EECE 571F: Advanced Topics in Deep Learning

Lecture 2: Invariance, Equivariance, and Deep Learning Models for Sets/Sequences

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University of British Columbia

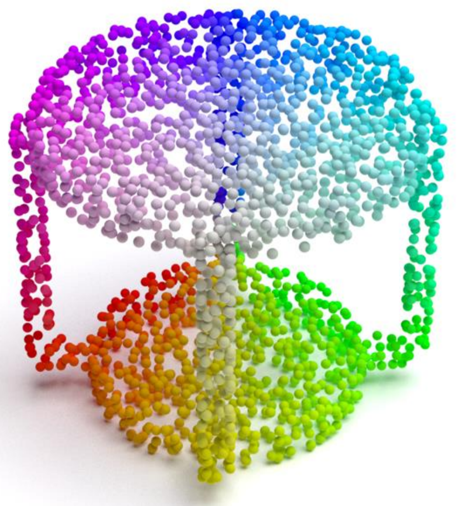
Winter, Term 2, 2025

Outline

- Invariance & Equivariance Principle
  - Translation equivariance in convolutions
  - Permutation equivariance and invariance
- Models for Sets
  - DeepSets: representation theorem of permutation-invariant set functions & architecture
  - DeepSets: permutation-equivariant linear mapping & architecture
- Models for Sequences
  - Transformers
  - Positional encoding vs. Rotary Positional Embeddings (RoPE)
  - Attention & Flash Attention
  - Pre-norm vs. post-norm
  - Vision Transformers (ViT) & Swin Transformers

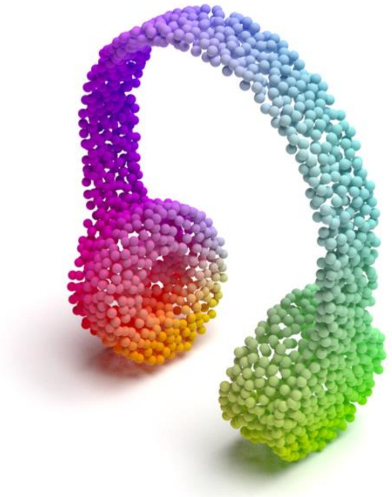
Motivating Applications for Sets

- Population Statistics
- Point Cloud Classification



Table

Airplane



Earphone

Image Credit: https://github.com/AnTao97/PointCloudDatasets

Invariance & Equivariance

- Invariance:

A mathematical object (or a class of mathematical objects) remains unchanged after operations or transformations of a certain type are applied to the objects

$$f(X) = f(g(X))$$

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- Equivariance:

Applying a transformation and then computing the function produces the same result as computing the function and then applying the transformation

$$g(f(X)) = f(g(X))$$

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Revisit Convolution

Matrix multiplication views of (discrete) convolution:

- Filter => Toeplitz matrix
- Data => Toeplitz matrix

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Consider a special Toeplitz matrix: circulant matrix (must be square!)

Convolution with padding

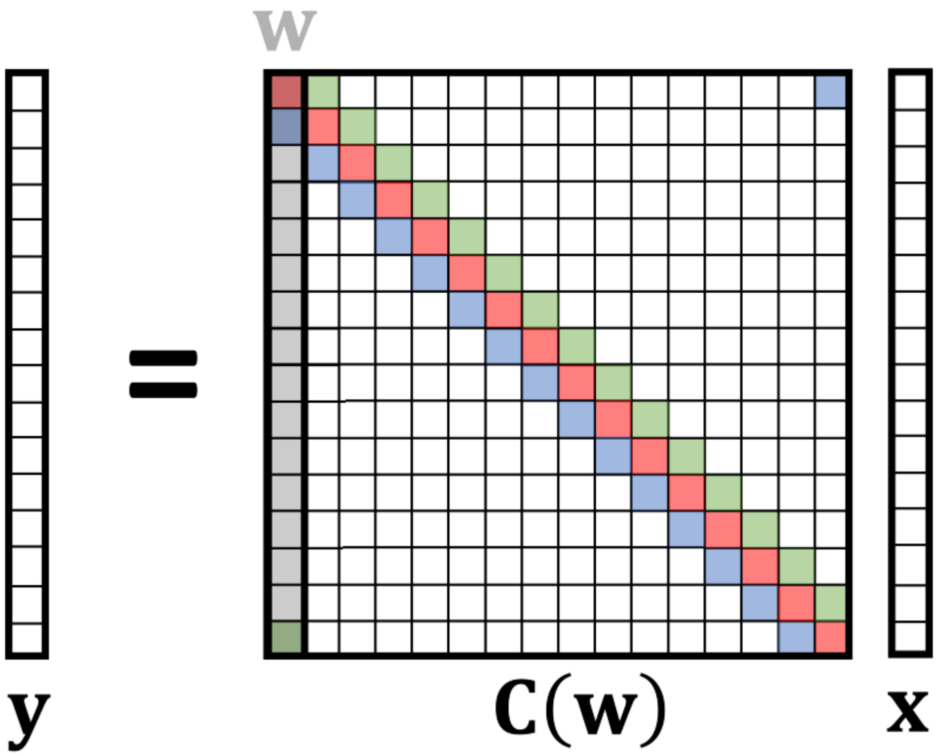
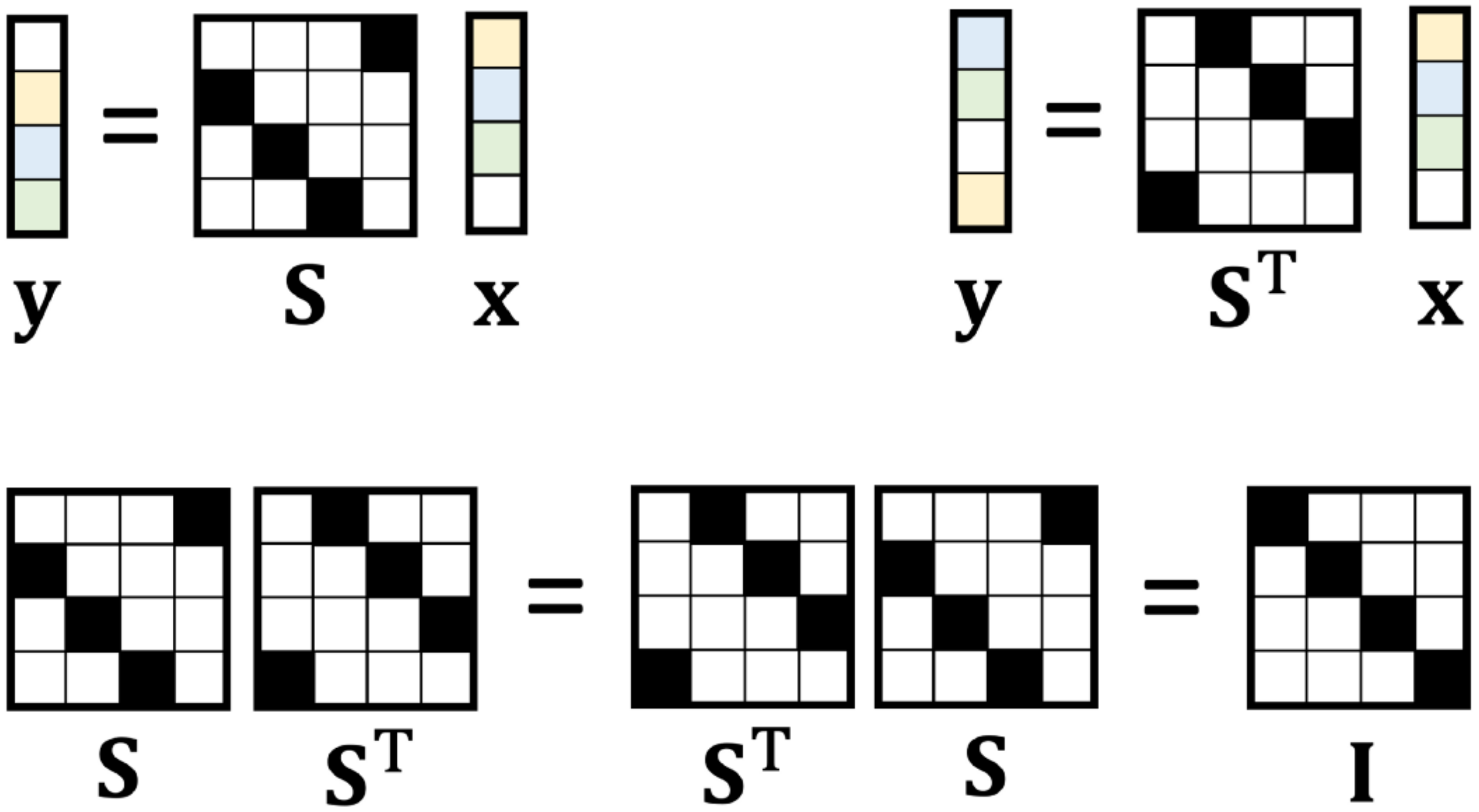


Image Credit: https://towardsdatascience.com/deriving-convolution-from-first-principles-4ff124888028

Translation/Shift Operator



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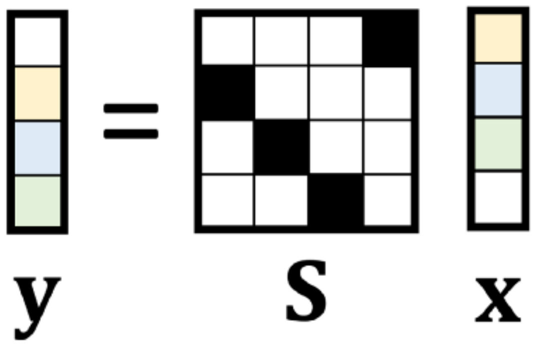
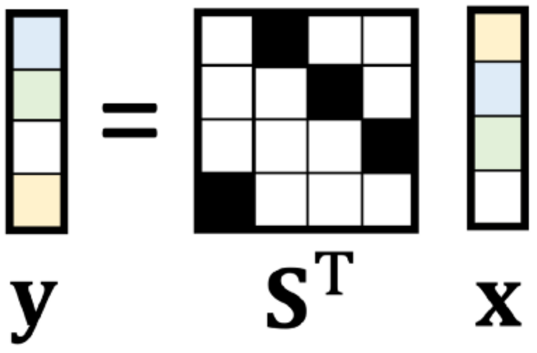
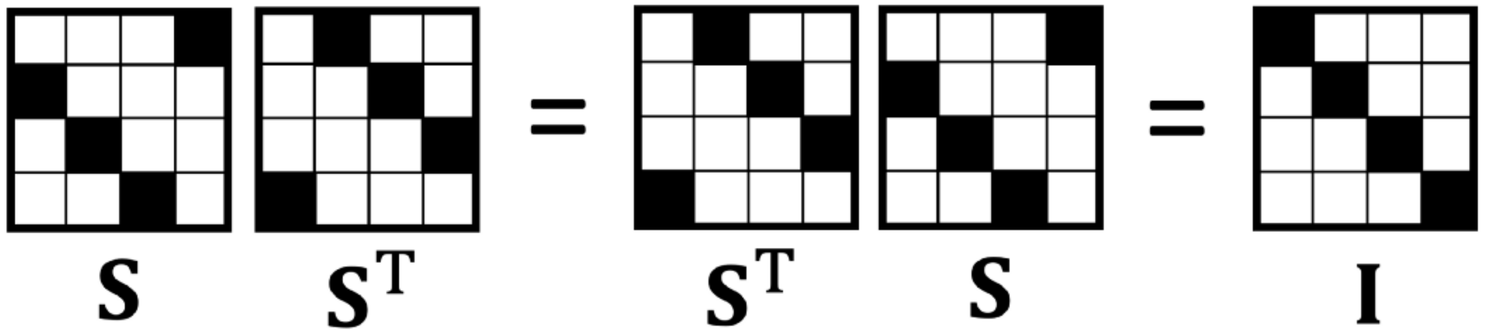
Translation/Shift Operator

Shift operator is also a circulant matrix!







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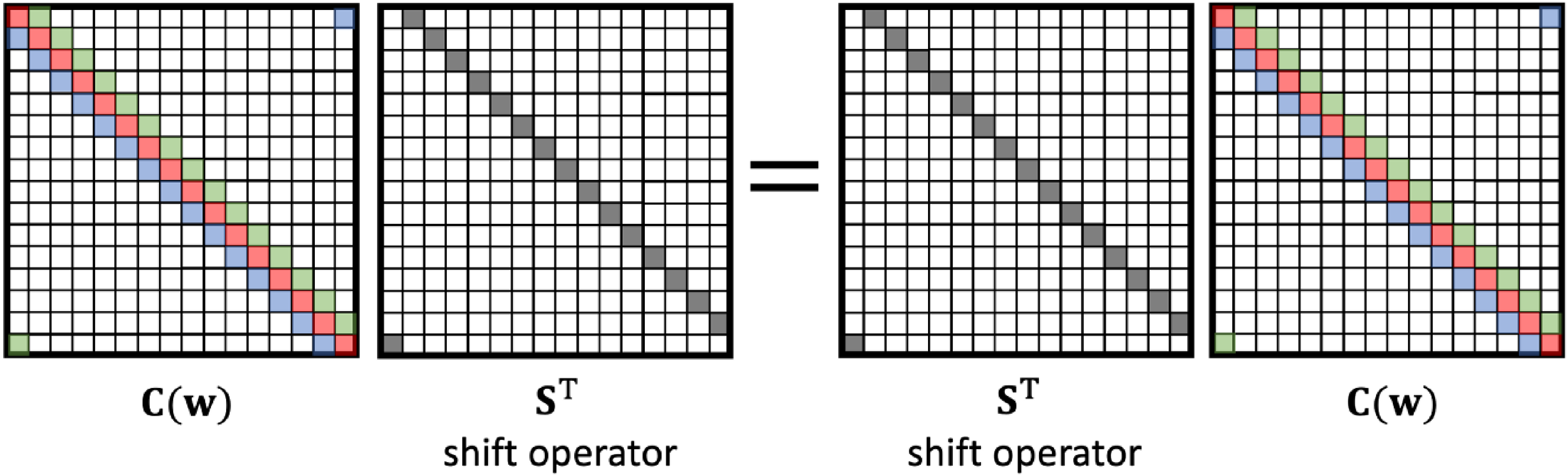
Translation/Shift Equivariance

Matrix multiplication is non-commutative. But not for circulant matrices!



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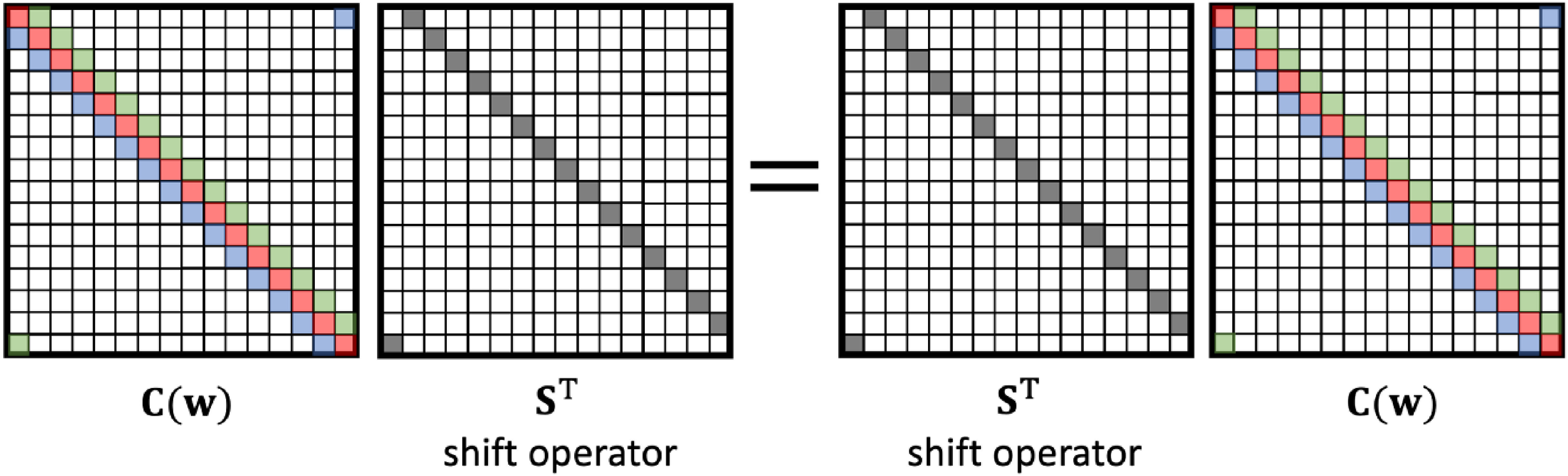


Convolution is translation equivariant, i.e., Conv(Shift(X)) = Shift(Conv(X))!

Image Credit: https://towardsdatascience.com/deriving-convolution-from-first-principles-4ff124888028

Translation/Shift Invariance

Global pooling gives you shift-invariance!

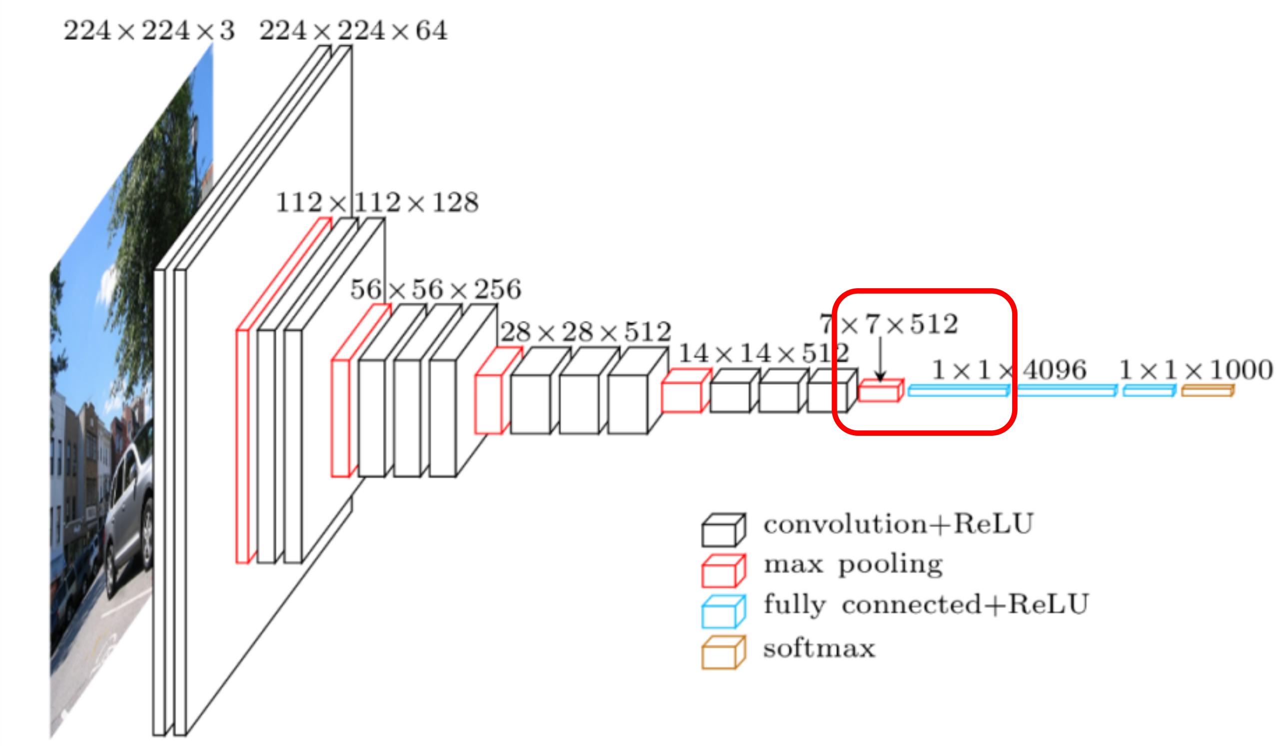
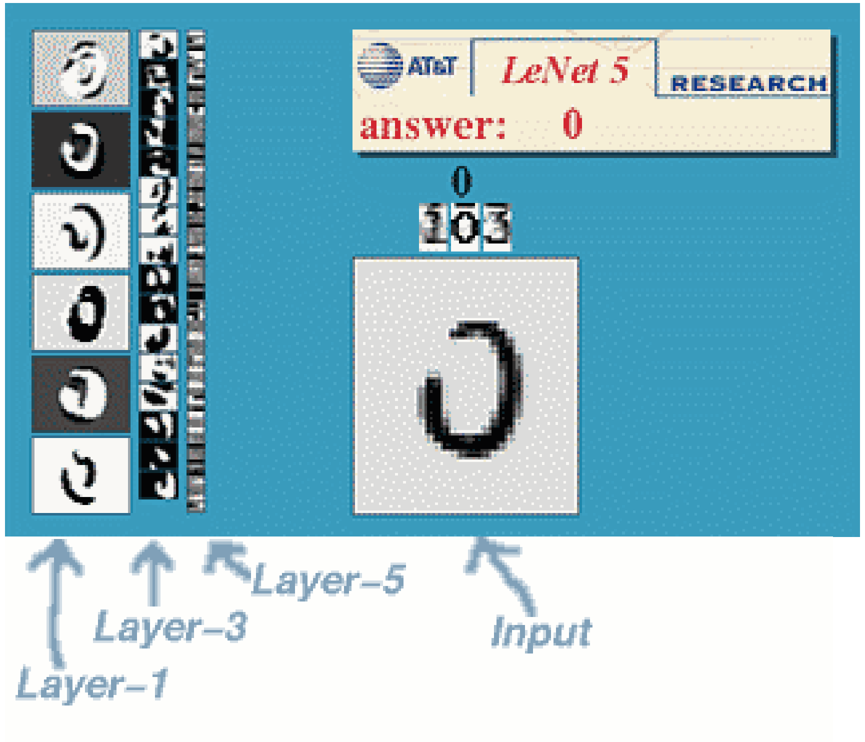


Image Credit: https://towardsdatascience.com/covolutional-neural-network-cb0883dd6529

Translation/Shift Equivariance Invariance

Yann LeCun's LeNet Demo:



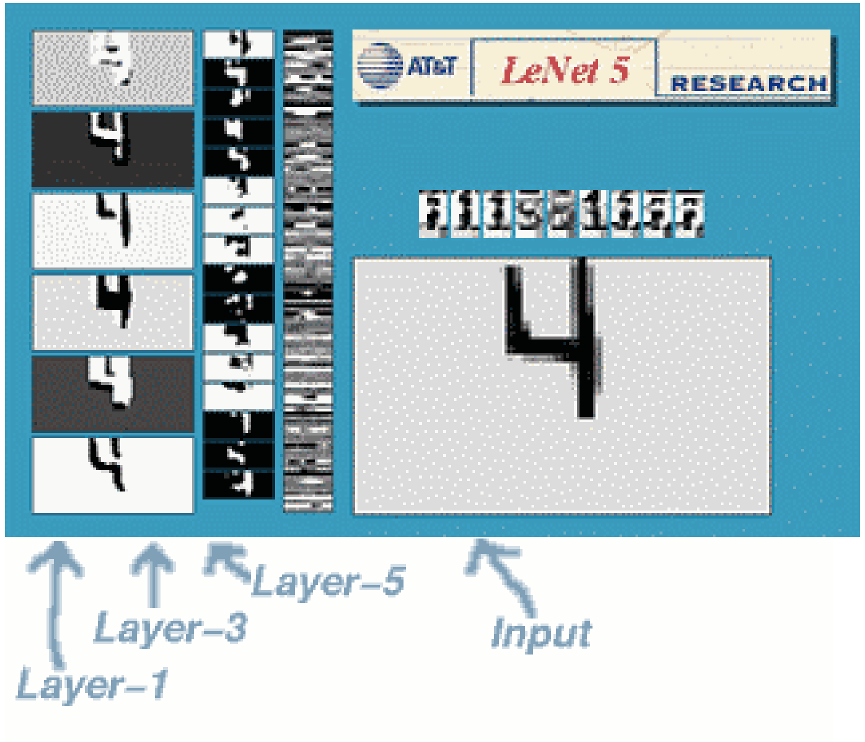


Image Credit: http://yann.lecun.com/exdb/lenet/translation.html

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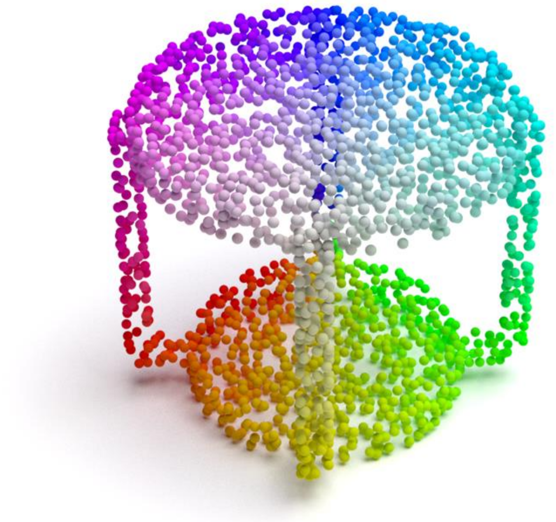
Permutation Invariance



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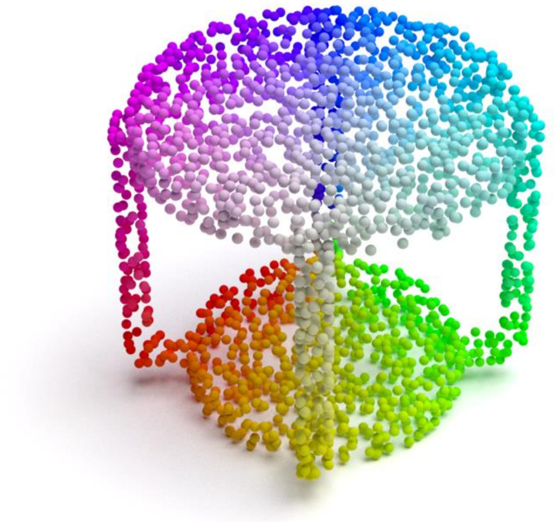
Point Clouds $X \in \mathbb{R}^{n \times 3}$

Probability of Classes $Y \in \mathbb{R}^{1 \times K}$

Permutation / Shuffle $P \in \mathbb{R}^{n \times n}$

Image Credit: https://github.com/AnTao97/PointCloudDatasets

Permutation Invariance



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$$\begin{bmatrix} 2 \\ 5 \\ 3 \\ 1 \\ 4 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{bmatrix}$$

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Geometric Interpretation of Permutation Matrix

Birkhoff Polytope

$$B_n = \{P \in \mathbb{R}^{n\times n} | \forall i \forall j \ P_{ij} \geq 0, \forall i \ \sum_j P_{ij} = 1, \forall j \ \sum_i P_{ij} = 1\}$$

Doubly Stochastic Matrix

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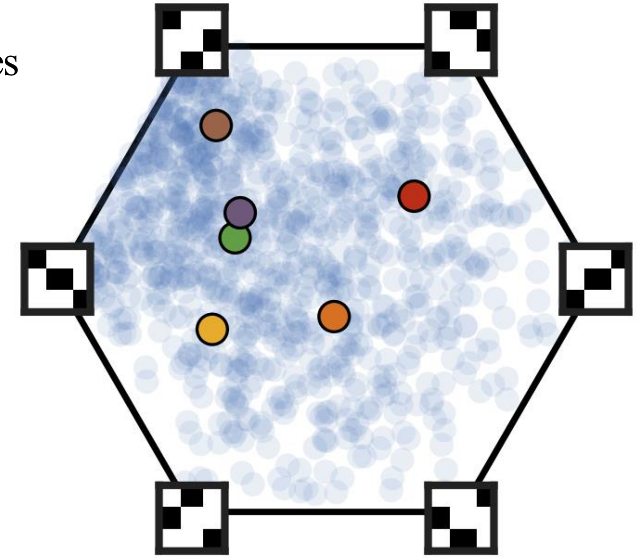

Image Credit: https://arxiv.org/pdf/1710.09508.pdf

Permutation Invariance

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$$Y = f(PX) \qquad \forall P \in S_n$$

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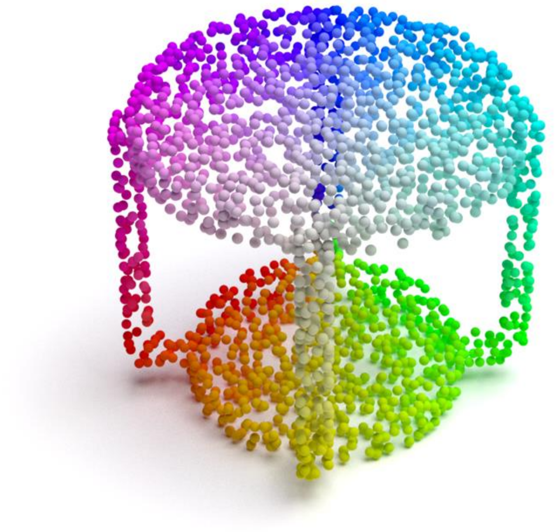
Permutation Equivariance



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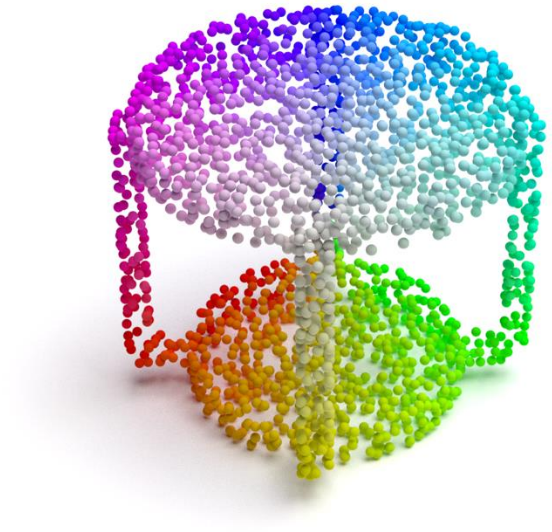

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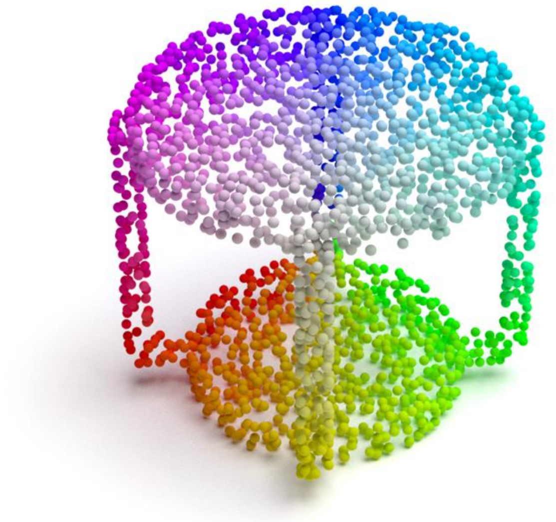

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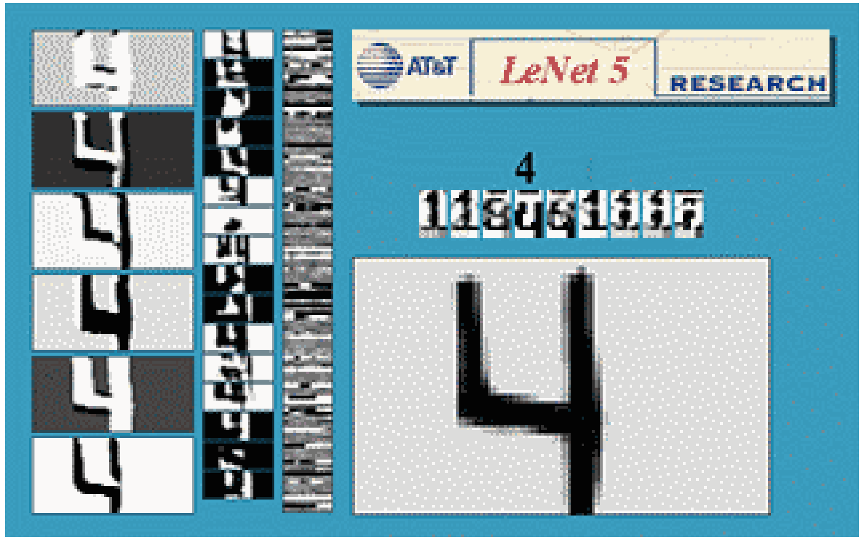
More on Invariance & Equivariance

- What about other transformations, e.g., scaling, 2D/3D rotations, Gauge transformation?



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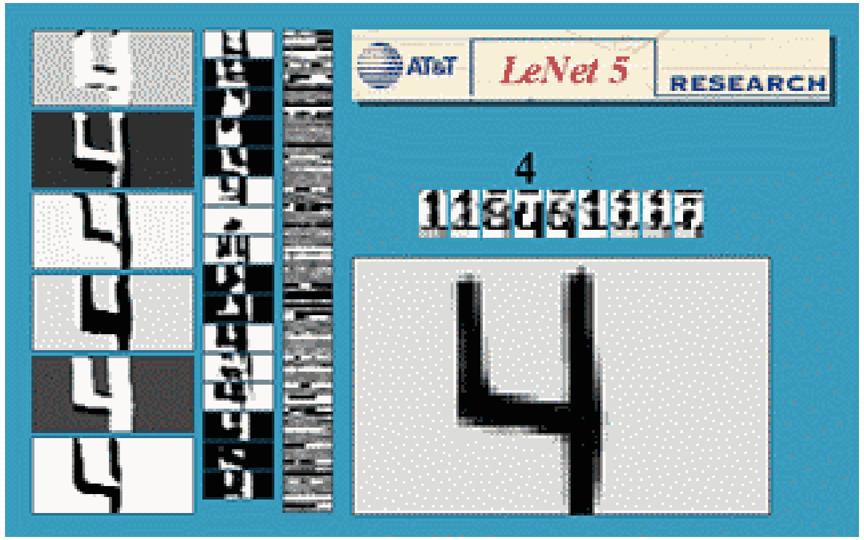

- Generalize to Group Invariance & Equivariance

Recommend Taco Cohen's PhD Thesis: https://pure.uva.nl/ws/files/60770359/Thesis.pdf

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Deep Learning for Sets

- Point-level Tasks

    Input: a vector per point

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- Set-level Tasks

  Input: a set of vectors, each corresponds to a point

  Output: a label/vector per set

  Prediction of a set depends on all points, e.g., point cloud classification

Deep Learning for Sets

Key Challenges:

- Varying-sized input sets
- Permutation equivariant and invariant models
- Expressive models

Deep Learning for Sets

- Deep Sets [1]

Theorem 2 *A function* $f(X)$ *operating on a set* X *having elements from a countable universe, is a valid set function,* i.e., ***invariant*** *to the permutation of instances in* X*, iff it can be decomposed in the form* $\rho\left(\sum_{x\in X}\phi(x)\right)$*, for suitable transformations* ϕ *and* ρ*.*

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Sketch of Proof

Sufficiency: summation is permutation invariant!

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Then the size-$|\mathfrak{X}|$ binary string of set $X_1 = \{1\}$ is $b_1 = 10\dots$ and its binary expansion is $\sum_{x \in X_1} \phi(x) = \sum_{i=1} \frac{b_1[i]}{2^i} = \frac{1}{2} = 0.5$

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Then the binary string of set $X_2 = \{2, 3, \dots\}$ is $b_2 = 011\dots$ and its binary expansion is $\sum_{x \in X_2} \phi(x) = \sum_{i=1}^{\infty} \frac{b_2[i]}{2^i} = \sum_{i=2}^{\infty} \frac{1}{2^i} = 0.5$

Deep Learning for Sets

Necessity:

1. Construct a mapping $c : \mathfrak{X} \to \mathbb{N}$
2. Let $\phi(x) = 4^{-c(x)}$
3. Injection $X \in 2^{\mathfrak{X}} \to \sum_{x \in X} \phi(x)$

Why base 4?

For better illustrate the problem, let us switch to base 2, i.e., $\phi(x) = 2^{-c(x)}$.

Therefore, the above “injection” essentially maps the binary string to a real number via the binary expansion.

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Dyadic rationals do not have unique binary expansions!

Deep Learning for Sets

Suppose we use base B, where B > 1. the value of a tail of a geometric series starting from index n+1 is:

$$\sum_{i=n+1}^{\infty} B^{-i} = \frac{B^{-(n+1)}}{1 - B^{-1}} = \frac{B^{-(n+1)}}{\frac{B-1}{B}} = \frac{1}{B^n(B-1)}$$

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We want to ensure that even if a set X contains every single element from index n+1 onwards, its sum still cannot "reach" the value of the n-th element alone. This requires:

$$\phi(x_n) > \sum_{i=n+1}^{\infty} \phi(x_i)$$

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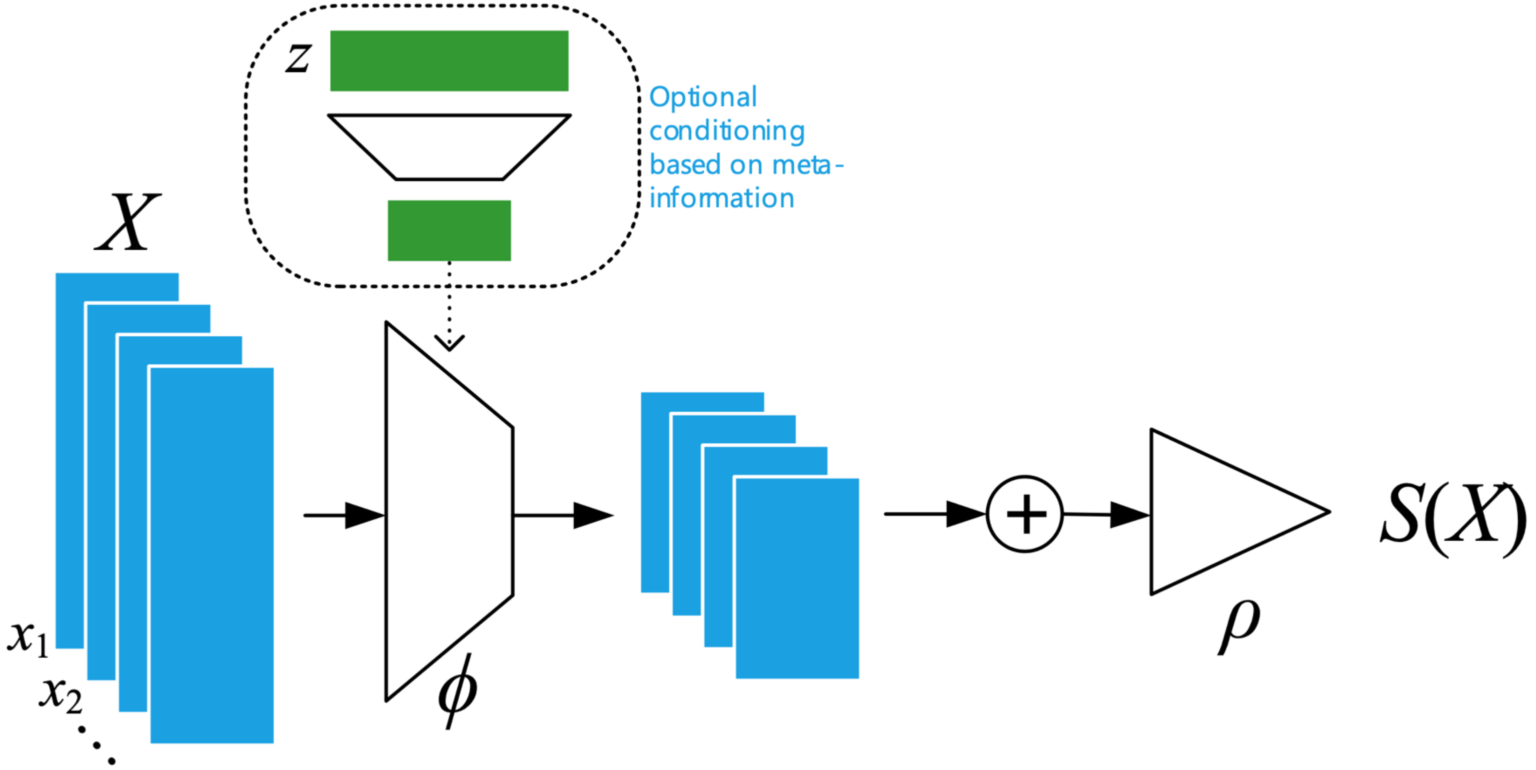
If we simplify this inequality, we get: $1 > \frac{1}{B-1} \implies B - 1 > 1 \implies B > 2$

Therefore, any base greater than 2 works!

Deep Learning for Sets

- Deep Sets [1]

Invariant Architecture



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Outline

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    - Translation equivariance in convolutions
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Deep Learning for Sets

- Deep Sets [1] $\mathbf{f}_\Theta(\mathbf{x}) \doteq \boldsymbol{\sigma}(\Theta\mathbf{x}) \quad \Theta \in \mathbb{R}^{M\times M}$

Lemma 3 *The function* $\mathbf{f}_\Theta : \mathbb{R}^M \to \mathbb{R}^M$ *defined above is permutation* ***equivariant*** *iff all the off-diagonal elements of* Θ *are tied together and all the diagonal elements are equal as well. That is,*

$\Theta = \lambda\mathbf{I} + \gamma\left(\mathbf{1}\mathbf{1}^\mathsf{T}\right) \qquad \lambda, \gamma \in \mathbb{R} \quad \mathbf{1} = [1,\ldots,1]^\mathsf{T} \in \mathbb{R}^M \qquad \mathbf{I} \in \mathbb{R}^{M\times M}$ *is the identity matrix*

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Sketch of Proof

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1. All diagonal elements are identical

   $\pi_{k,l}\Theta = \Theta\pi_{k,l} \;\Rightarrow\; \pi_{k,l}\Theta\pi_{l,k} = \Theta \;\Rightarrow\; (\pi_{k,l}\Theta\pi_{l,k})_{l,l} = \Theta_{l,l} \;\Rightarrow\; \Theta_{k,k} = \Theta_{l,l}$

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2. All off-diagonal elements are identical

$$\pi_{j',j}\pi_{i,i'}\Theta = \Theta\pi_{j',j}\pi_{i,i'} \;\Rightarrow \pi_{j',j}\pi_{i,i'}\Theta(\pi_{j',j}\pi_{i,i'})^{-1} = \Theta \qquad \Rightarrow$$
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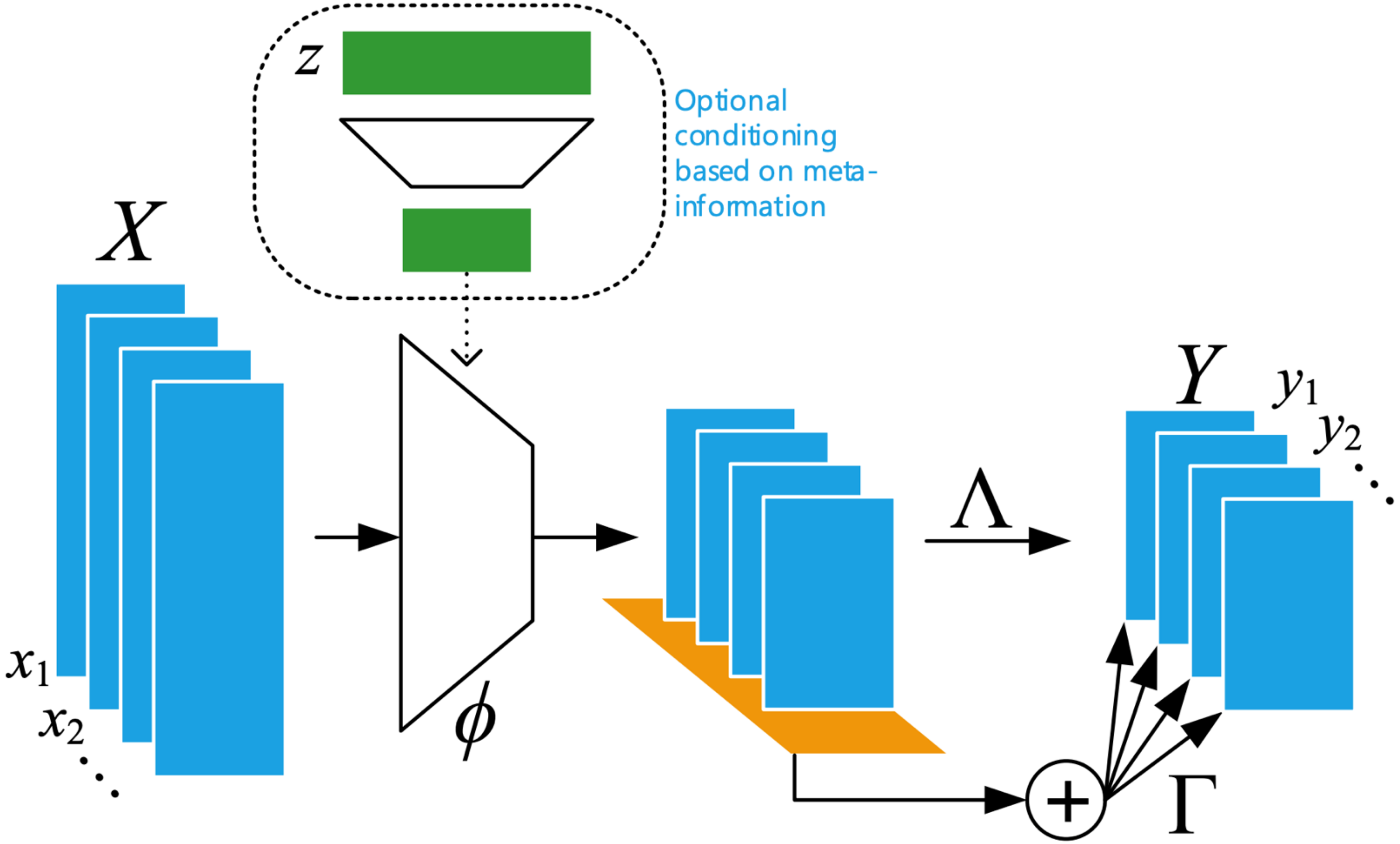
Deep Learning for Sets

- Deep Sets [1]

Equivariant Architecture

$$f(\mathbf{x}) = \sigma\left(\mathbf{x}\Lambda - \mathbf{1}\mathbf{1}^{\mathsf{T}}\mathbf{x}\Gamma\right)$$



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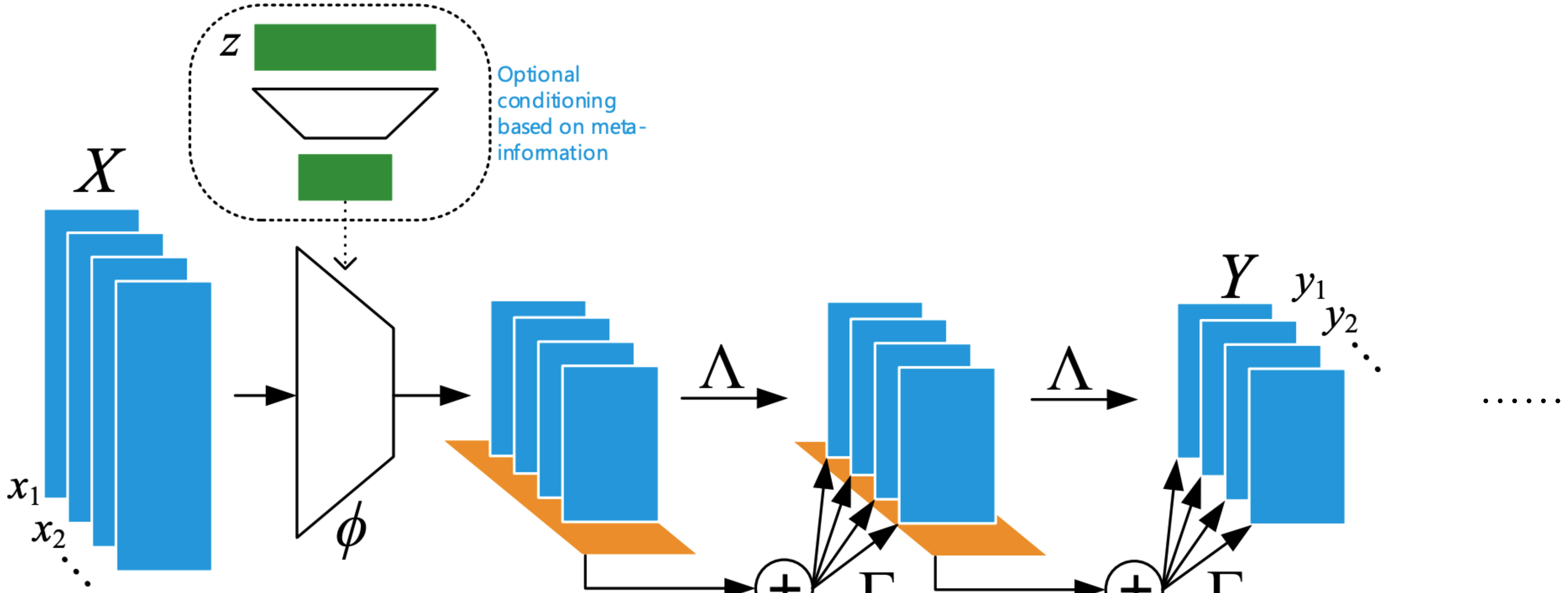
Deep Learning for Sets

- Deep Sets [1]

Recipe for making the model deep:

Stack multiple equivariant layers (+ invariant layer at the end), e.g., PointNet [2]



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Deep Learning for Sequences

- Language Models

$$P(\boldsymbol{x}^{(t+1)} \mid \boldsymbol{x}^{(t)}, \ldots, \boldsymbol{x}^{(1)})$$

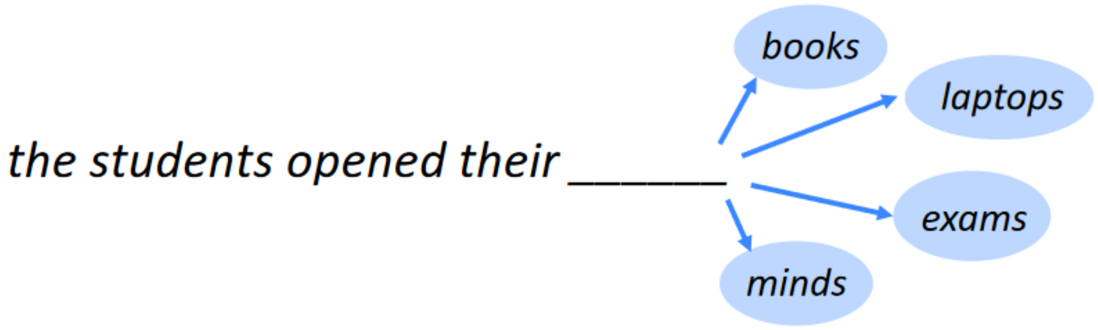

Image Credit: http://web.stanford.edu/class/cs224n/

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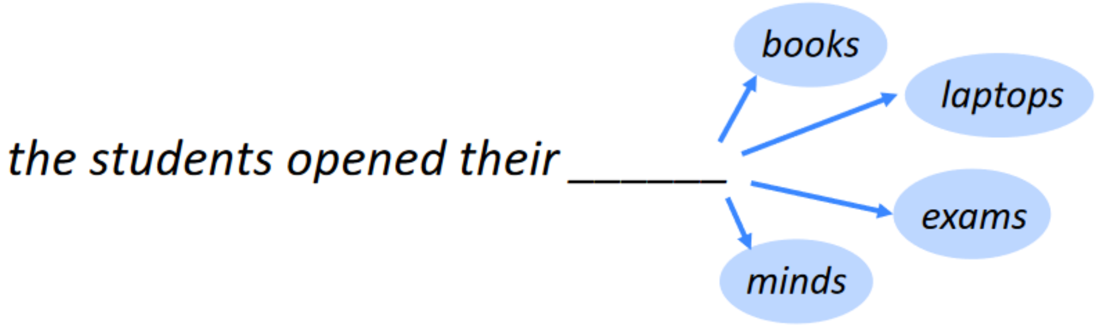

- Machine Translation

Image Credit: http://web.stanford.edu/class/cs224n/ https://jalammar.github.io/illustrated-transformer/

Deep Learning for Sequences

Key Challenges:

- Varying-sized input sequences

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Aoccdrnig to a rscheearch at Cmabrigde Uinervtisy, it deosn't mttaer in waht oredr the ltteers in a wrod are, the olny iprmoetnt tihng is taht the frist and lsat ltteer be at the rghit pclae. The rset can be a toatl mses and you can sitll raed it wouthit porbelm. Tihs is bcuseae the huamn mnid deos not raed ervey lteter by istlef, but the wrod as a wlohe.

Image Credit: https://www.mrc-cbu.cam.ac.uk/people/matt.davis/cmabridge

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LSTM [1]
GRU [2]
Seq2Seq [3]
Transformer [4]

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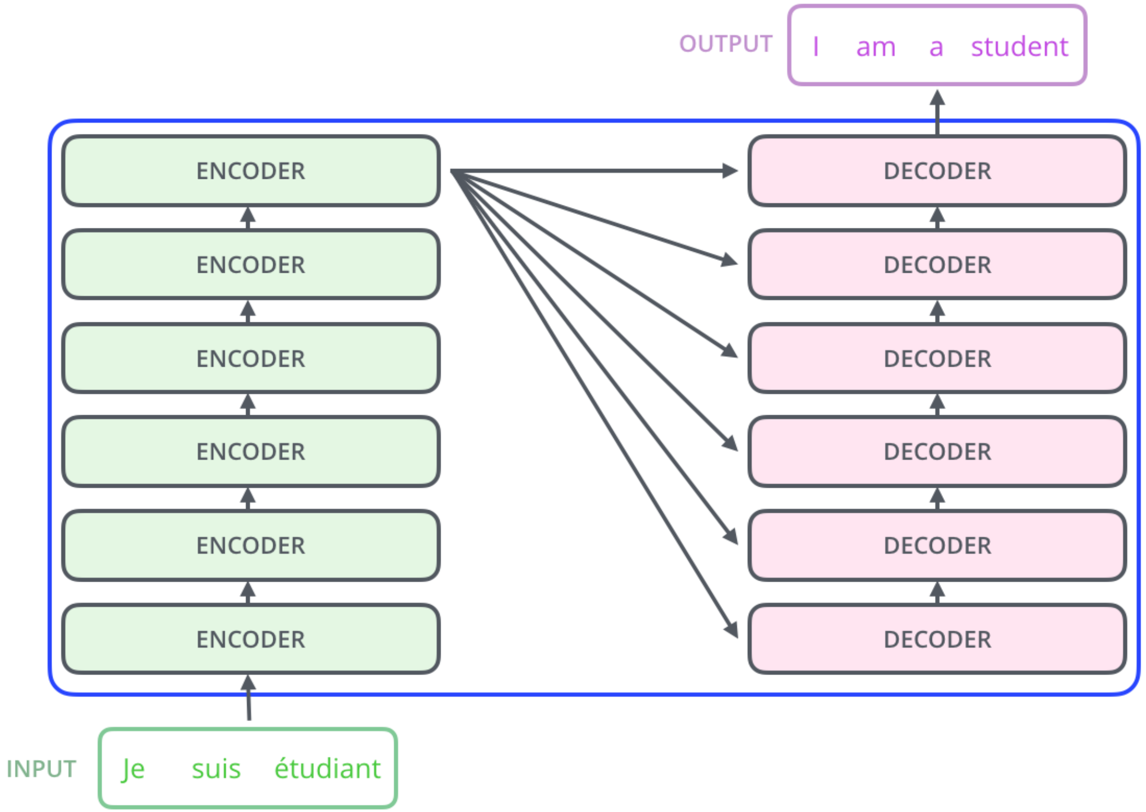
[1] Hochreiter, S. "Long Short-term Memory." Neural Computation MIT-Press (1997). [2] Cho, Kyunghyun. "Learning phrase representations using RNN encoder-decoder for statistical machine translation." arXiv preprint arXiv:1406.1078 (2014). [3] Sutskever, I. "Sequence to Sequence Learning with Neural Networks." arXiv preprint arXiv:1409.3215 (2014). [4] Vaswani, A. "Attention is all you need." Advances in Neural Information Processing Systems (2017).

Transformers



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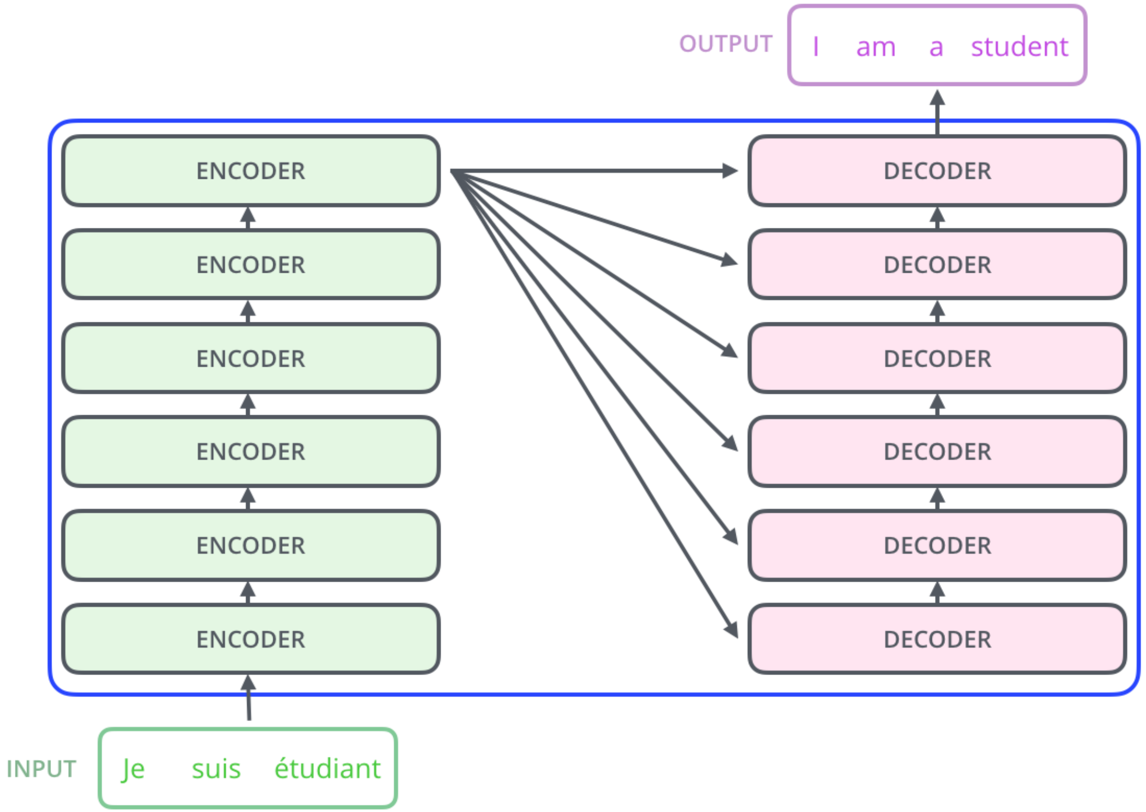

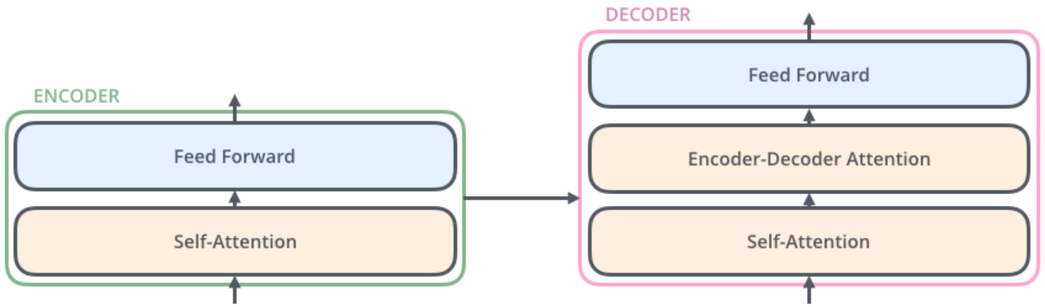

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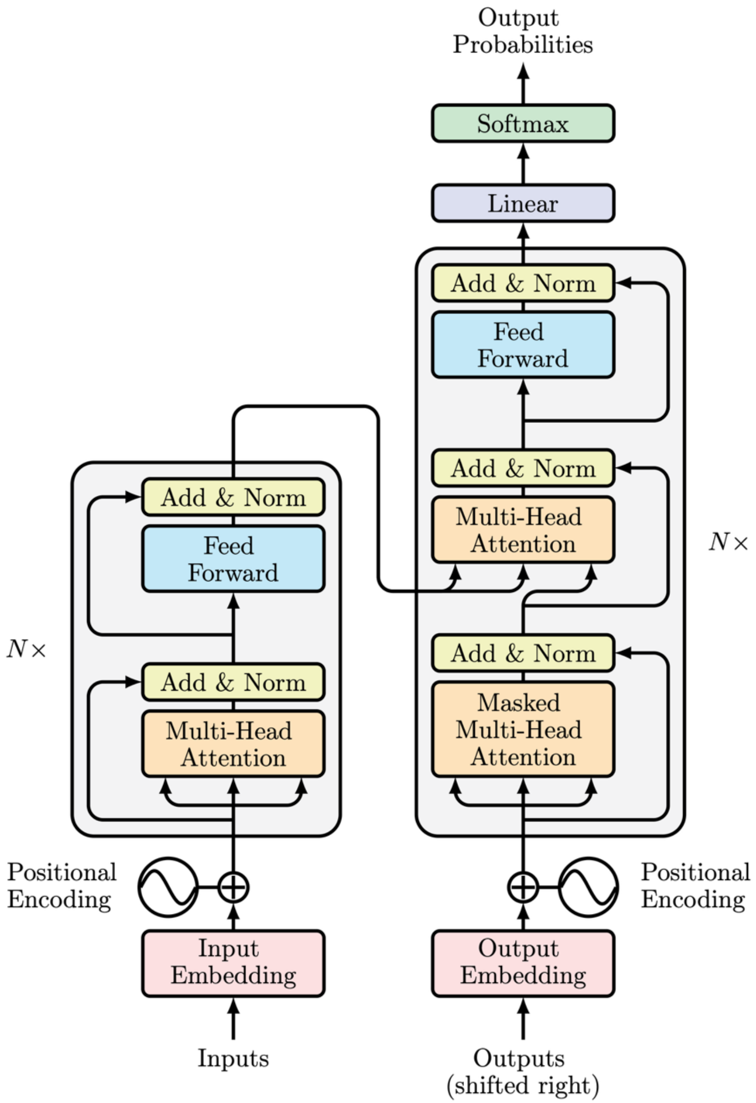

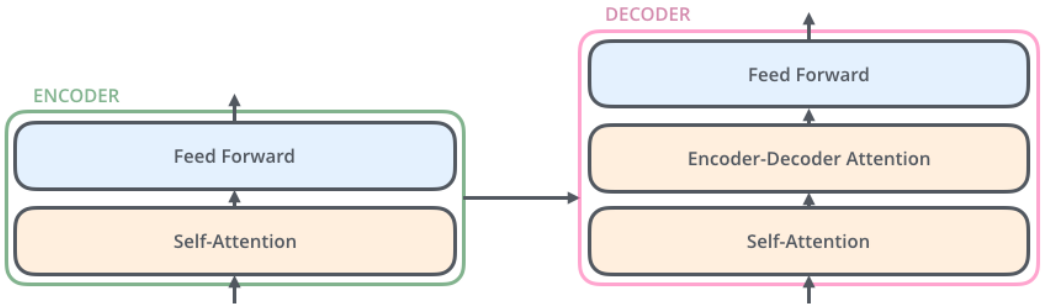

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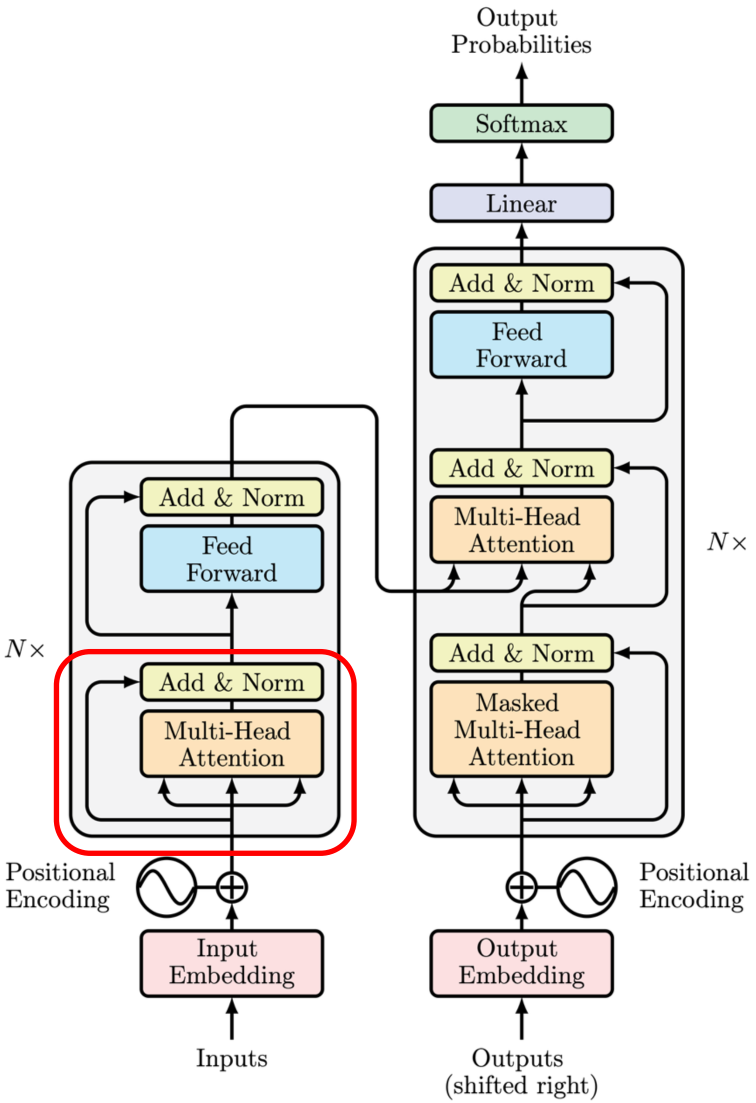

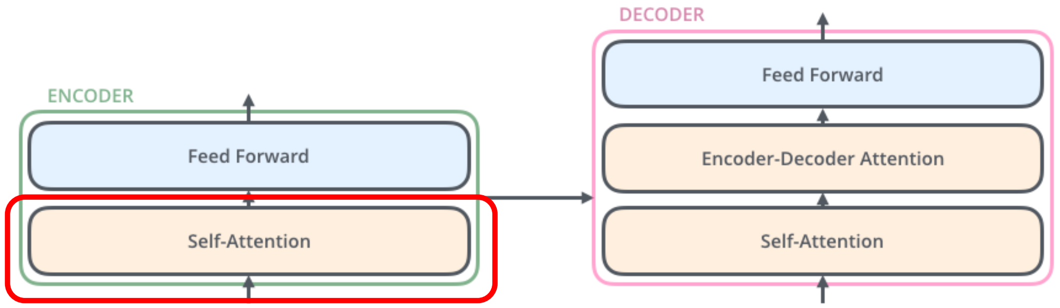

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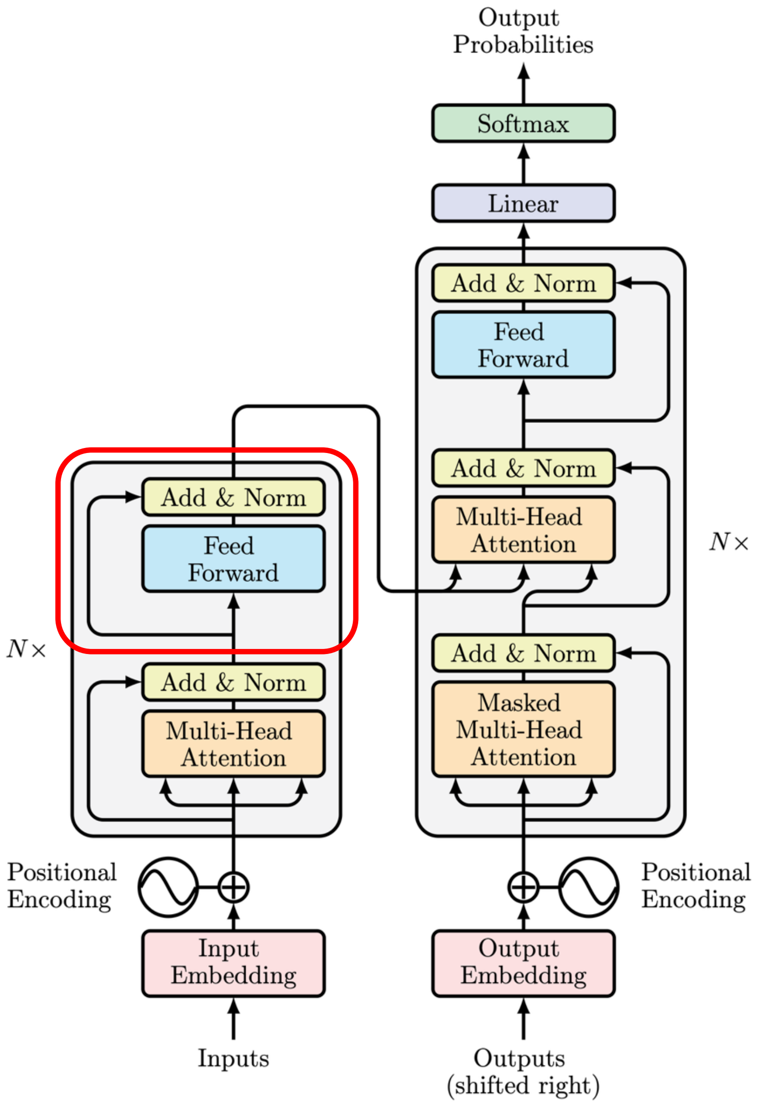

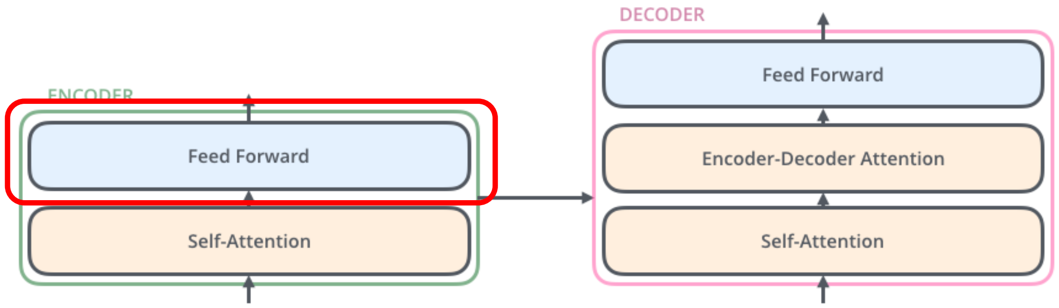

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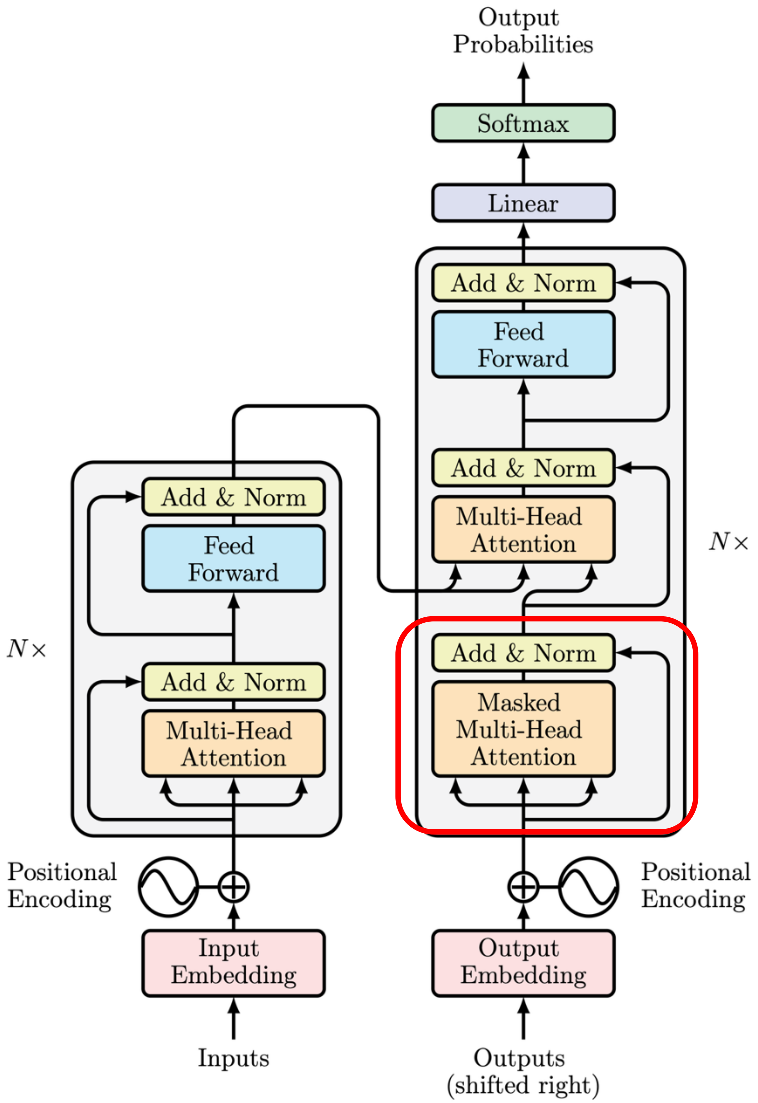

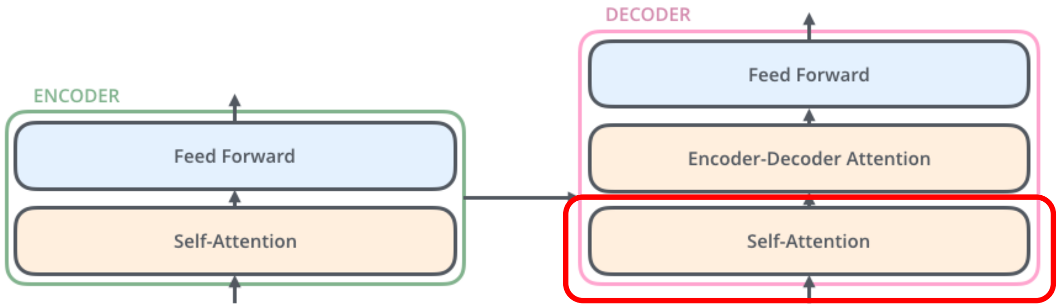

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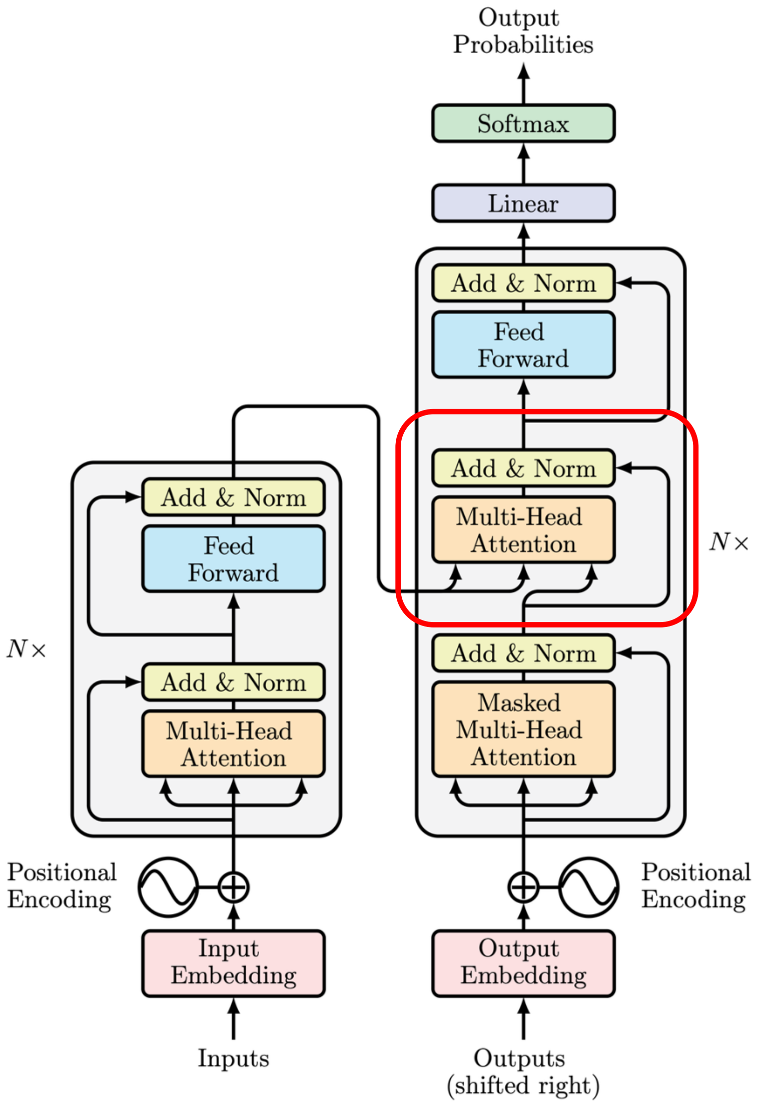

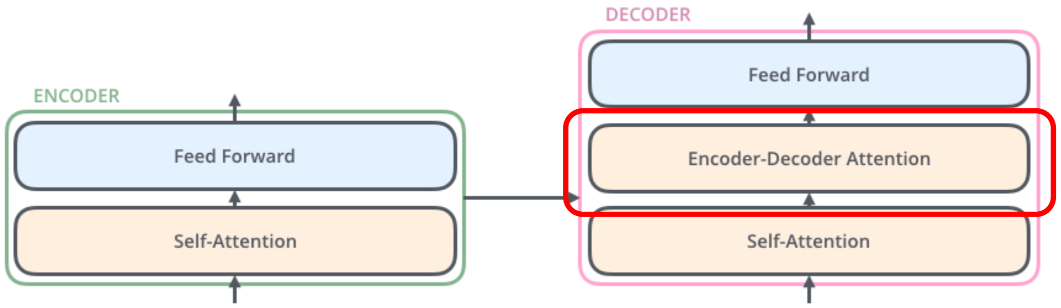

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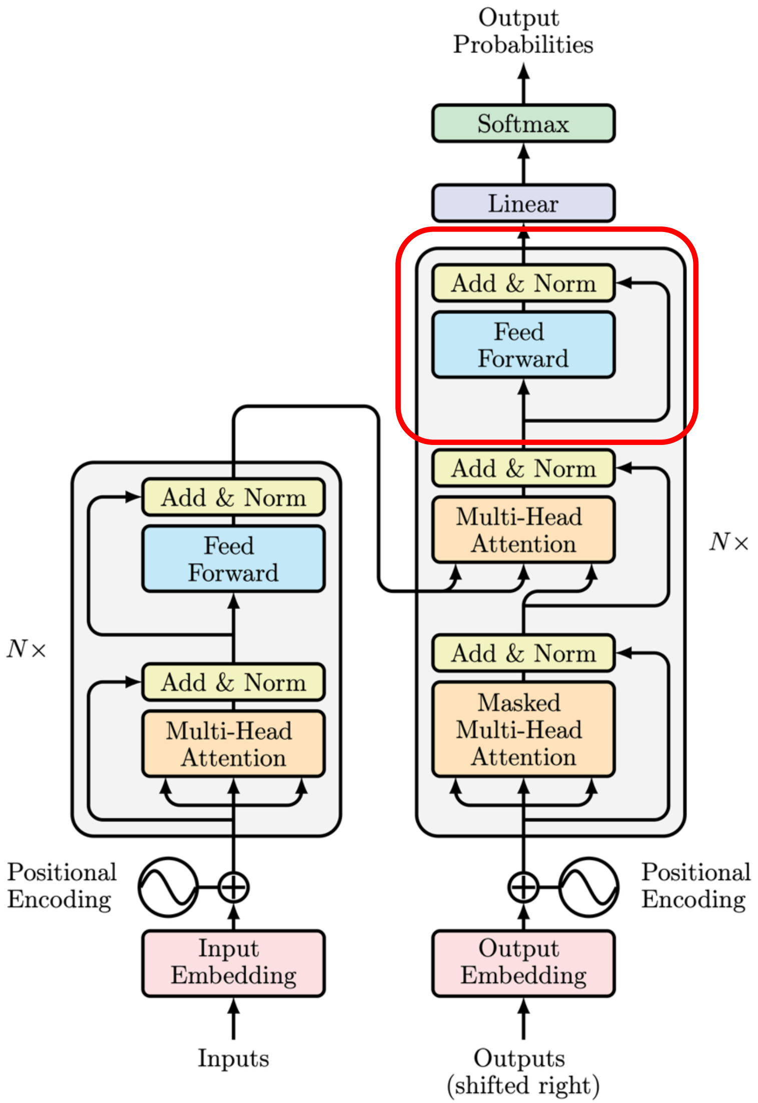

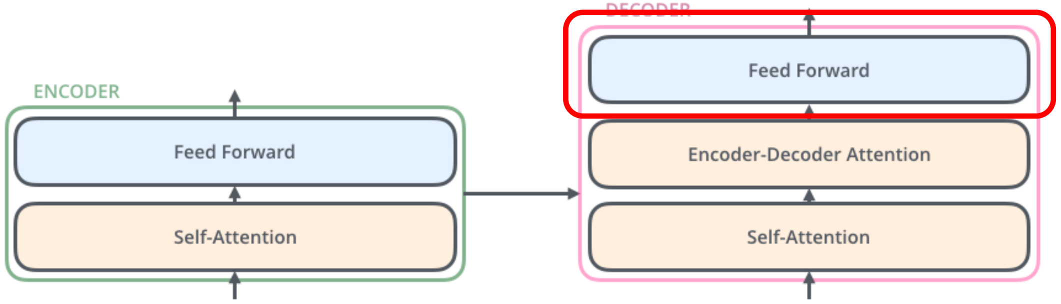

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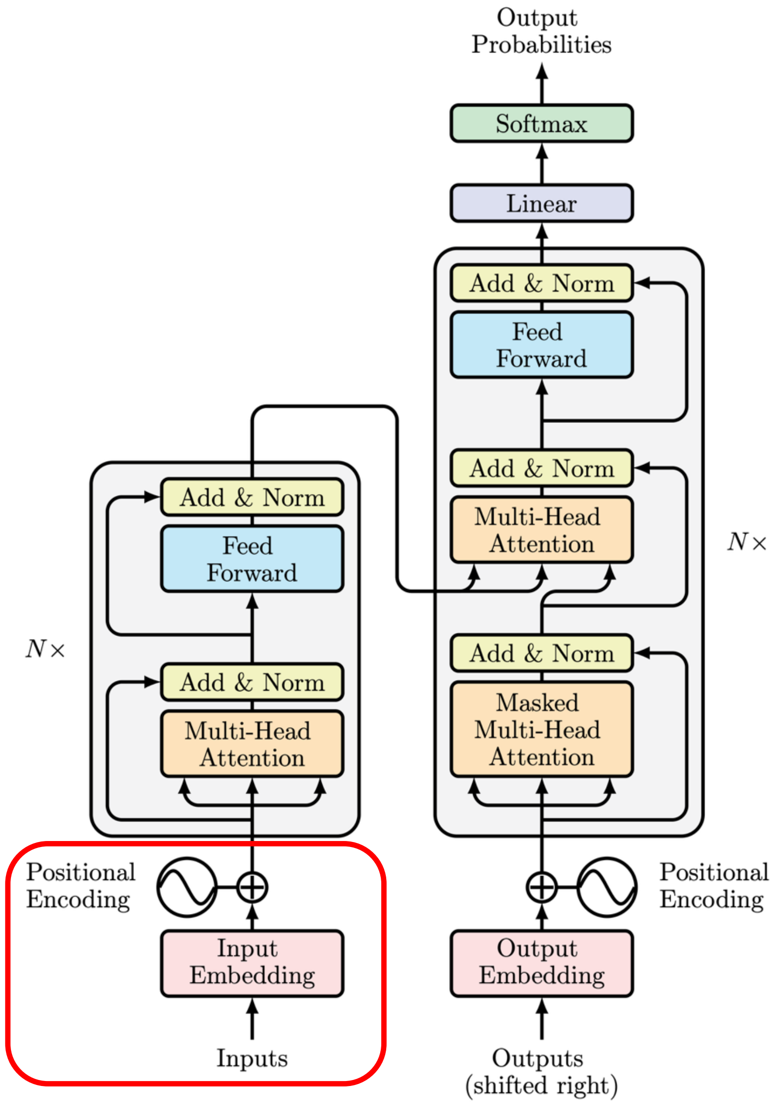
Input Encoding



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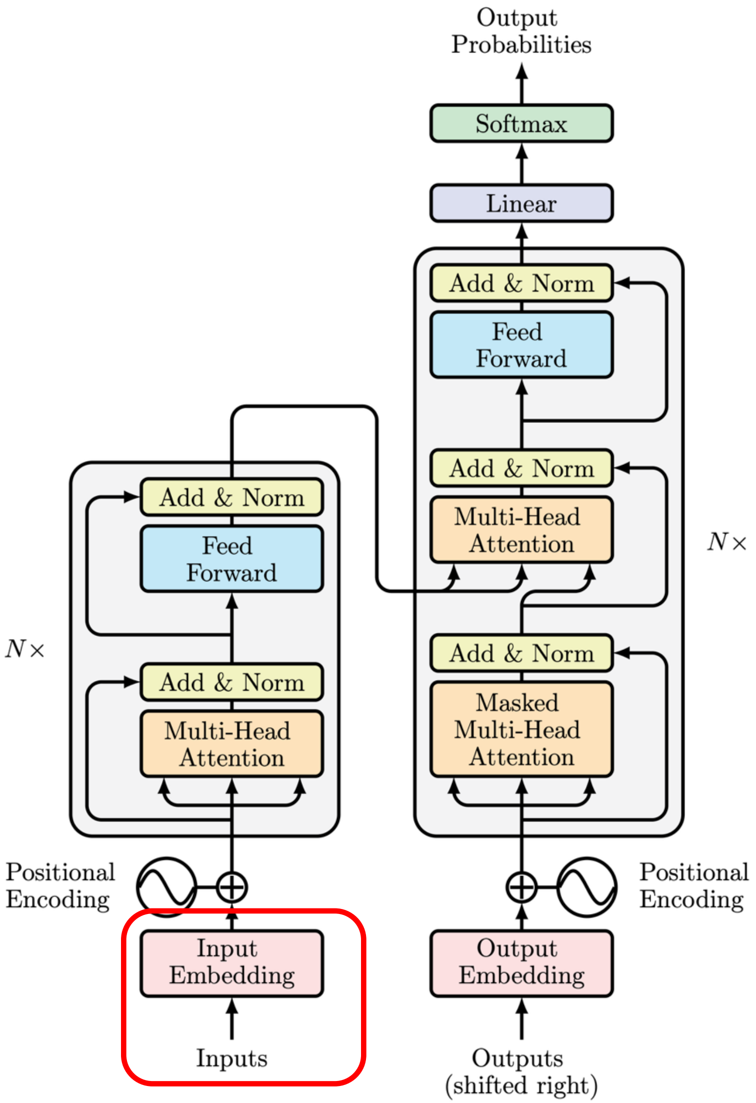

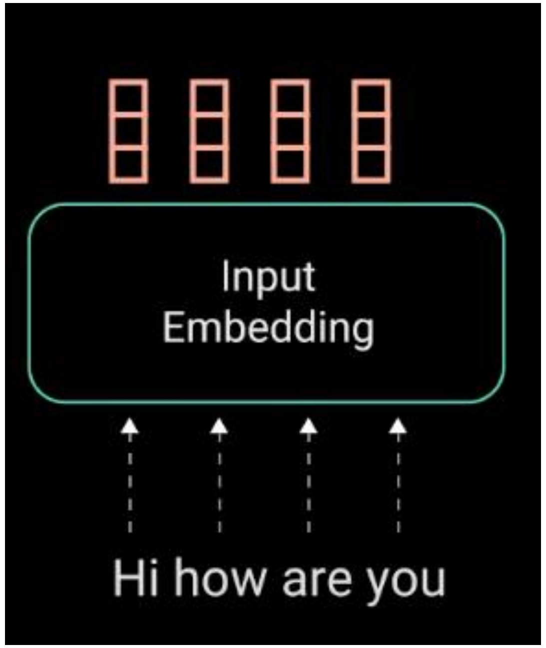

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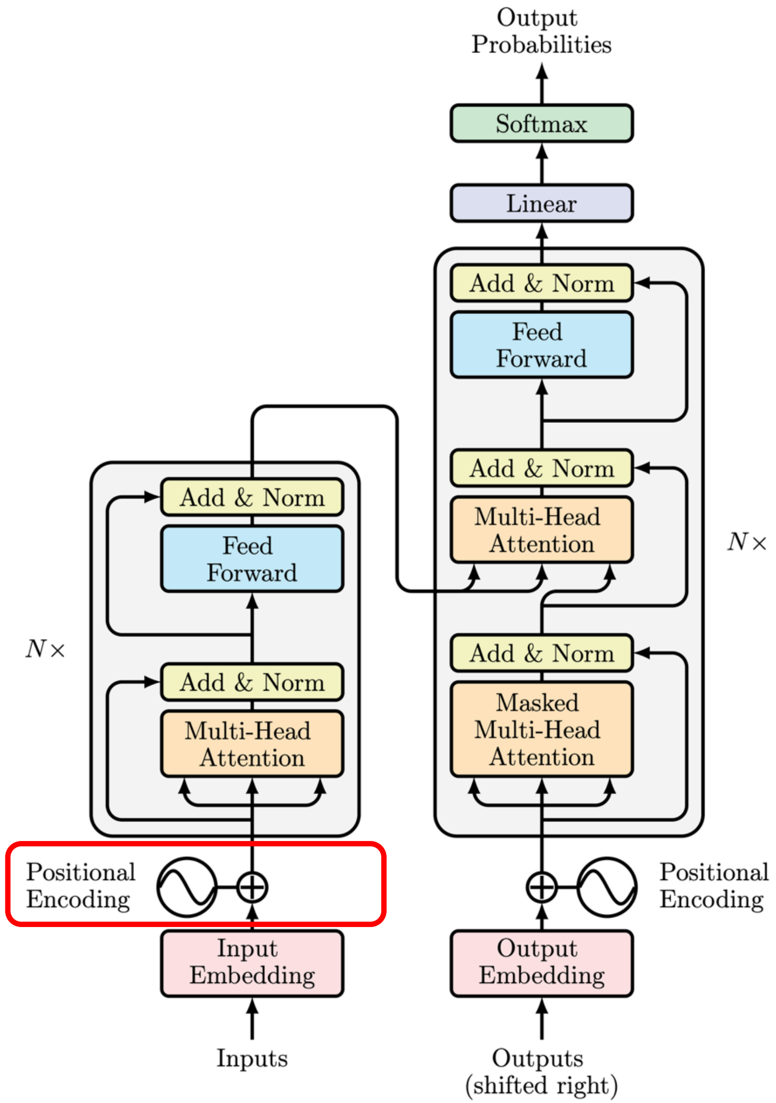
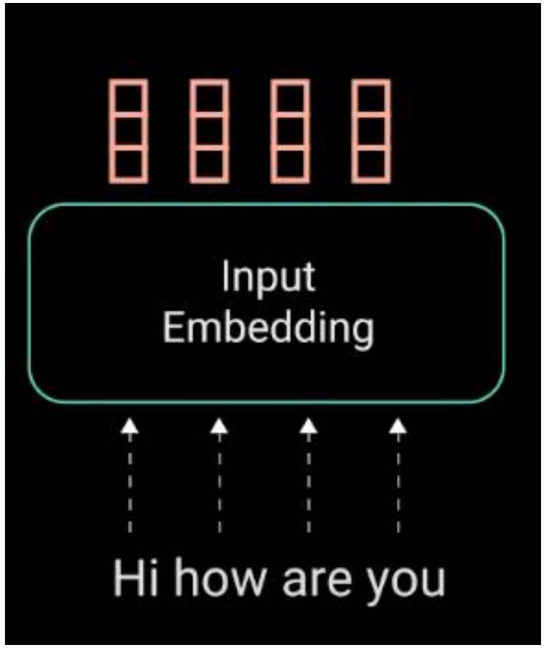
Positional Encoding





$$PE_{(pos,2i)} = sin(pos/10000^{2i/d_{model}})$$

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

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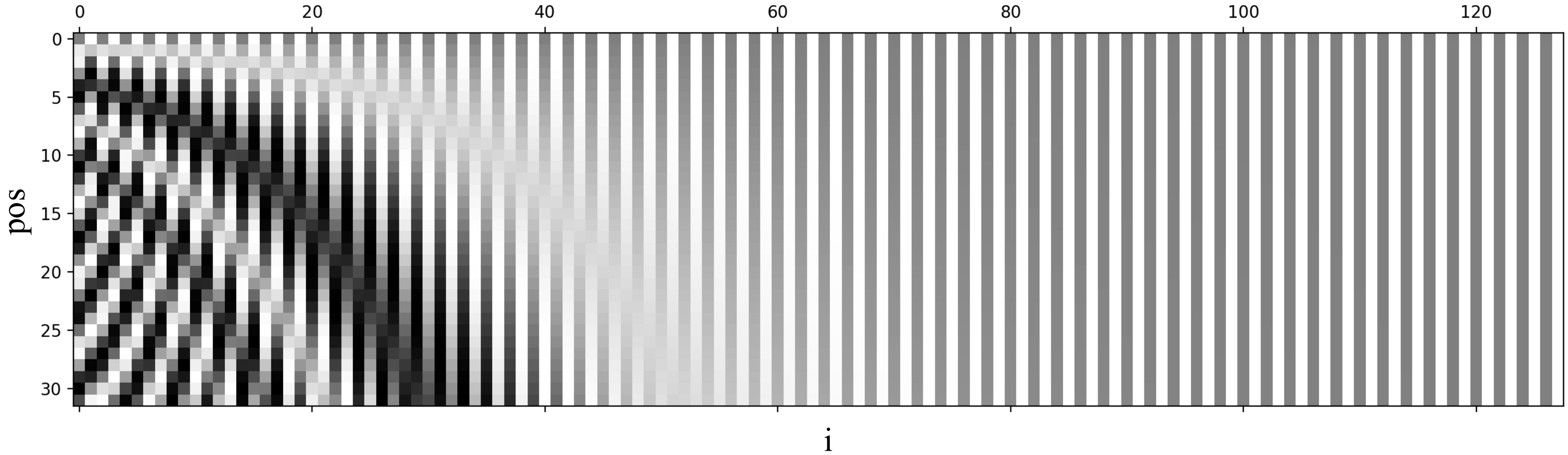
Positional Encoding



$$PE_{(pos,2i)} = sin(pos/10000^{2i/d_{model}})$$

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

Image Credit: https://lilianweng.github.io/lil-log/2020/04/07/the-transformer-family.html

Absolute vs. Relative Positional Encoding

Encode relative position information could help better model the dependency among tokens.

How to encode relative positions?

- We can inject the relative position into the bias of attention.
- We can use Rotary Position Embedding (RoPE) [1], which is more effective empirically.

To understand RoPE, let us recap how to rotate a 2D vector:

$$\begin{bmatrix} x_1' \\ x_2' \end{bmatrix} = \underbrace{\begin{bmatrix} \cos m\theta & -\sin m\theta \\ \sin m\theta & \cos m\theta \end{bmatrix}}_{\mathbf{R}_{\theta,m}} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

Rotation matrix is orthogonal and preserves the norm!

[1] Su, Jianlin, et al. "RoFormer: Enhanced Transformer with Rotary Position Embedding." arXiv preprint arXiv:2104.09864 (2021).

Rotary Positional Embedding

RoPE first divide d-dimension vector space in d/2 subspaces and then rotate them based on the position:

$$\begin{bmatrix} x'_1 \\ \vdots \\ x'_d \end{bmatrix} = \underbrace{\begin{bmatrix} \cos m\theta_1 & -\sin m\theta_1 & 0 & 0 & \cdots & 0 & 0 \\ \sin m\theta_1 & \cos m\theta_1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cos m\theta_2 & -\sin m\theta_2 & \cdots & 0 & 0 \\ 0 & 0 & \sin m\theta_2 & \cos m\theta_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & \cos m\theta_{d/2} & -\sin m\theta_{d/2} \\ 0 & 0 & 0 & 0 & \cdots & \sin m\theta_{d/2} & \cos m\theta_{d/2} \end{bmatrix}}_{\mathbf{R}^d_{\Theta,m}} \begin{bmatrix} x_1 \\ \vdots \\ x_d \end{bmatrix}$$

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

In practice, we can apply 2D rotations to pairs $(x_1, x_{1+d/2}), (x_2, x_{2+d/2}), \ldots, (x_{d/2}, x_d)$

Rotary Positional Embedding

RoPE first divide d-dimension vector space in d/2 subspaces and then rotate them based on the position:

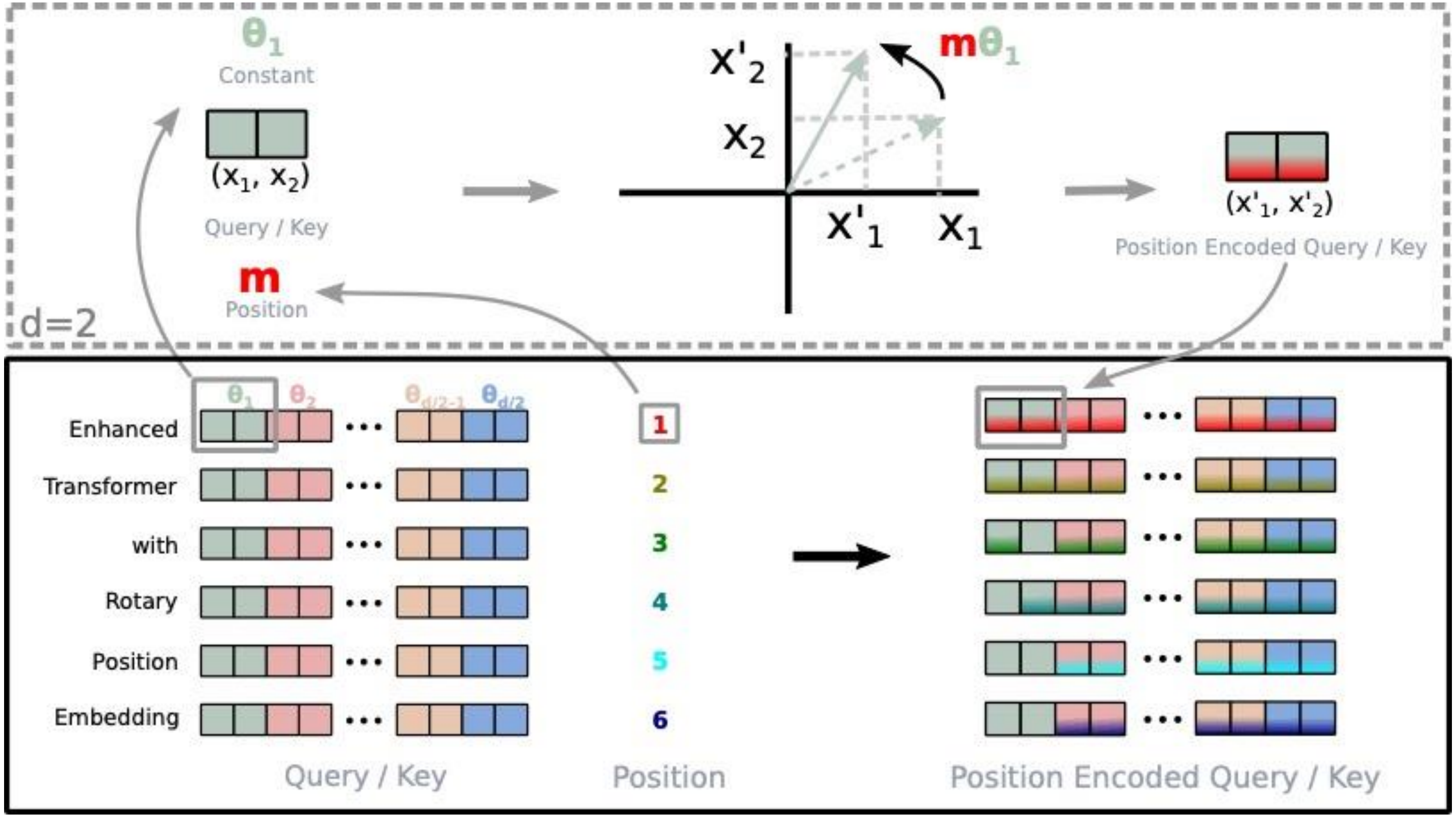


Image Credit: Su, Jianlin, et al. "RoFormer: Enhanced Transformer with Rotary Position Embedding." arXiv preprint arXiv:2104.09864 (2021).

Rotary Positional Embedding

What do we gain in RoPE?

- Inner product depends on the relative position

Let us look at the case of 2D:

$$\left\langle \begin{bmatrix} x_1' \\ x_2' \end{bmatrix}, \begin{bmatrix} y_1' \\ y_2' \end{bmatrix} \right\rangle = \left\langle \underbrace{\begin{bmatrix} \cos m\theta & -\sin m\theta \\ \sin m\theta & \cos m\theta \end{bmatrix}}_{\mathbf{R}_{\theta,m}} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}, \underbrace{\begin{bmatrix} \cos n\theta & -\sin n\theta \\ \sin n\theta & \cos n\theta \end{bmatrix}}_{\mathbf{R}_{\theta,n}} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} \right\rangle$$

$$= \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^\top \begin{bmatrix} \cos m\theta & -\sin m\theta \\ \sin m\theta & \cos m\theta \end{bmatrix}^\top \begin{bmatrix} \cos n\theta & -\sin n\theta \\ \sin n\theta & \cos n\theta \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

$$= \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^\top \begin{bmatrix} \cos m\theta \cos n\theta + \sin m\theta \sin n\theta & -\cos m\theta \sin n\theta + \sin m\theta \cos n\theta \\ -\sin m\theta \cos n\theta + \cos m\theta \sin n\theta & \sin m\theta \sin n\theta + \cos m\theta \cos n\theta \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

$$= \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^\top \begin{bmatrix} \cos(m-n)\theta & \sin(m-n)\theta \\ \sin(n-m)\theta & \cos(m-n)\theta \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

$$= \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^\top \underbrace{\begin{bmatrix} \cos(m-n)\theta & -\sin(m-n)\theta \\ \sin(m-n)\theta & \cos(m-n)\theta \end{bmatrix}^\top}_{\mathbf{R}_{\theta,m-n}} \underbrace{\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}}_{\mathbf{R}_{\theta,0}} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \left\langle \mathbf{R}_{\theta,m-n} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}, \mathbf{R}_{\theta,0} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} \right\rangle$$

Rotary Positional Embedding

What do we gain in RoPE?

- Inner product depends on the relative position

Let us look at the case of 2D:

This holds for d-dimension as we construct a block-diagonal matrix with 2D rotation matrices!

$$\left\langle \begin{bmatrix} x_1' \\ x_2' \end{bmatrix}, \begin{bmatrix} y_1' \\ y_2' \end{bmatrix} \right\rangle = \left\langle \underbrace{\begin{bmatrix} \cos m\theta & -\sin m\theta \\ \sin m\theta & \cos m\theta \end{bmatrix}}_{\mathbf{R}_{\theta,m}} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}, \underbrace{\begin{bmatrix} \cos n\theta & -\sin n\theta \\ \sin n\theta & \cos n\theta \end{bmatrix}}_{\mathbf{R}_{\theta,n}} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} \right\rangle$$

$$= \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^\top \begin{bmatrix} \cos m\theta & -\sin m\theta \\ \sin m\theta & \cos m\theta \end{bmatrix}^\top \begin{bmatrix} \cos n\theta & -\sin n\theta \\ \sin n\theta & \cos n\theta \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

$$= \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^\top \begin{bmatrix} \cos m\theta \cos n\theta + \sin m\theta \sin n\theta & -\cos m\theta \sin n\theta + \sin m\theta \cos n\theta \\ -\sin m\theta \cos n\theta + \cos m\theta \sin n\theta & \sin m\theta \sin n\theta + \cos m\theta \cos n\theta \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

$$= \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^\top \begin{bmatrix} \cos(m-n)\theta & \sin(m-n)\theta \\ \sin(n-m)\theta & \cos(m-n)\theta \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

$$= \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^\top \underbrace{\begin{bmatrix} \cos(m-n)\theta & -\sin(m-n)\theta \\ \sin(m-n)\theta & \cos(m-n)\theta \end{bmatrix}^\top}_{\mathbf{R}_{\theta,m-n}} \underbrace{\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}}_{\mathbf{R}_{\theta,0}} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \left\langle \mathbf{R}_{\theta,m-n} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}, \mathbf{R}_{\theta,0} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} \right\rangle$$

Rotary Positional Embedding

What do we gain in RoPE?

- Long-term decay of inner product w.r.t. relative positions

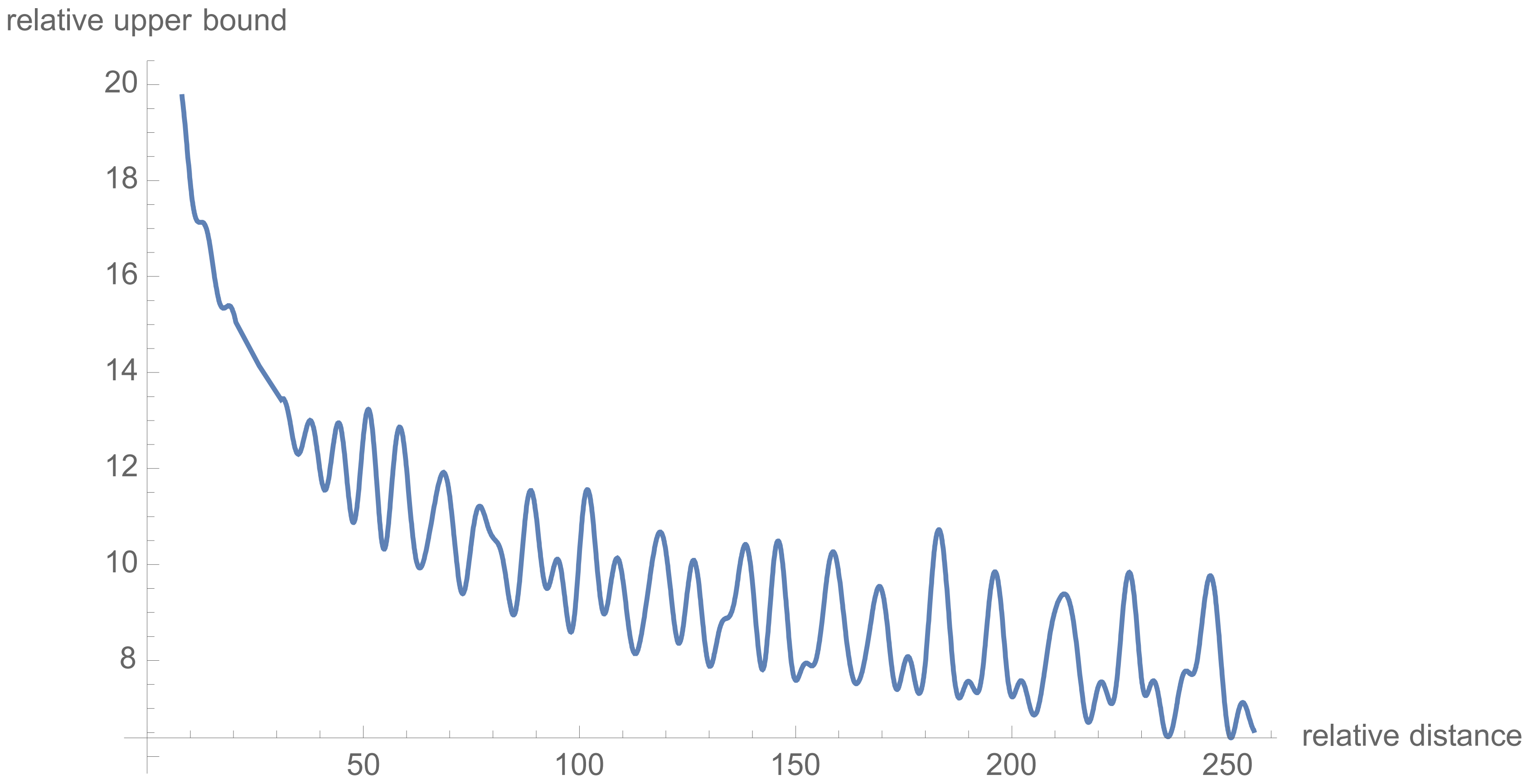


Image Credit: Su, Jianlin, et al. "RoFormer: Enhanced Transformer with Rotary Position Embedding." arXiv preprint arXiv:2104.09864 (2021).

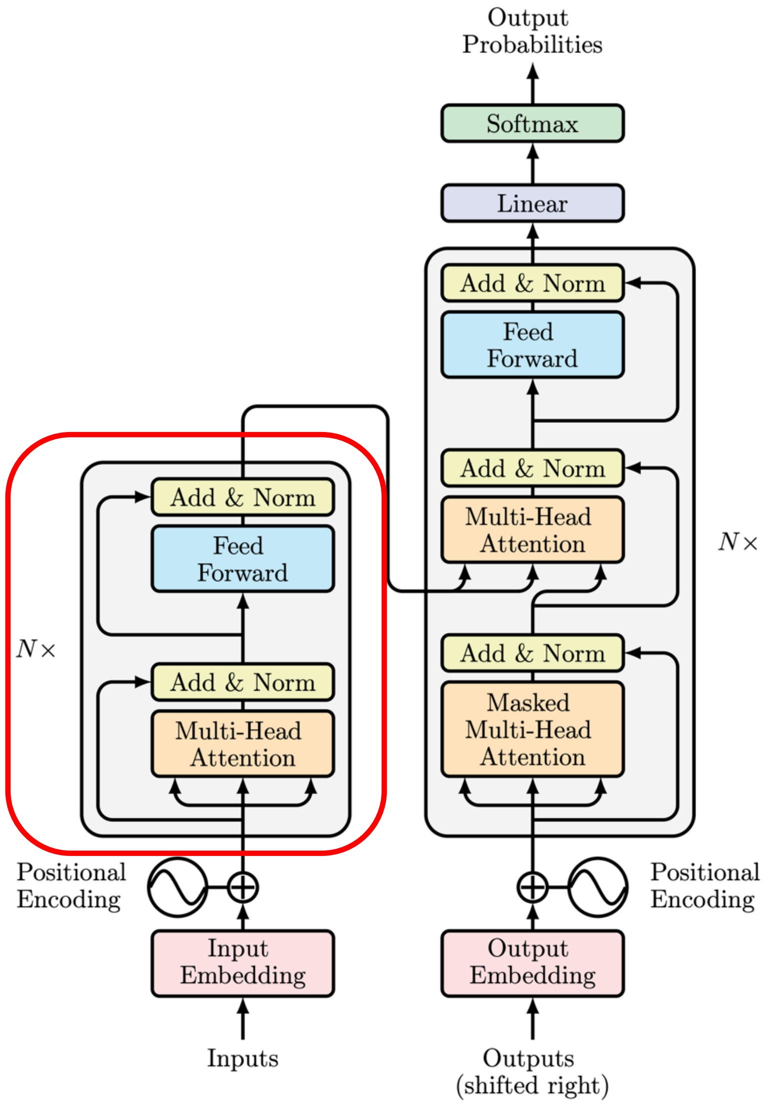
Outline

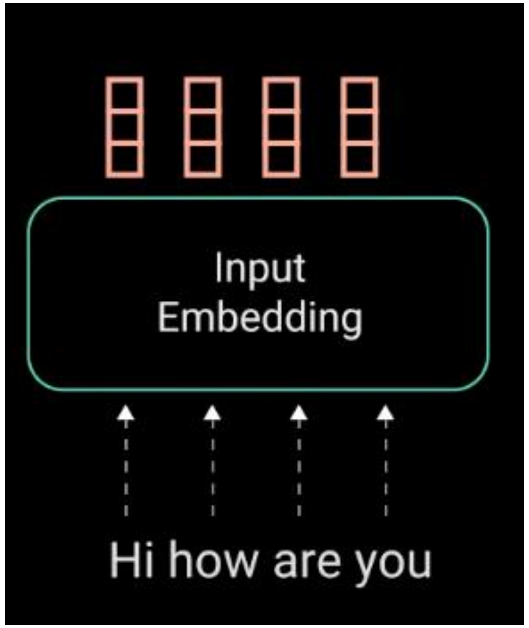
- Invariance & Equivariance Principle
  - Translation equivariance in convolutions
  - Permutation equivariance and invariance

- Models for Sets
  - DeepSets: representation theorem of permutation-invariant set functions & architecture
  - DeepSets: permutation-equivariant linear mapping & architecture

- Models for Sequences
  - Transformers
  - Positional encoding vs. Rotary Positional Embeddings (RoPE)
  - **Attention & Flash Attention**
  - Pre-norm vs. post-norm
  - Vision Transformers (ViT) & Swin Transformers

Encoder





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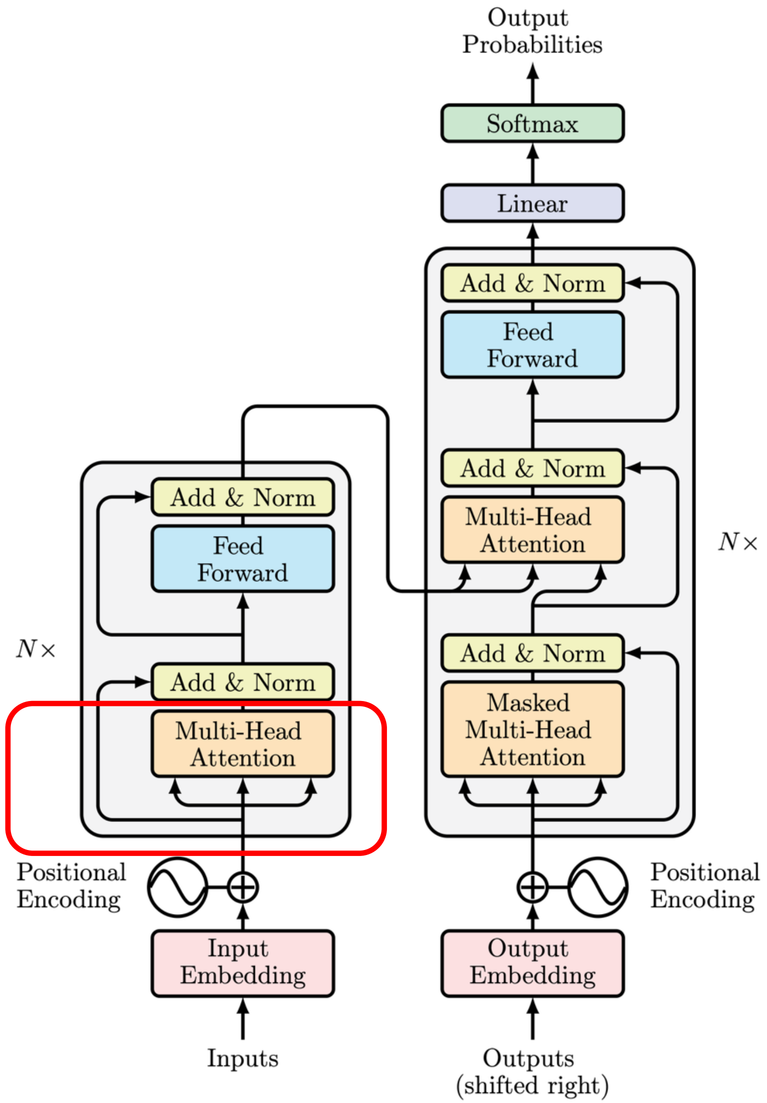
Multi-Head Attention



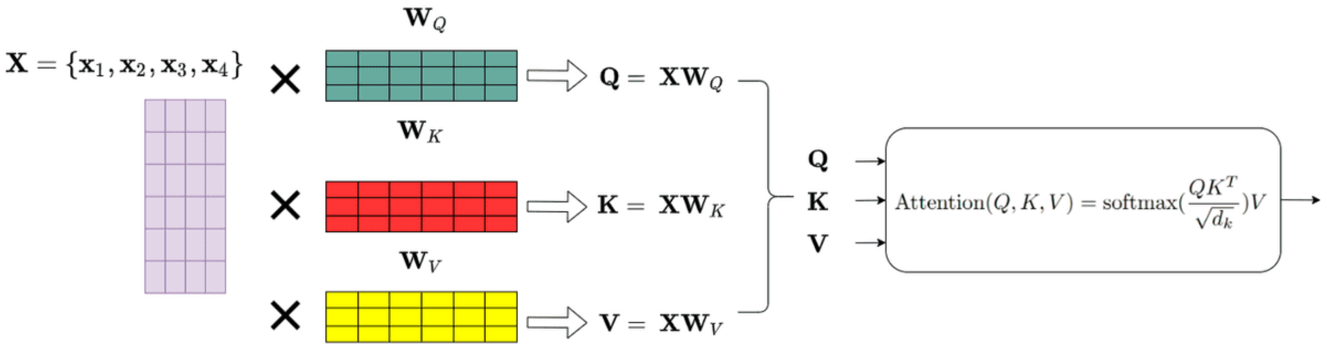
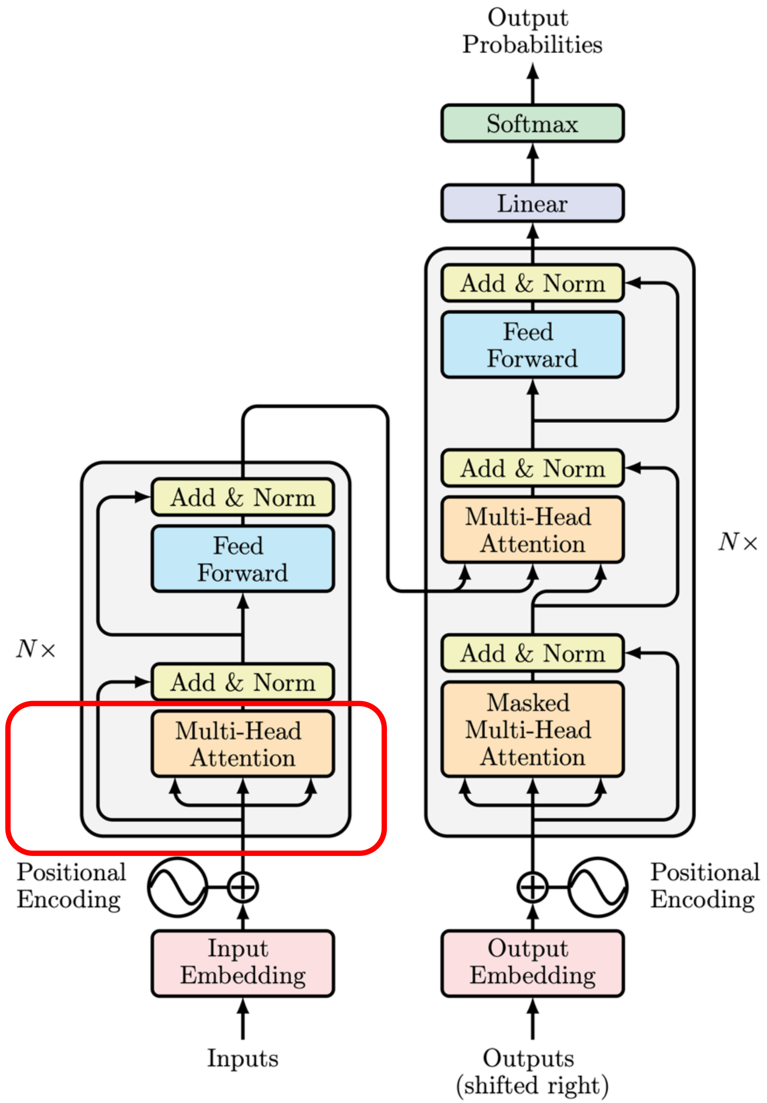
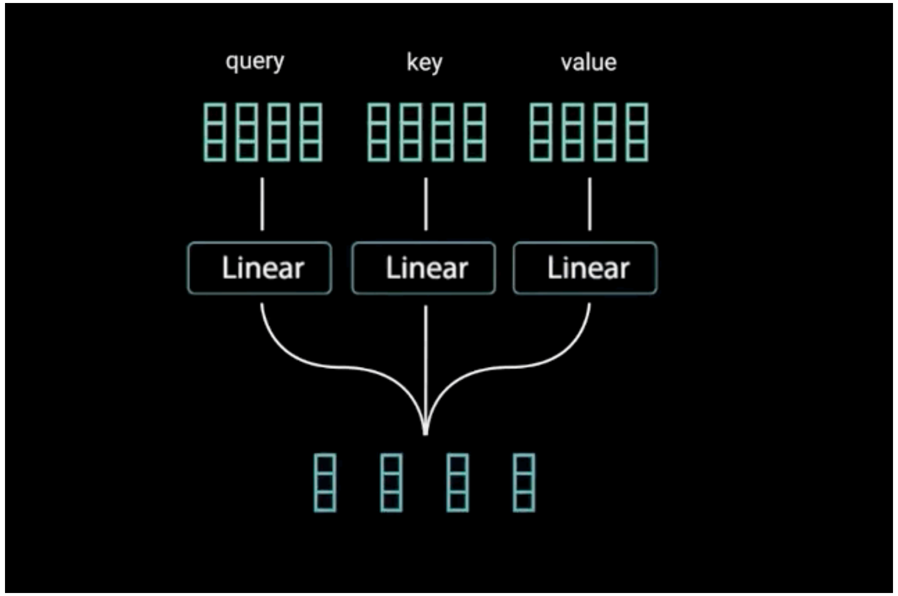


Image Credit: Vaswani, A. "Attention is all you need." Advances in Neural Information Processing Systems (2017). https://theaisummer.com/transformer/

Multi-Head Attention





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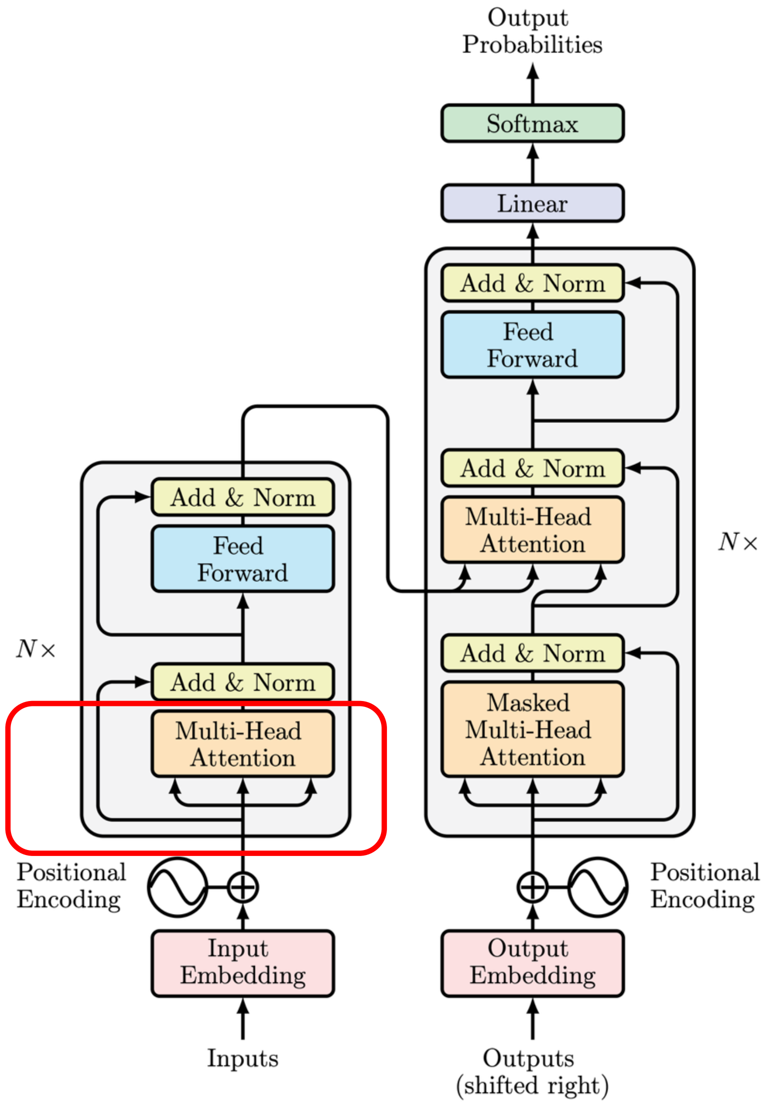

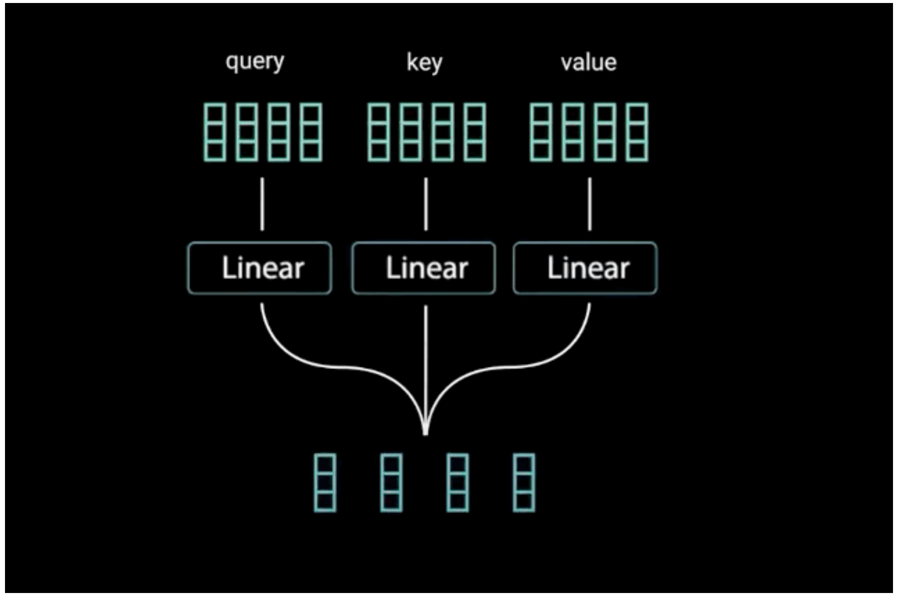

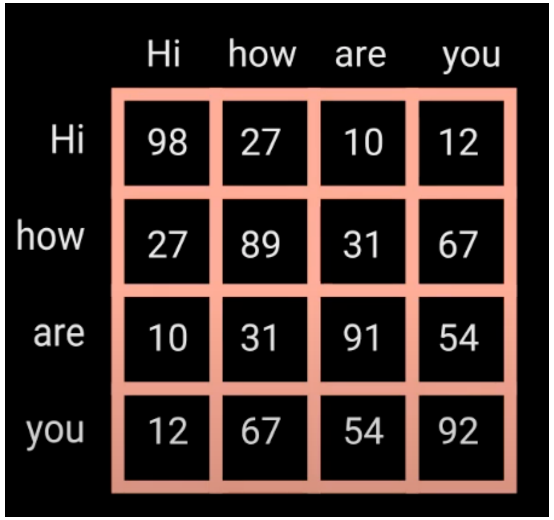

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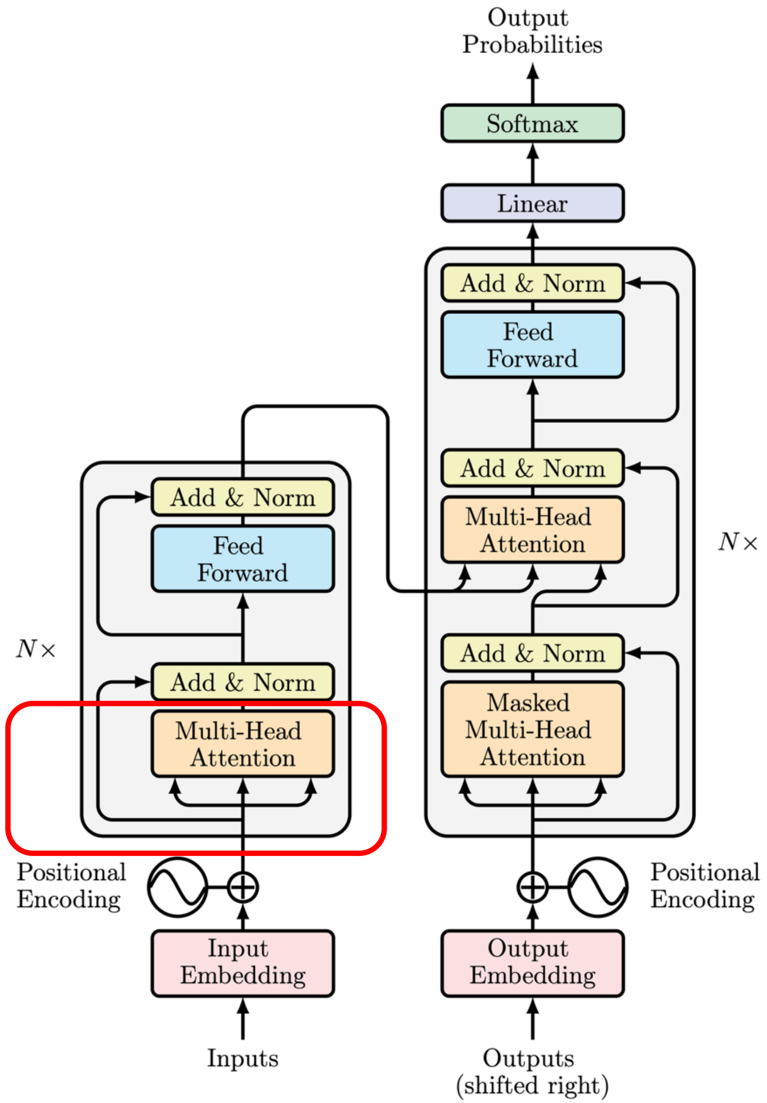

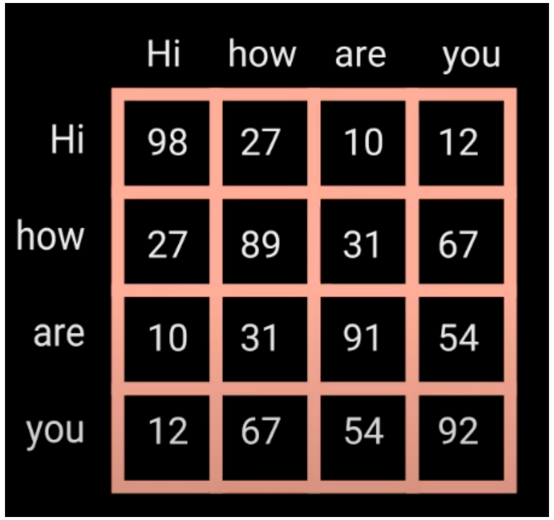

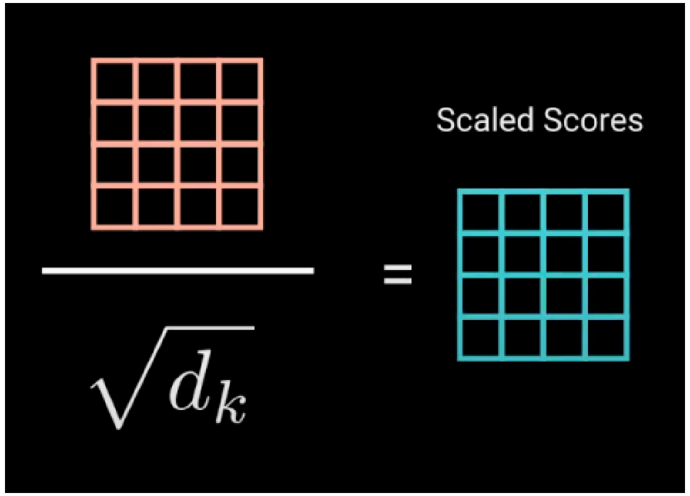

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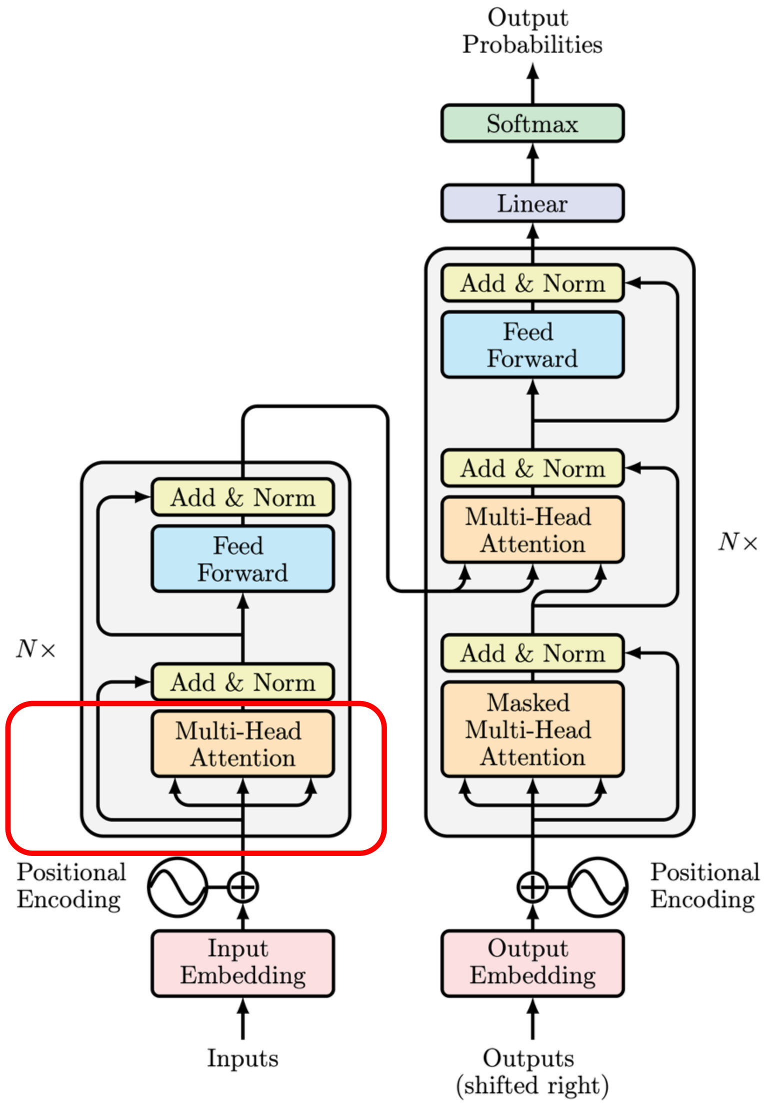

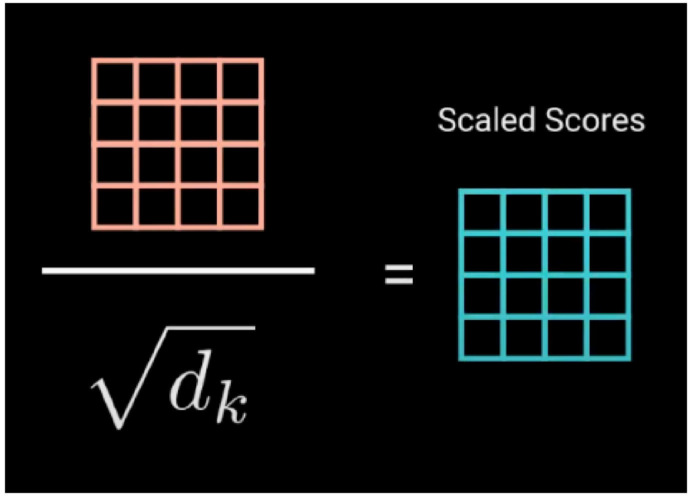

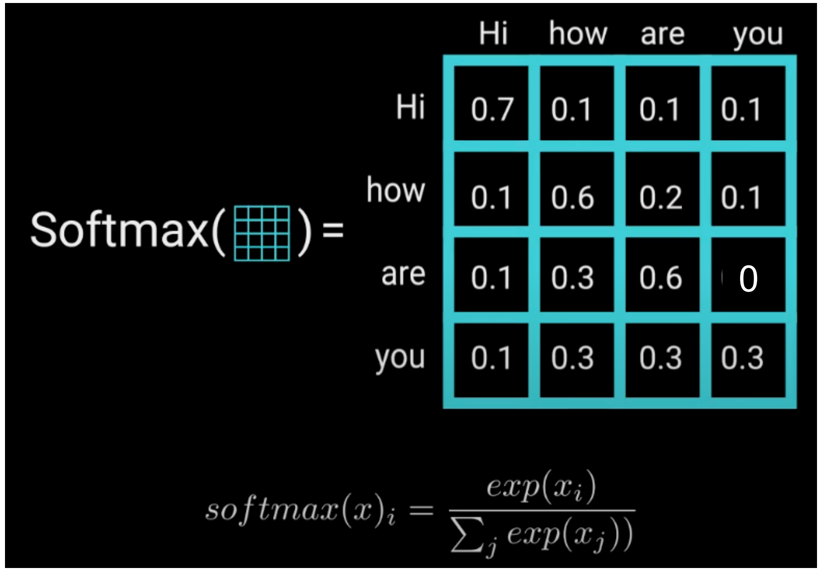

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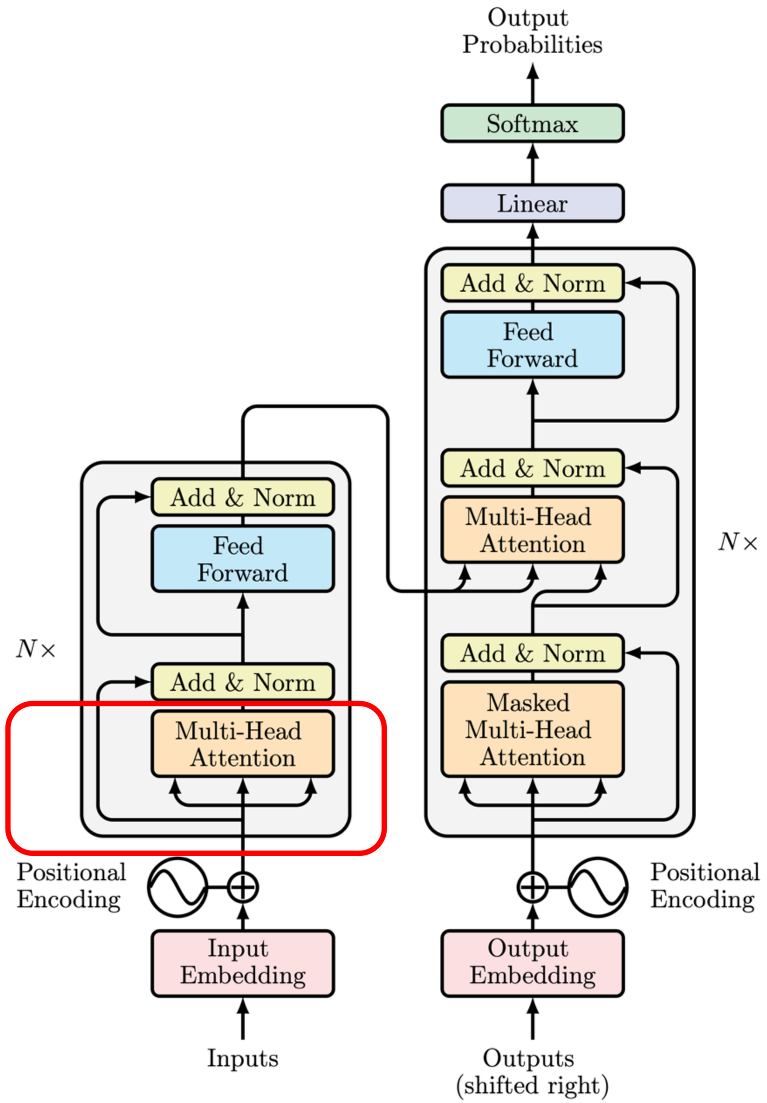
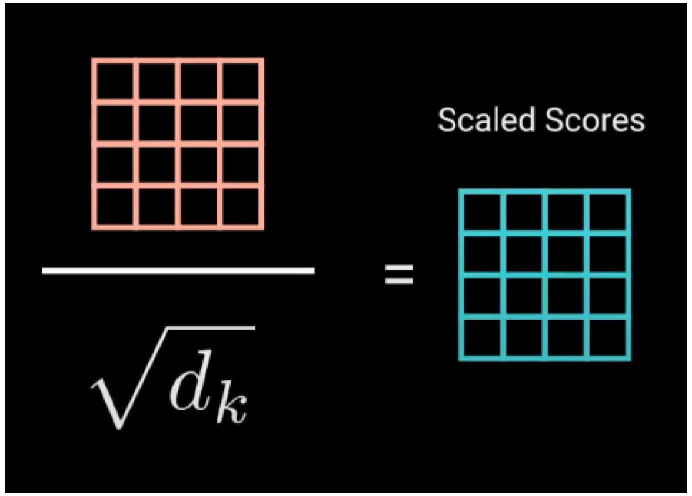
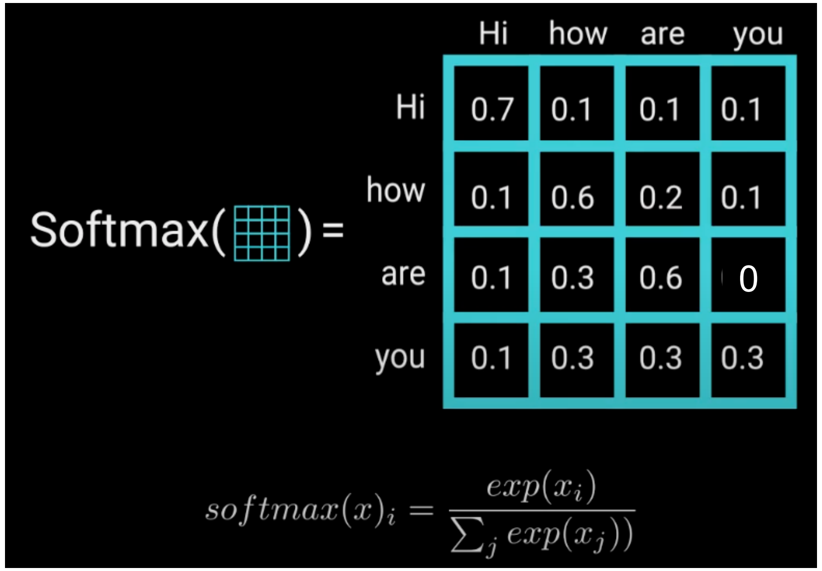




Why square root?



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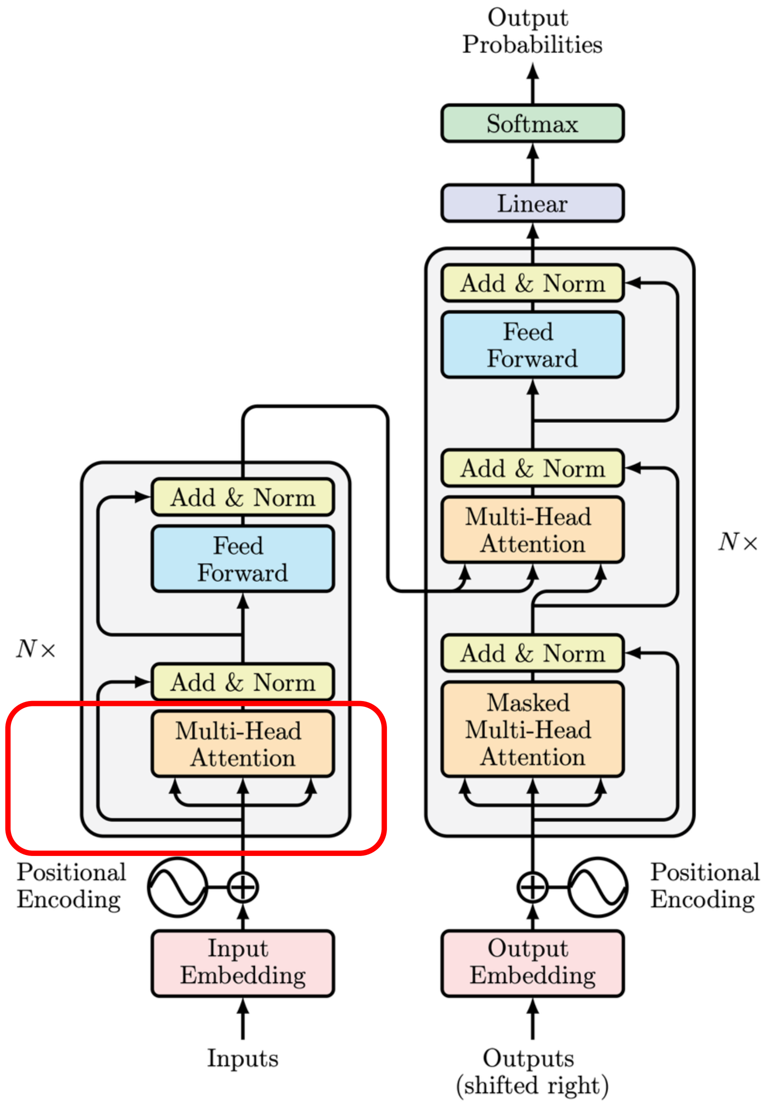

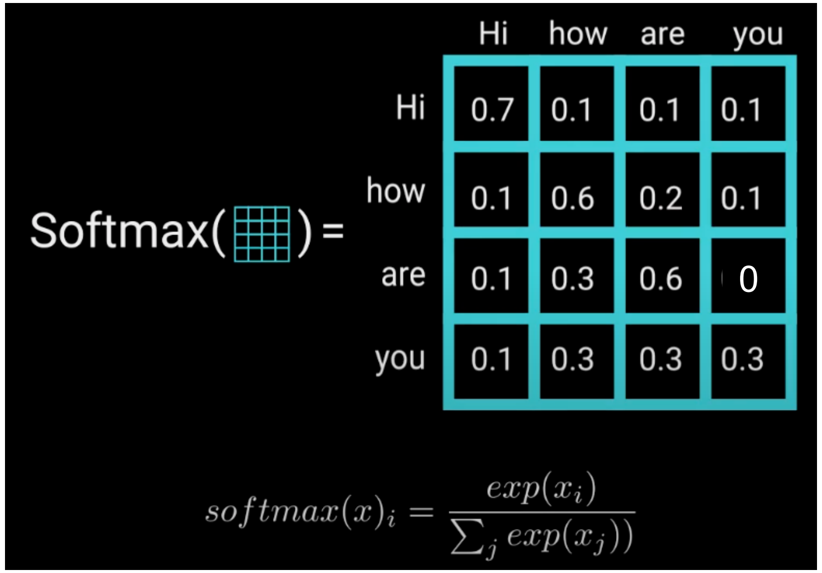

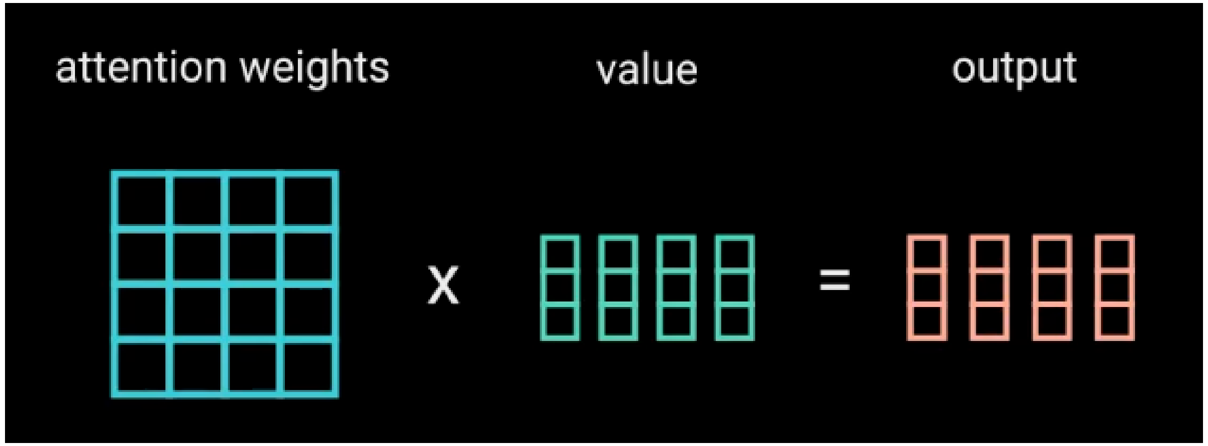

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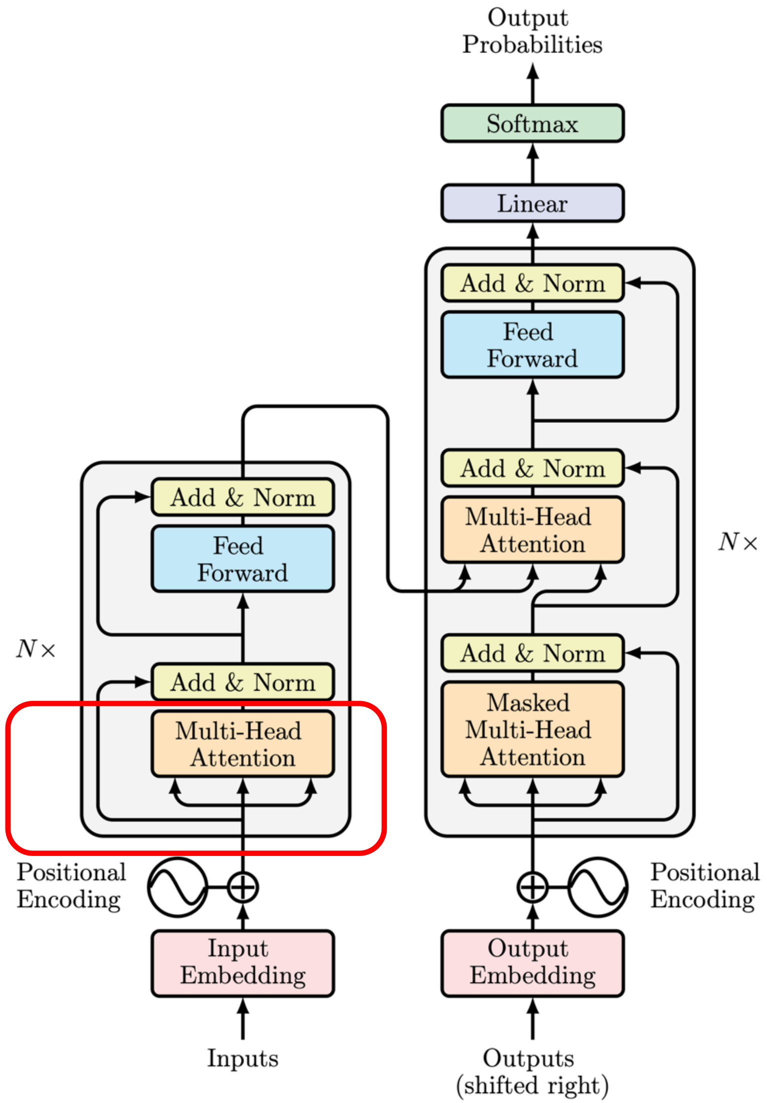

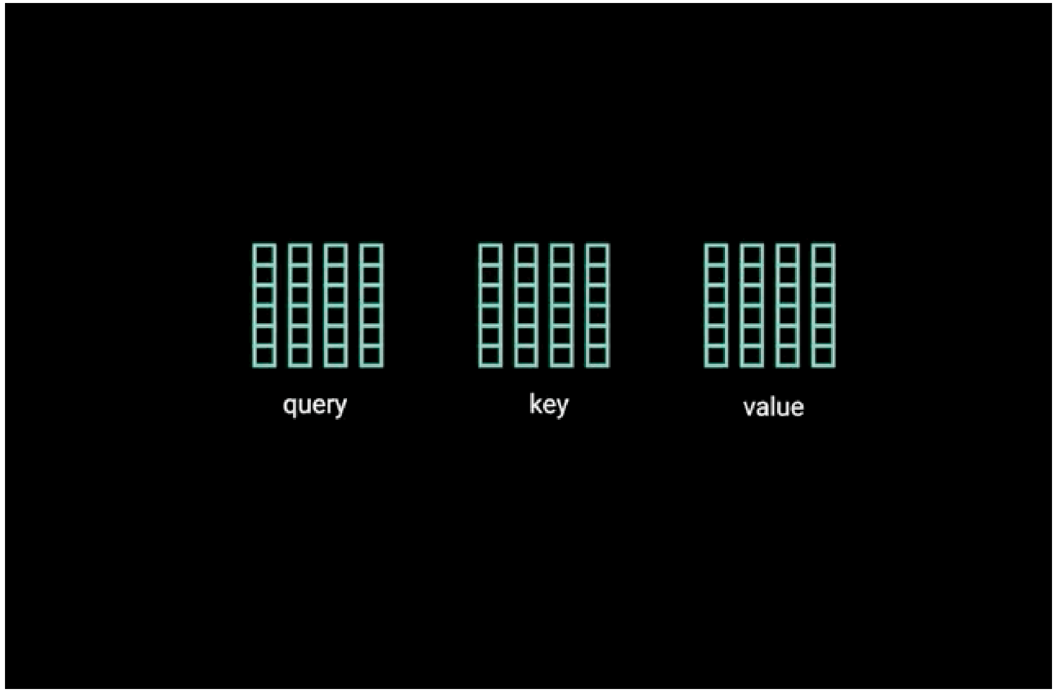

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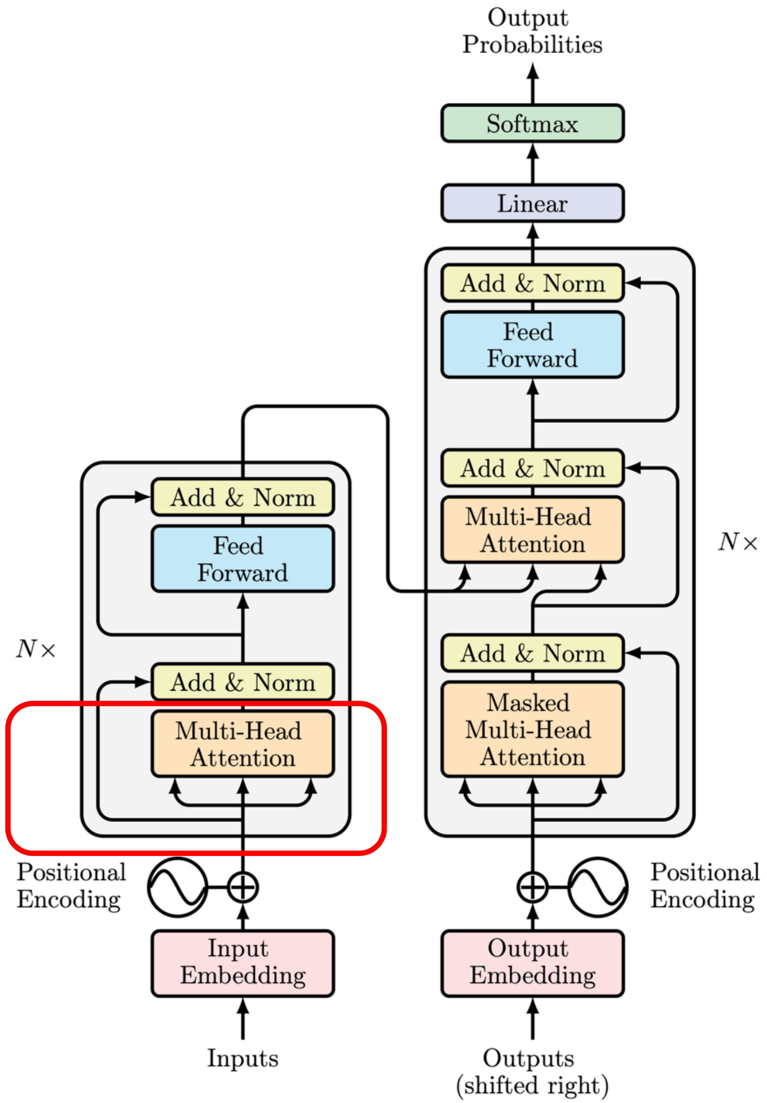
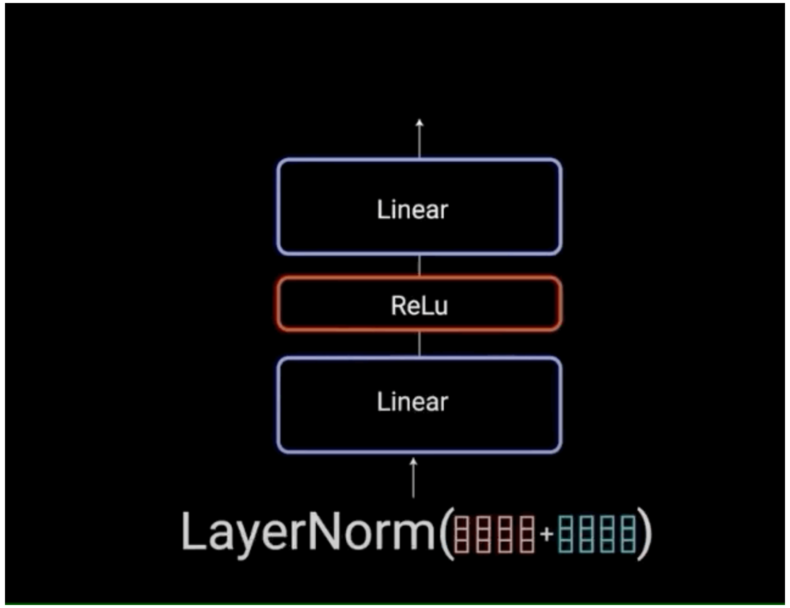
Layer Norm [1] & Residual Connection





$$\mu_i = \frac{1}{K}\sum_{k=1}^{K} x_{i,k}$$

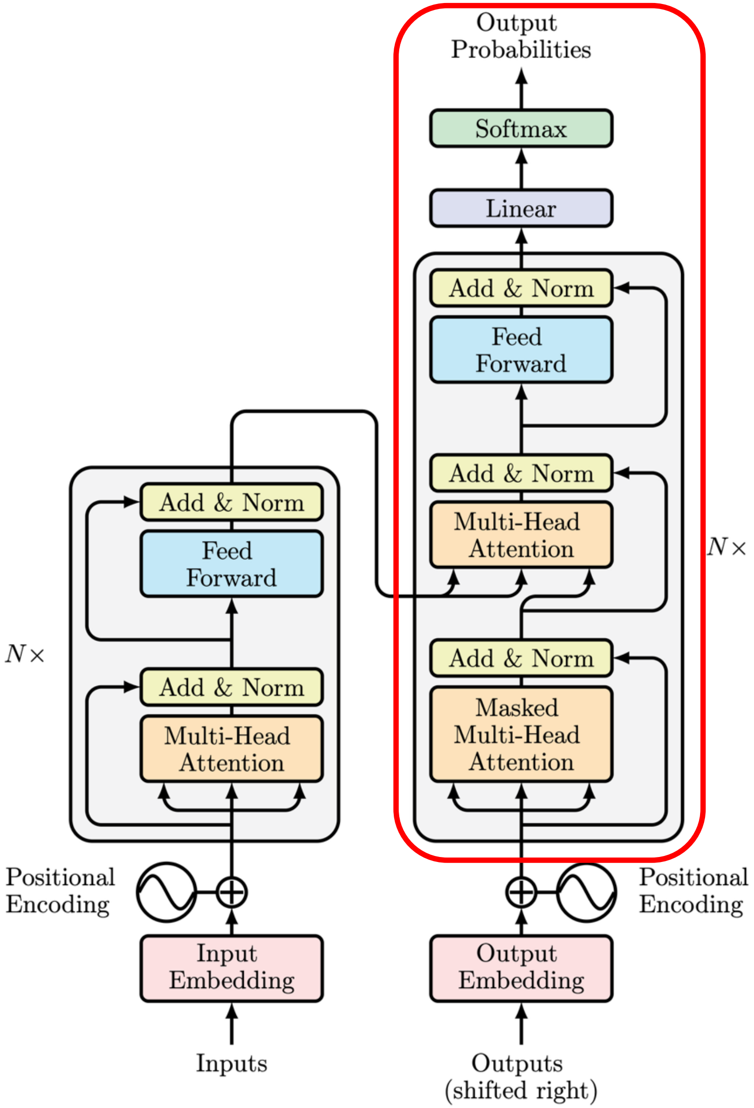
$$\sigma_i^2 = \frac{1}{K}\sum_{k=1}^{K}(x_{i,k}-\mu_i)^2$$

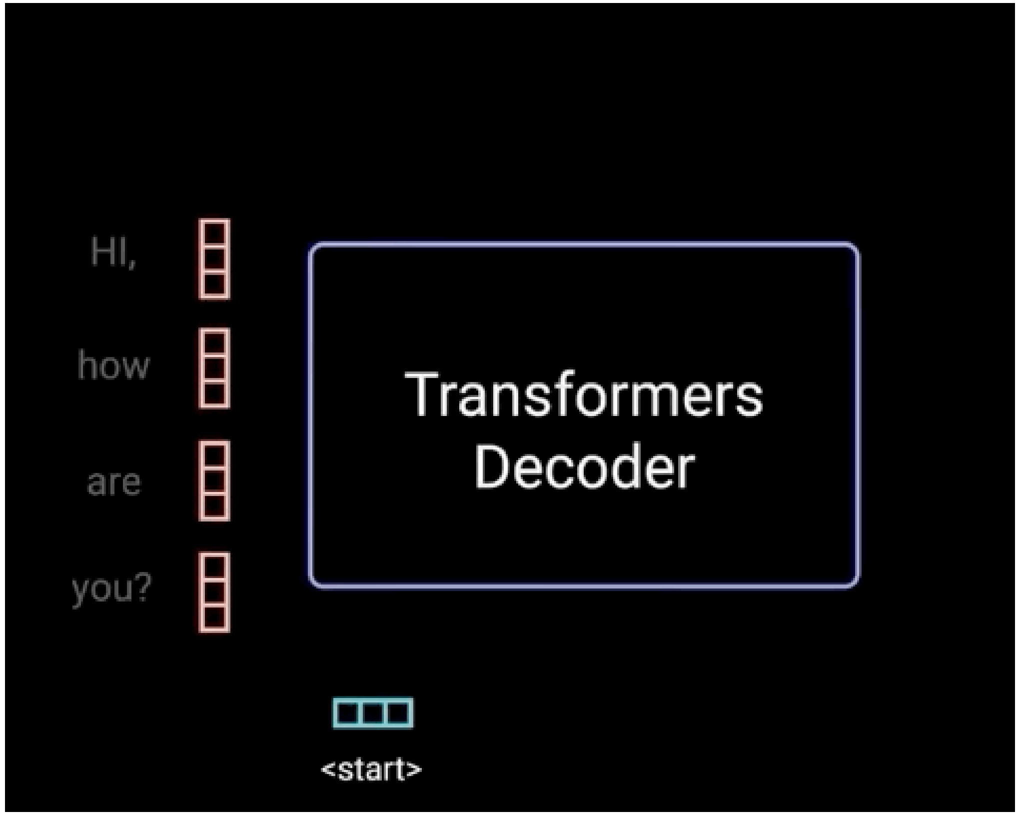
$$\hat{x}_{i,k} = \frac{x_{i,k}-\mu_i}{\sqrt{\sigma_i^2+\epsilon}}$$

$$y_i = \gamma\hat{x}_i + \beta \equiv \mathrm{LN}_{\gamma,\beta}(x_i)$$

[1] Ba, Jimmy Lei. "Layer normalization." arXiv preprint arXiv:1607.06450 (2016). Image Credit: Vaswani, A. "Attention is all you need." Advances in Neural Information Processing Systems (2017).
https://towardsdatascience.com/illustrated-guide-to-transformers-step-by-step-explanation-f74876522bc0

Decoder

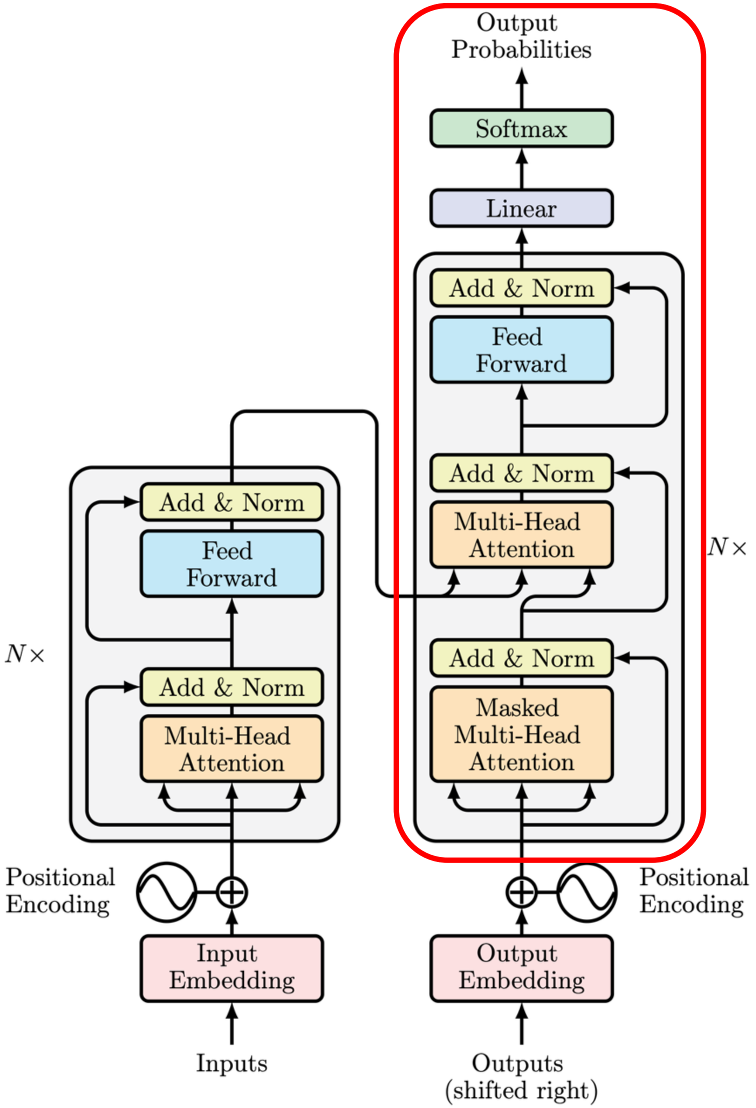


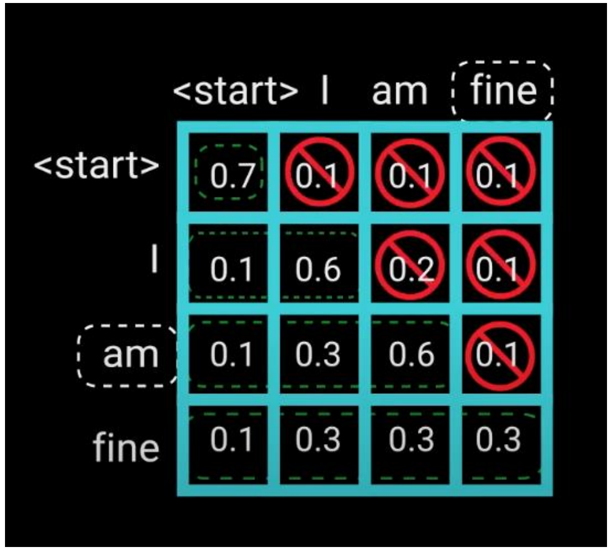


For certain applications like language models, decoder should be autoregressive!

Image Credit: Vaswani, A. "Attention is all you need." Advances in Neural Information Processing Systems (2017). https://towardsdatascience.com/illustrated-guide-to-transformers-step-by-step-explanation-f74876522bc0

Masked Multi-Head Attention





Prevent attending from future!

Image Credit: Vaswani, A. "Attention is all you need." Advances in Neural Information Processing Systems (2017). https://towardsdatascience.com/illustrated-guide-to-transformers-step-by-step-explanation-f74876522bc0

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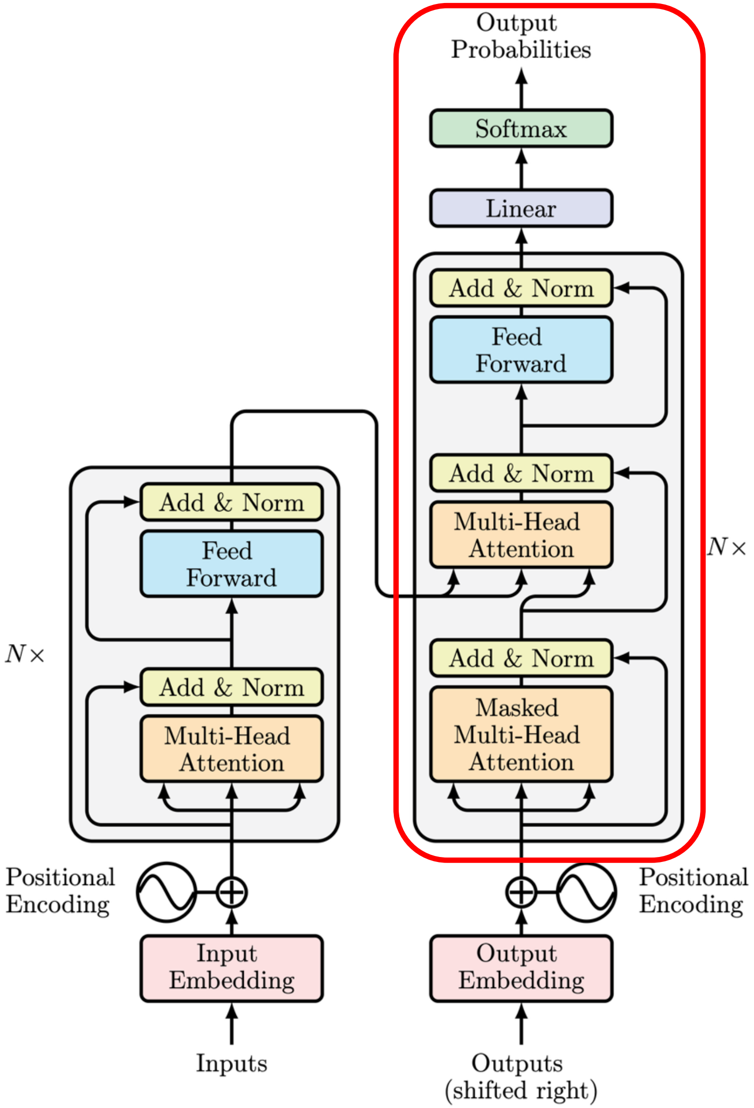
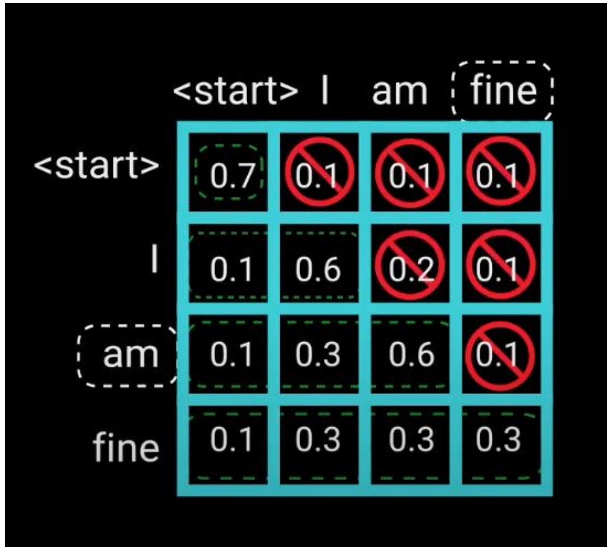




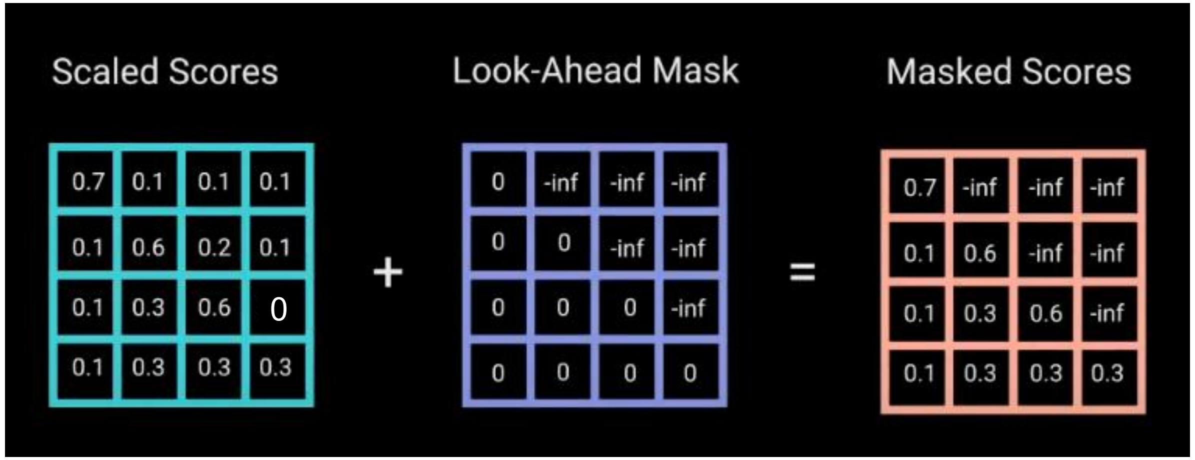
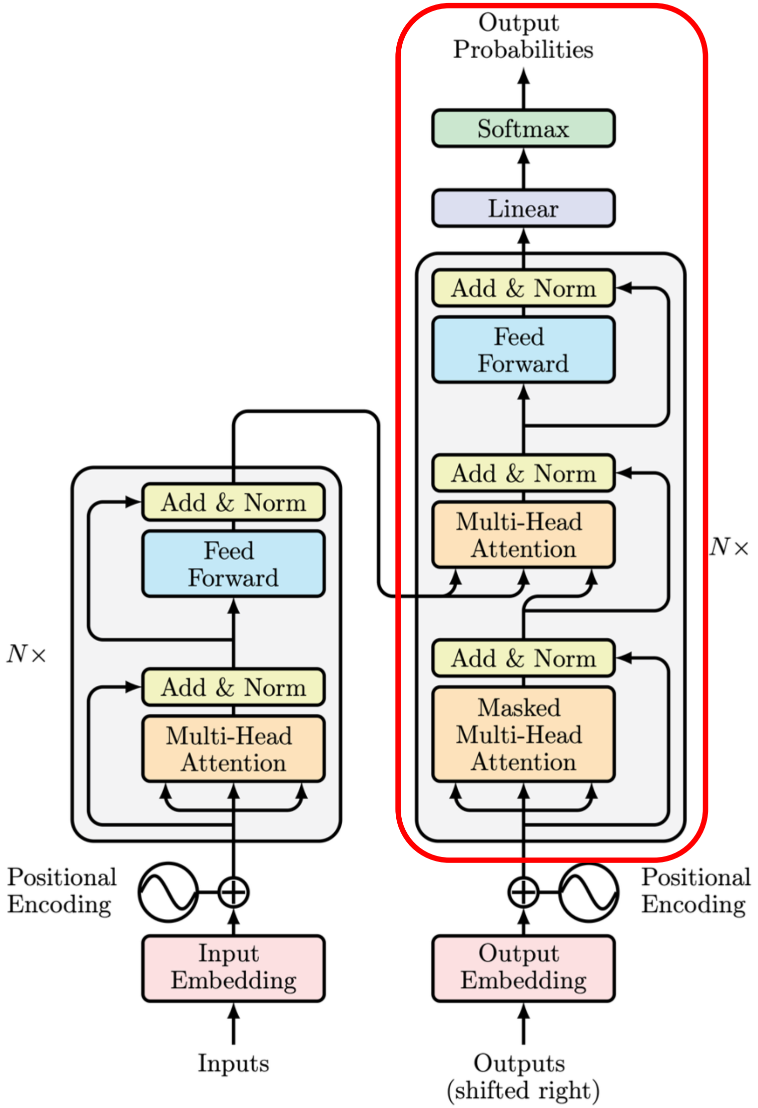
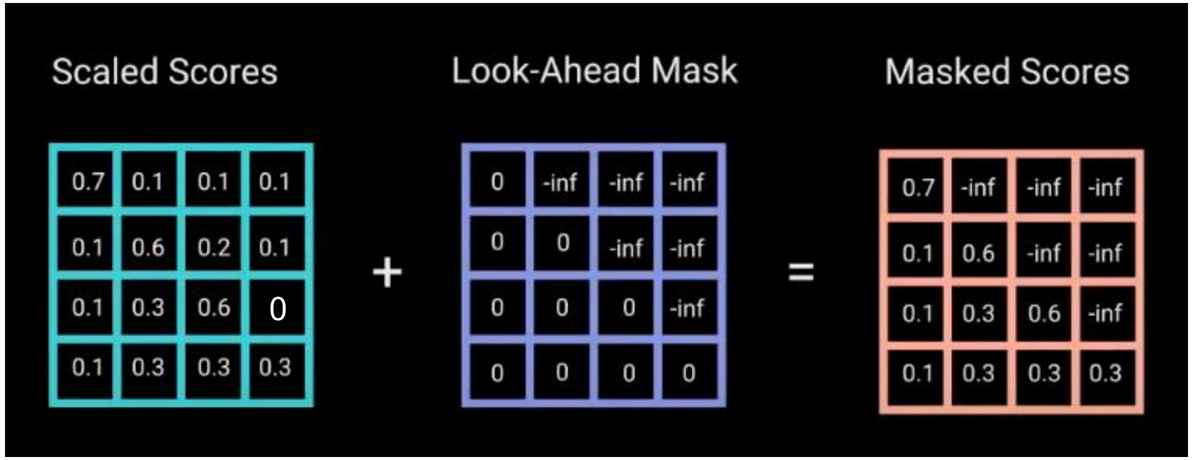
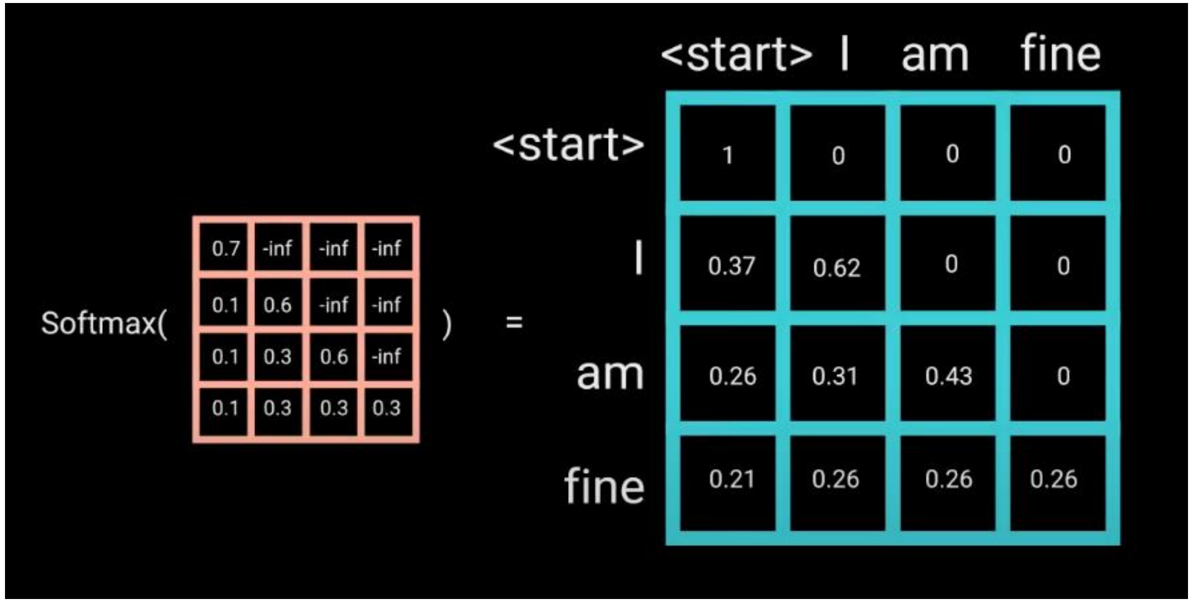


Image Credit: Vaswani, A. "Attention is all you need." Advances in Neural Information Processing Systems (2017). https://towardsdatascience.com/illustrated-guide-to-transformers-step-by-step-explanation-f74876522bc0

Masked Multi-Head Attention







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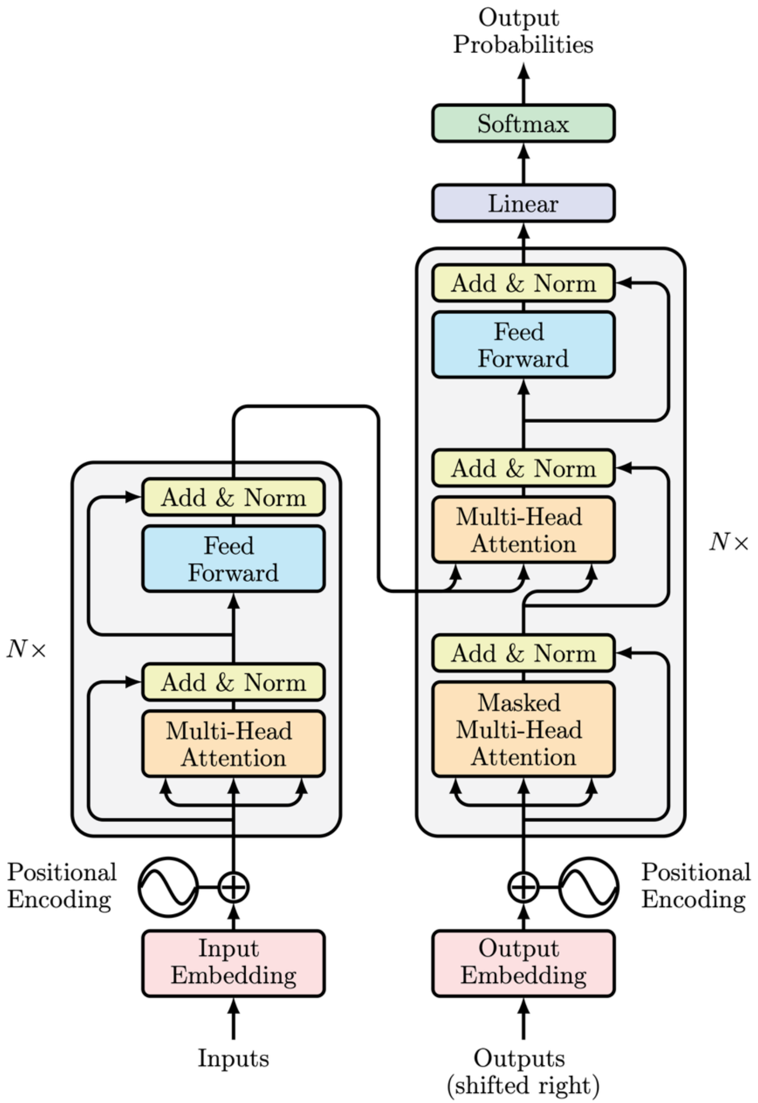
Limitations



- O(L^2) time/memory cost for self-attention

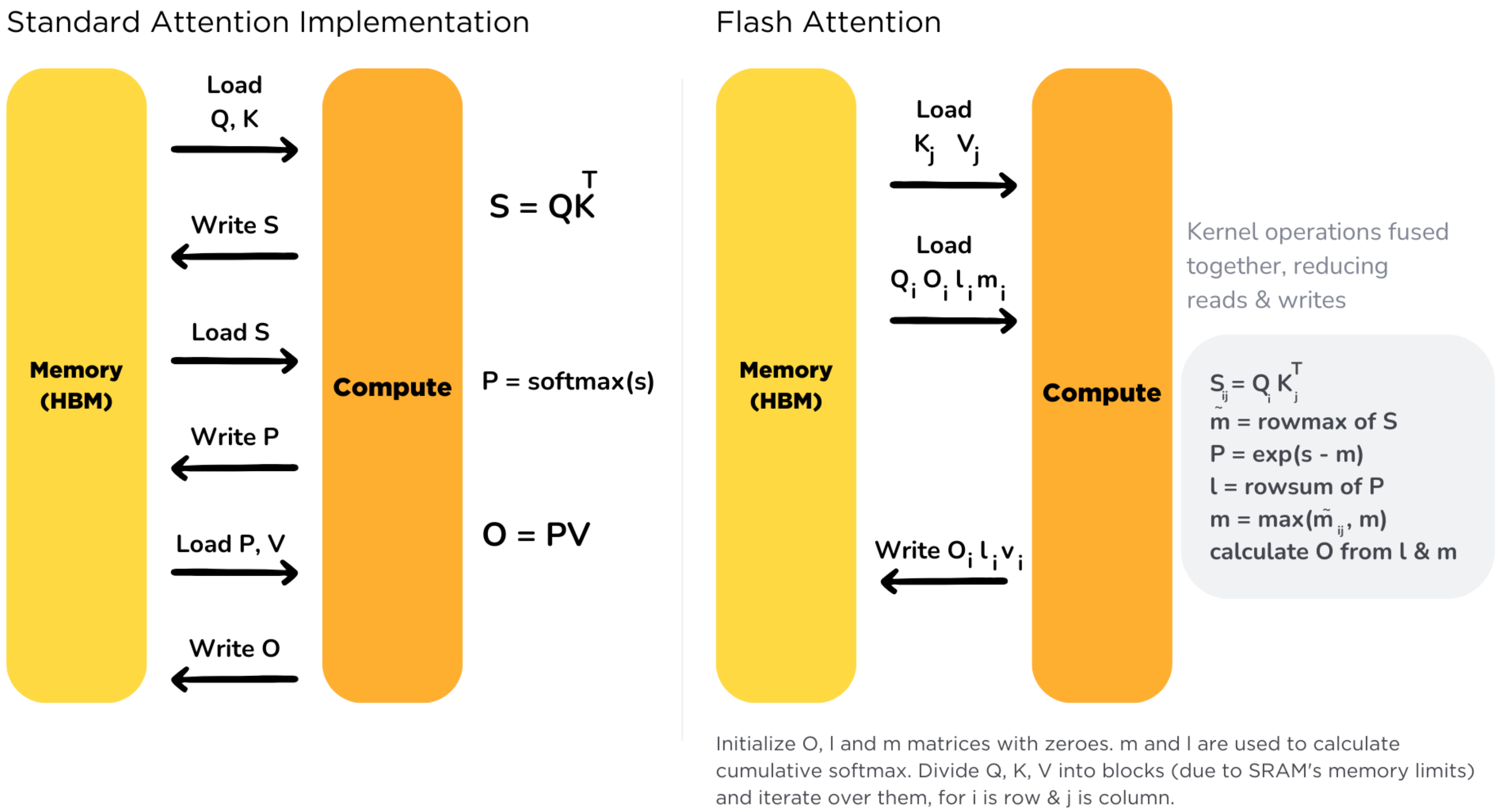
  Methods like Reformer [1] speed up attention to O(L log L) using locality-sensitive hashing techniques

- How can we incorporate prior knowledge into attention rather than having a fully connected attention?
  - Encourage sparse attention
  - Inject known graph structures
  - ……

[1] Kitaev, Nikita, Łukasz Kaiser, and Anselm Levskaya. "Reformer: The efficient transformer." arXiv preprint arXiv:2001.04451 (2020). Image Credit: Vaswani, A. "Attention is all you need." Advances in Neural Information Processing Systems (2017).

Flash Attention [1]

Flash attention accelerates attention by using on-chip static random-access memory (SRAM, small memory but fast) to reduce the IO with high bandwidth memory (HBM, large memory but slow).



[1] Dao, Tri, et al. "Flashattention: Fast and memory-efficient exact attention with io-awareness." Advances in Neural Information Processing Systems 35 (2022): 16344-16359. Image Credit: https://huggingface.co/docs/text-generation-inference/en/conceptual/flash_attention

Outline

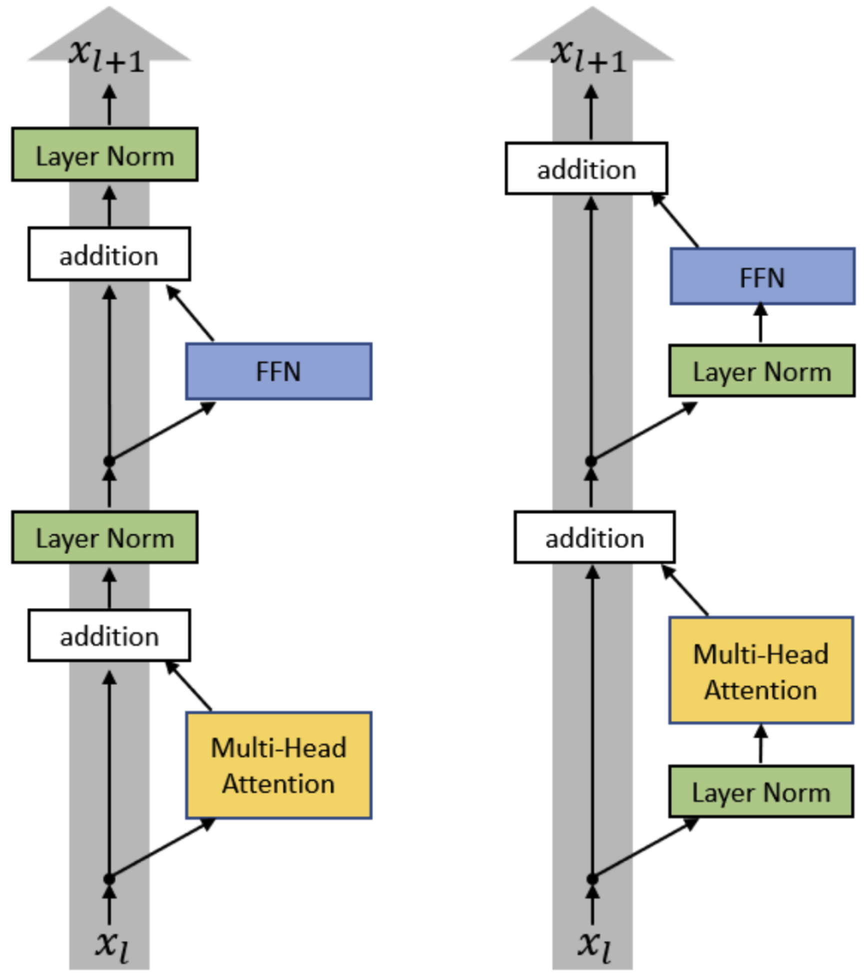
- Invariance & Equivariance Principle
  - Translation equivariance in convolutions
  - Permutation equivariance and invariance

- Models for Sets
  - DeepSets: representation theorem of permutation-invariant set functions & architecture
  - DeepSets: permutation-equivariant linear mapping & architecture

- Models for Sequences
  - Transformers
  - Positional encoding vs. Rotary Positional Embeddings (RoPE)
  - Attention & Flash Attention
  - **Pre-norm vs. post-norm**
  - Vision Transformers (ViT) & Swin Transformers

Pre-Norm vs. Post-Norm

Where to place the Layer Normalization?



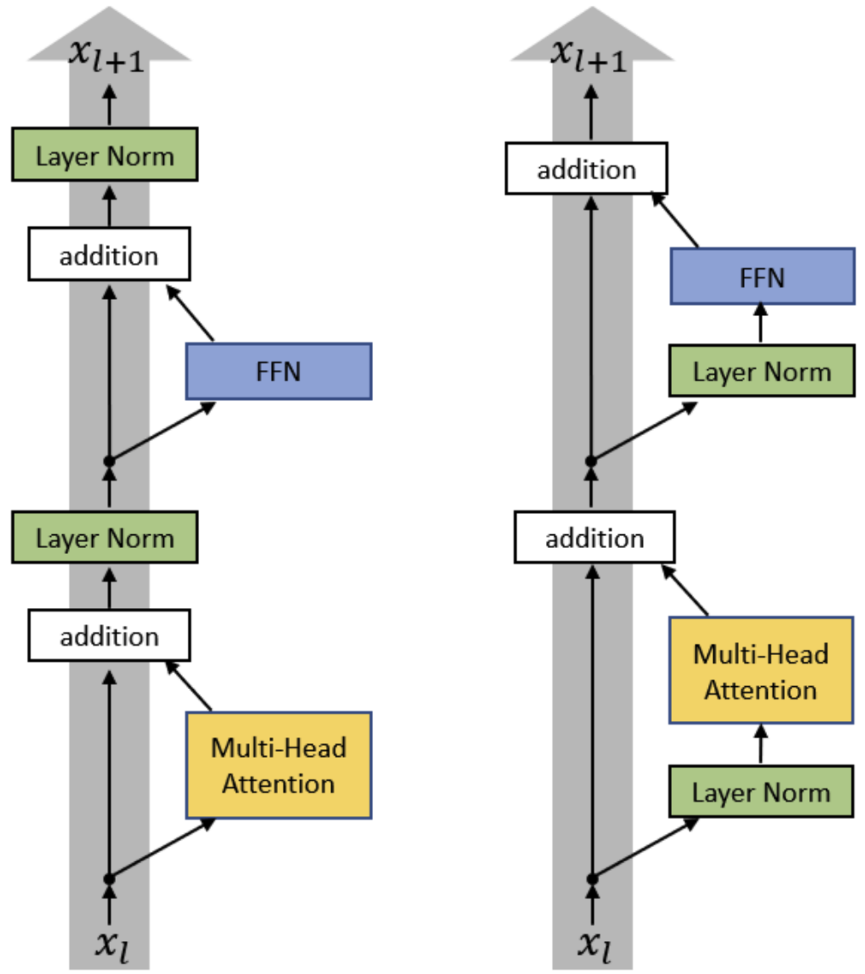
Post-Norm Pre-Norm

Image Credit: Xiong, Ruibin, et al. "On layer normalization in the transformer architecture." International Conference on Machine Learning. PMLR, 2020.

Pre-Norm vs. Post-Norm

Where to place the Layer Normalization?

- Gradient norm in the Post-Norm Transformer is large for parameters near the output and will be likely to decay as the layer gets closer to input



Post-Norm Pre-Norm

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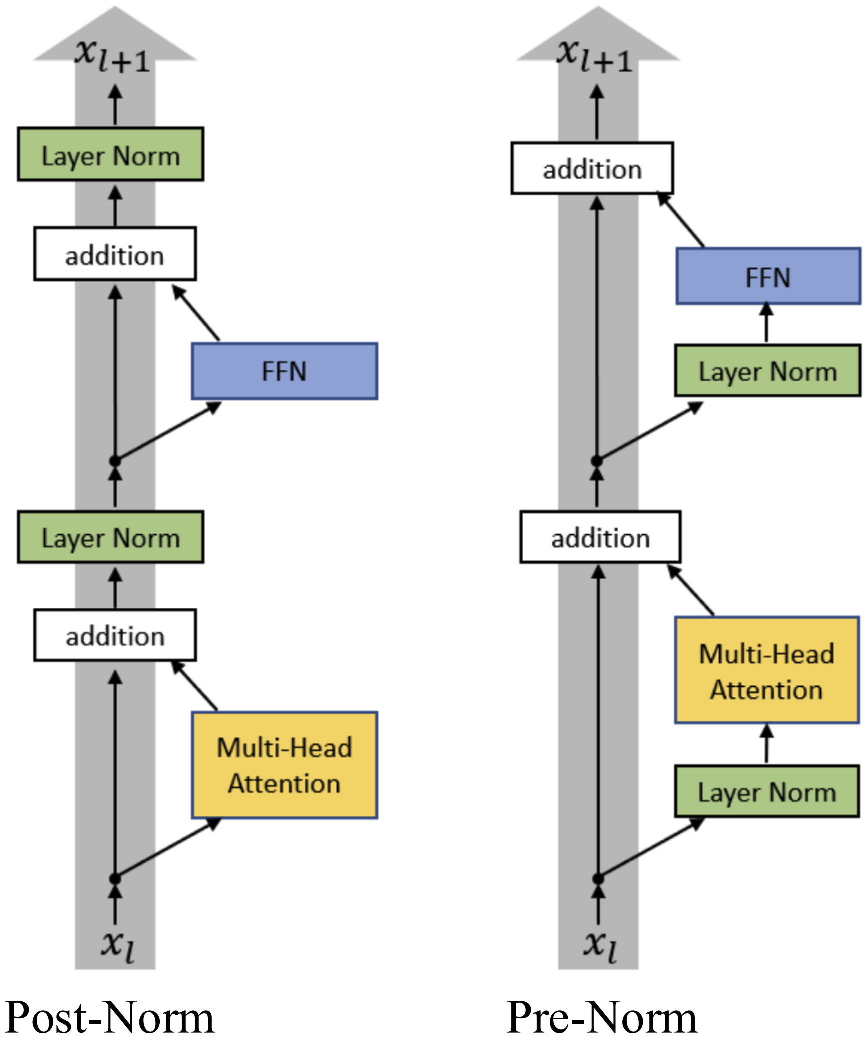
Pre-Norm vs. Post-Norm

Where to place the Layer Normalization?

- Gradient norm in the Post-Norm Transformer is large for parameters near the output and will be likely to decay as the layer gets closer to input

- Training the Pre-Norm Transformer does not rely on the learning rate warm-up stage and can be trained much faster than the Post-Norm



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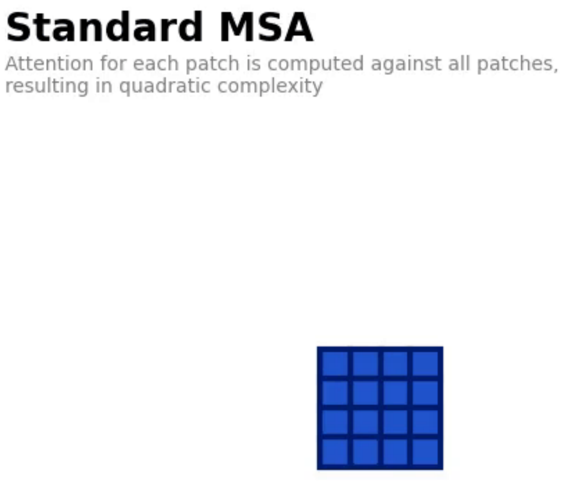
Extensions: Vision Transformers [1]

[1] Dosovitskiy, Alexey, et al. "An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale." International Conference on Learning Representations. 2020. Image Credit: https://github.com/lucidrains/vit-pytorch

Extensions: Swin Transformers [1]

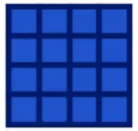


[1] Liu, Ze, et al. "Swin transformer: Hierarchical vision transformer using shifted windows." Proceedings of the IEEE/CVF international conference on computer vision. 2021. Image Credit: https://towardsdatascience.com/a-comprehensive-guide-to-swin-transformer-64965f89d14c

Extensions: Swin Transformers

Standard MSA

Attention for each patch is computed against all patches, resulting in quadratic complexity

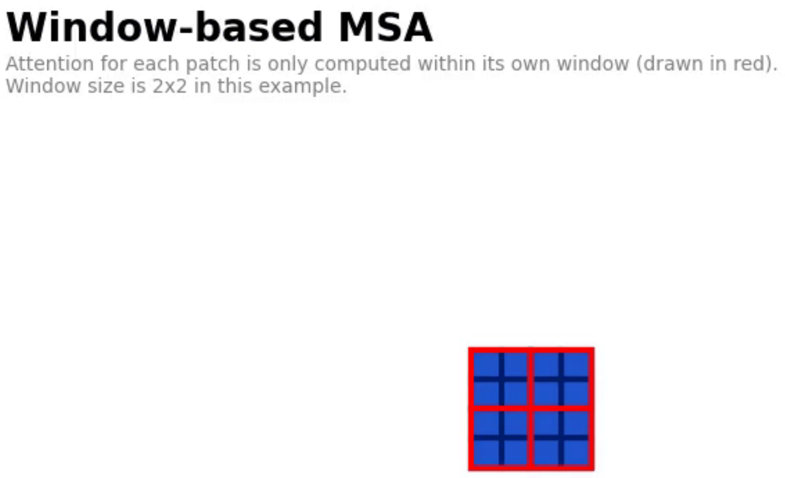


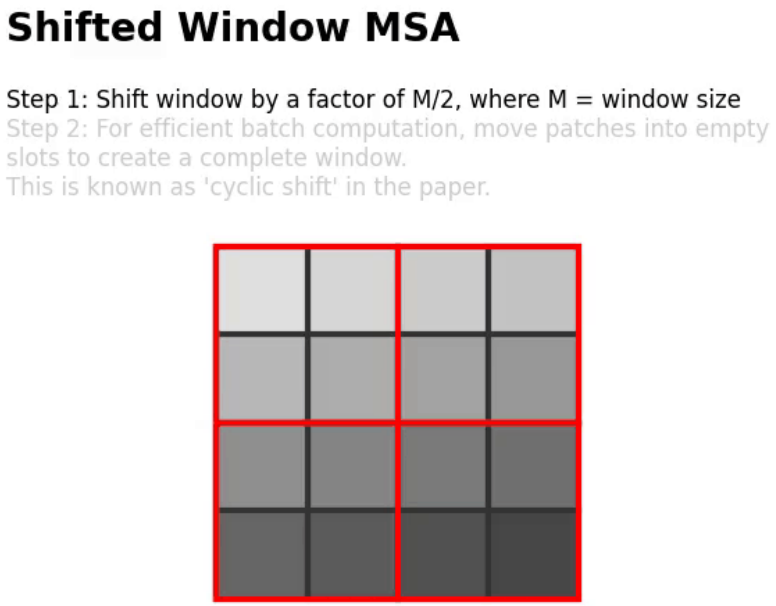
Window-based MSA

Attention for each patch is only computed within its own window (drawn in red). Window size is 2x2 in this example.

Image Credit: https://towardsdatascience.com/a-comprehensive-guide-to-swin-transformer-64965f89d14c

Extensions: Swin Transformers





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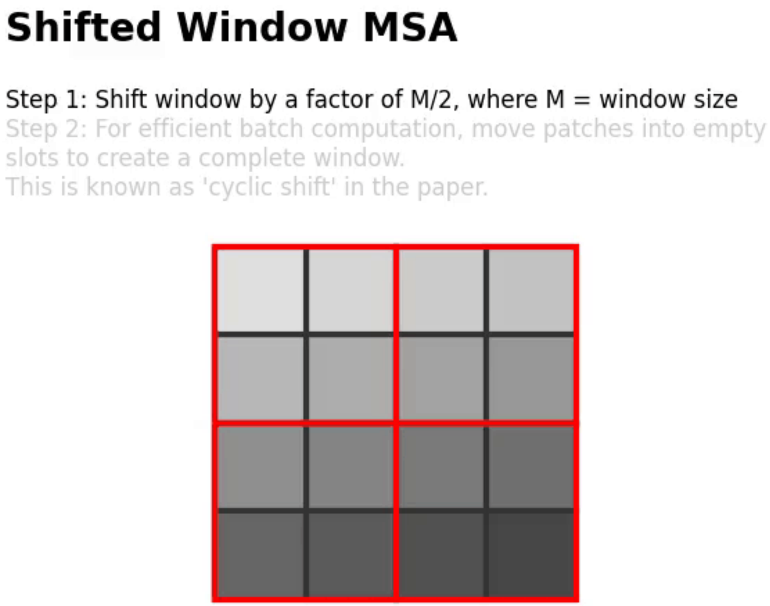
Extensions: Swin Transformers



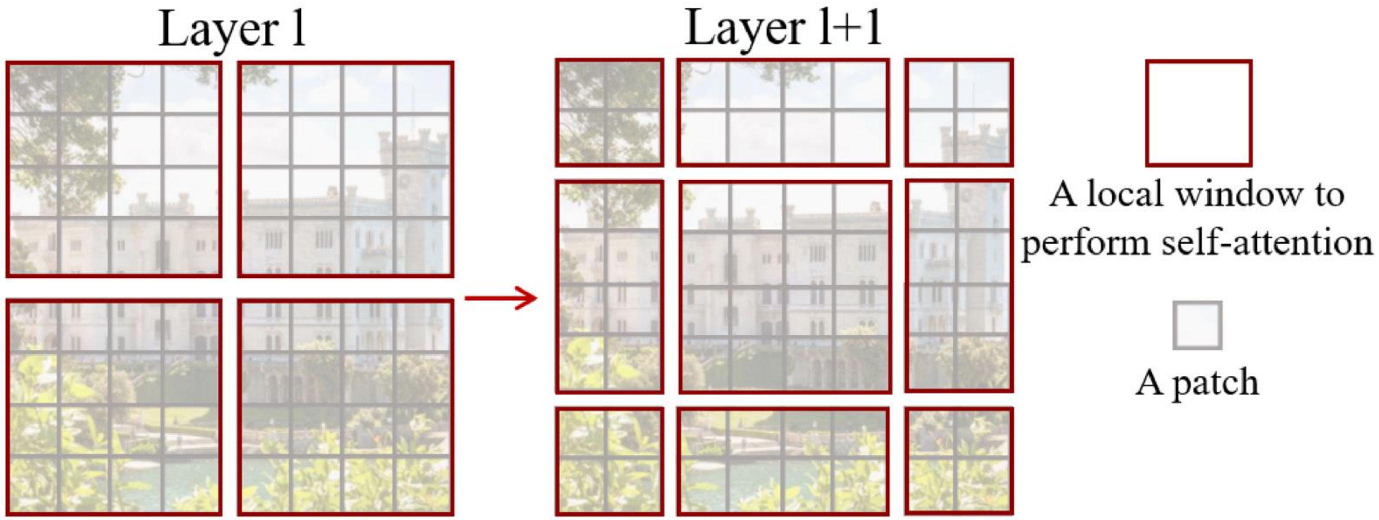
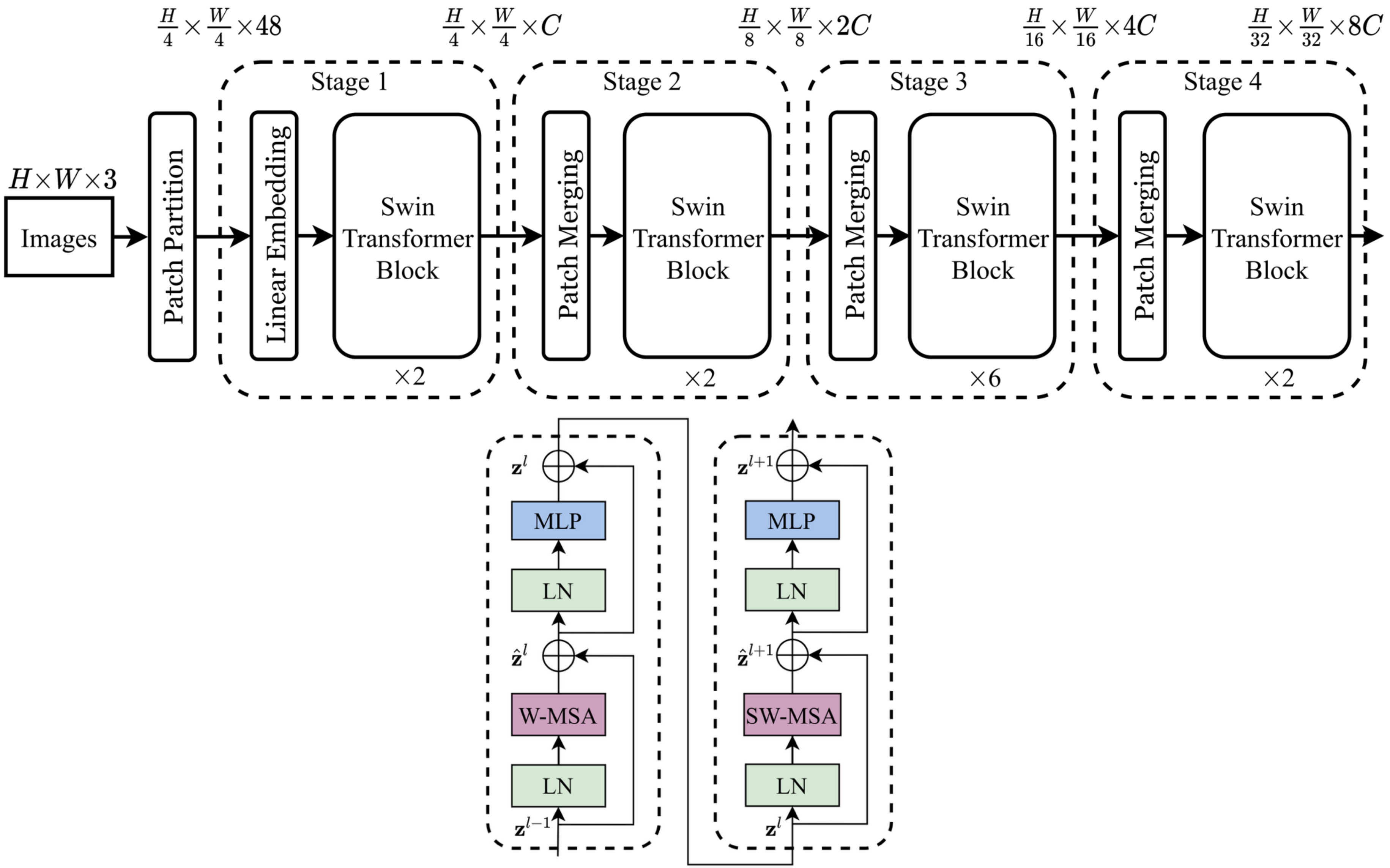


Image Credit: https://towardsdatascience.com/a-comprehensive-guide-to-swin-transformer-64965f89d14c Liu, Ze, et al. "Swin transformer: Hierarchical vision transformer using shifted windows." Proceedings of the IEEE/CVF international conference on computer vision. 2021.

Extensions: Swin Transformers



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Questions?