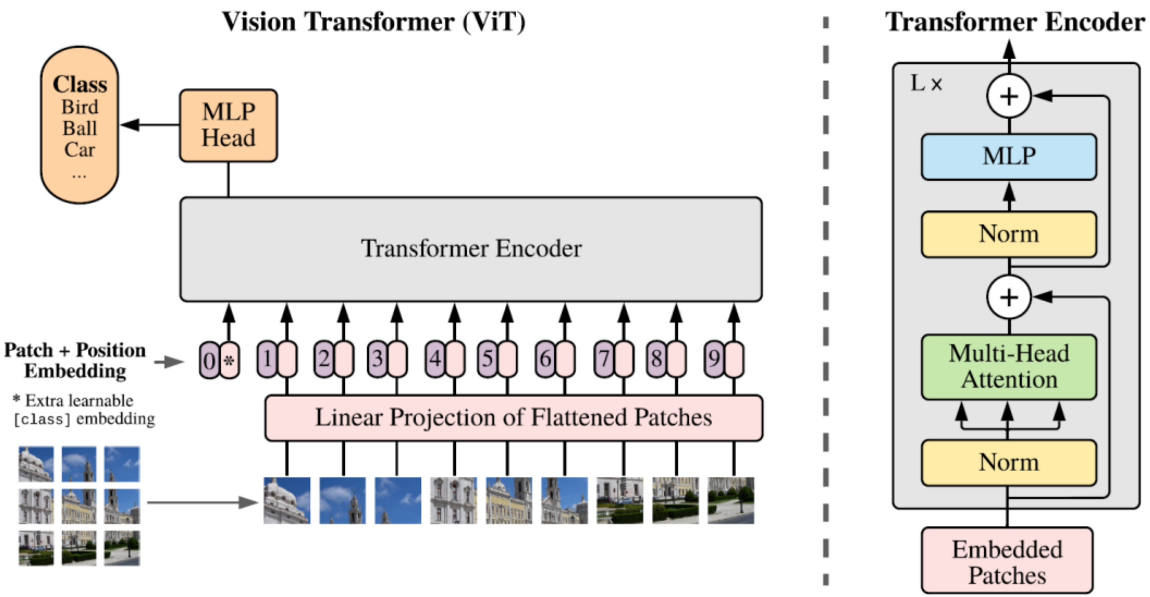
Transformer

- Limitations of transformer: Quadratic computation cost
  - Linear for RNNs
  - Large cost for large sequence length, e.g., $L > 10^4$

- Follow-ups:
  - Large-scale training: transformer-XL; XL-net (‘20)
  - Projection tricks to $O(L)$: Linformer ('20)
  - Math tricks to $O(L)$: Performer (‘20)
  - Sparse interactions: Big Bird (‘20)
  - Deeper transformers: DeepNet (’22)

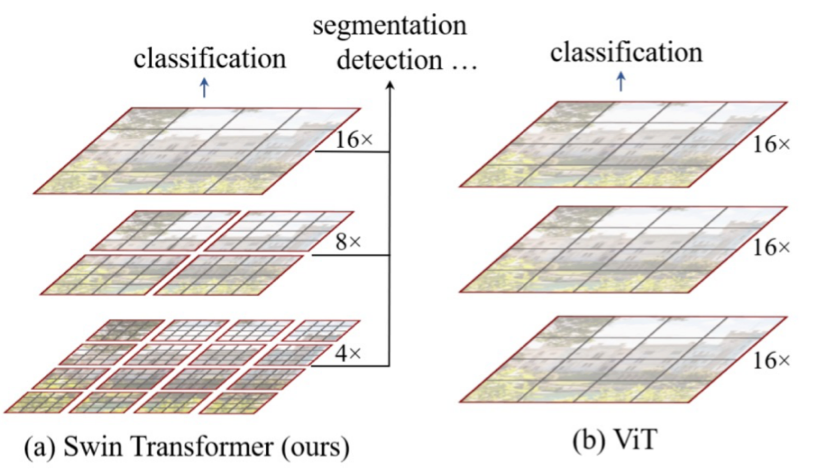
Transformer for Images

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



Transformer for Images

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



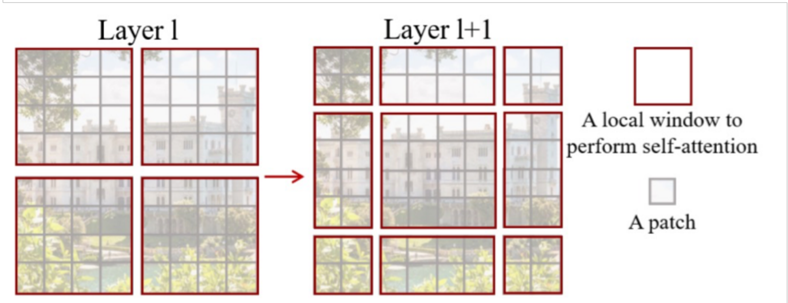
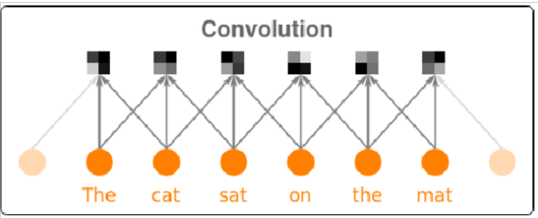
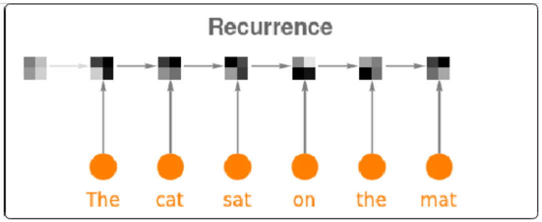
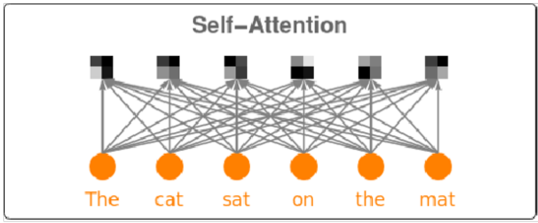


Figure 2. An illustration of the *shifted window* approach for com-

CNN vs. RNN vs. Attention







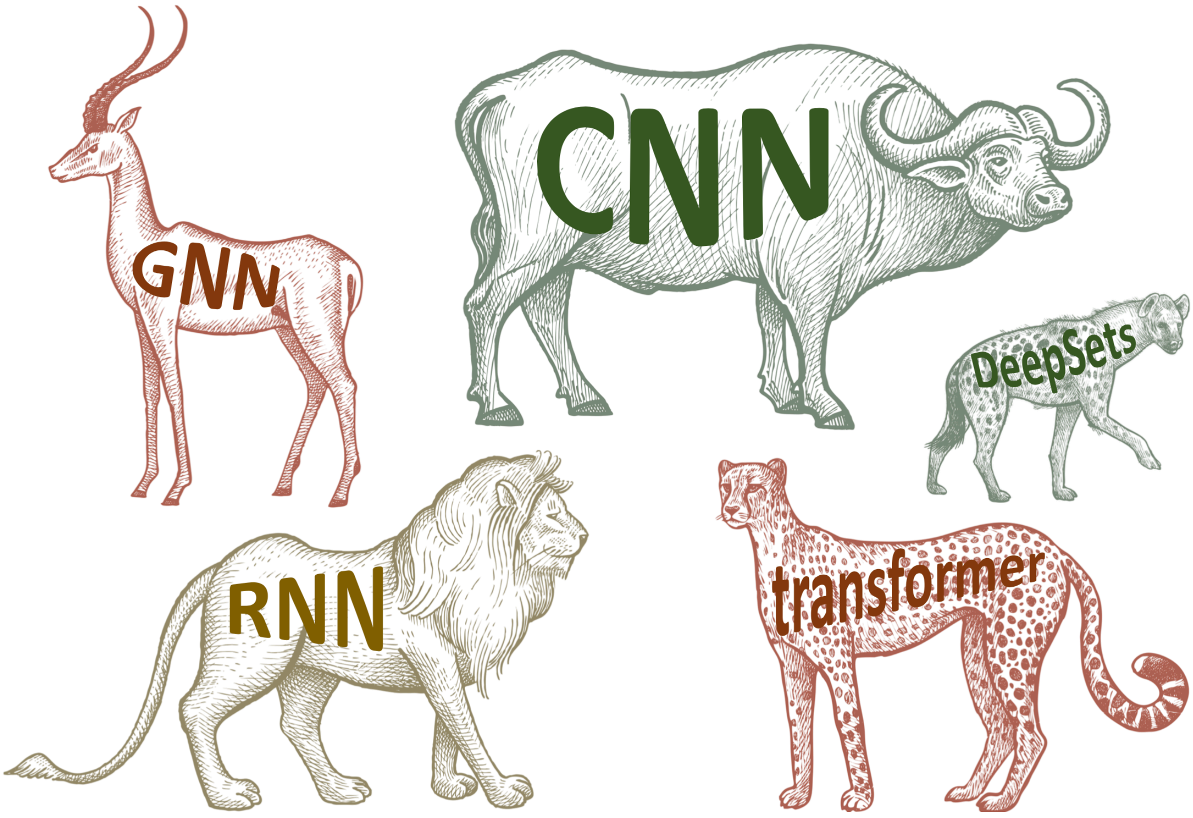
Summary

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

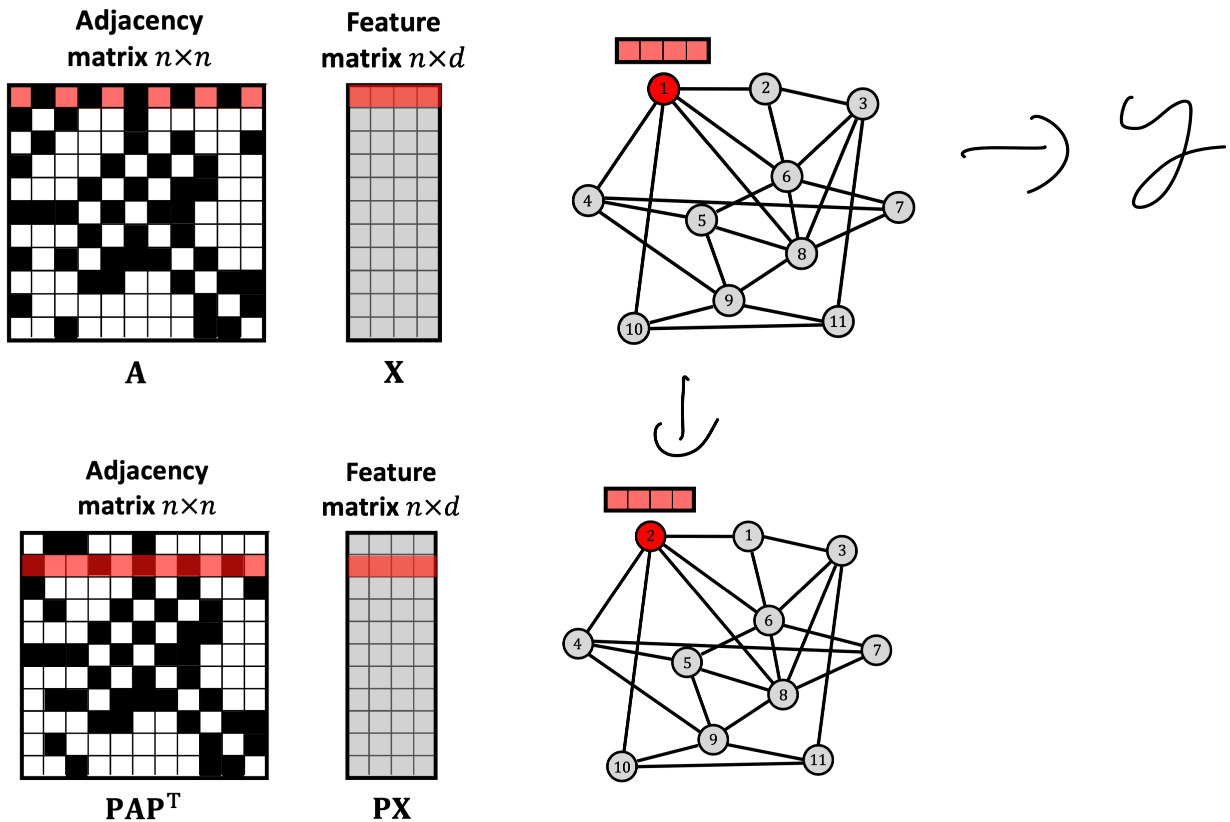
- Attention mechanism
  - So far the most successful idea for sequence data in deep learning
  - A scale/order-invariant representation
  - Transformer: a fully attention-based architecture for sequence data
  - Transformer + Pretraining: the core idea in today's NLP tasks

- LSTM is still useful in lightweight scenarios

Other architectures



Graph Neural Networks

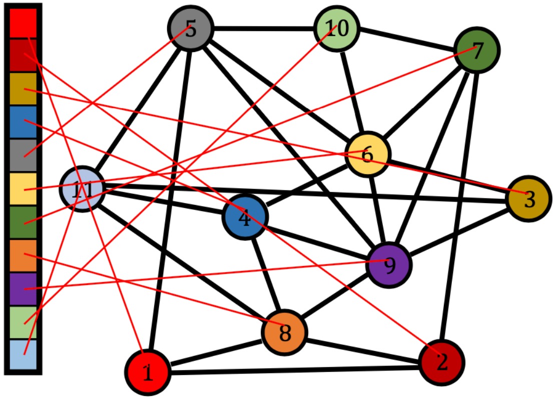


arbitrary ordering of nodes

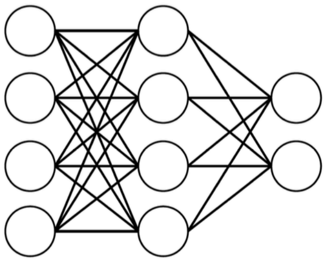
Graph Neural Networks

permutation-equivariant

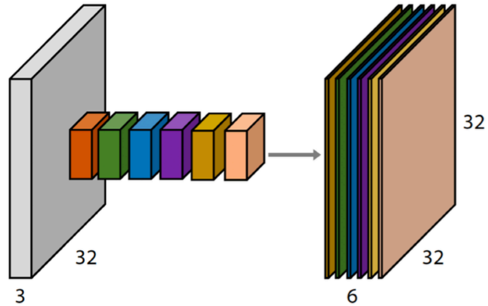
$$\mathbf{F}\left(\mathbf{PX}, \mathbf{PAP}^\top\right) = \mathbf{PF}(\mathbf{X}, \mathbf{A})$$



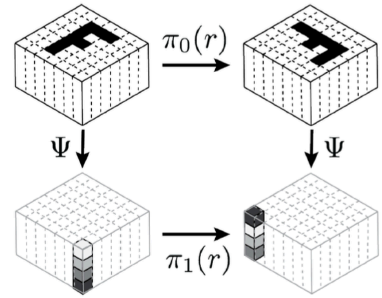
Geometric Deep Learning



Perceptrons
Function regularity

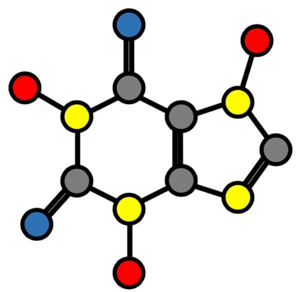


CNNs
Translation



Group-CNNs
Translation+Rotation

DeepSets / Transformers
Permutation



GNNs
Permutation

Intrinsic CNNs
Local frame choice