EECE 571F: Deep Learning with Structures

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

Renjie Liao

University of British Columbia

Winter, Term 1, 2023

Course Scope

- Brief Intro to Deep Learning

- Geometric Deep Learning

  - Deep Learning Models for Sets and Sequences: Deep Sets & Transformers
  - Deep Learning Models for Graphs: Message Passing & Graph Convolution GNNs
  - Group Equivariant Deep Learning

- Probabilistic Deep Learning

  - Auto-regressive models, Large Language Models (LLMs)
  - Variational Auto-Encoders (VAEs) and Generative Adversarial Networks (GANs)
  - Energy based models (EBMs)
  - Diffusion/Score based models

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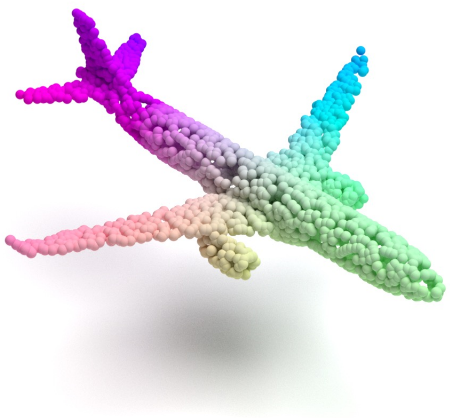
Motivating Applications for Sets

- 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

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

Revisit Convolution

Matrix multiplication views of (discrete) convolution:

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

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Matrix multiplication views of (discrete) convolution:

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

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

Convolution with padding

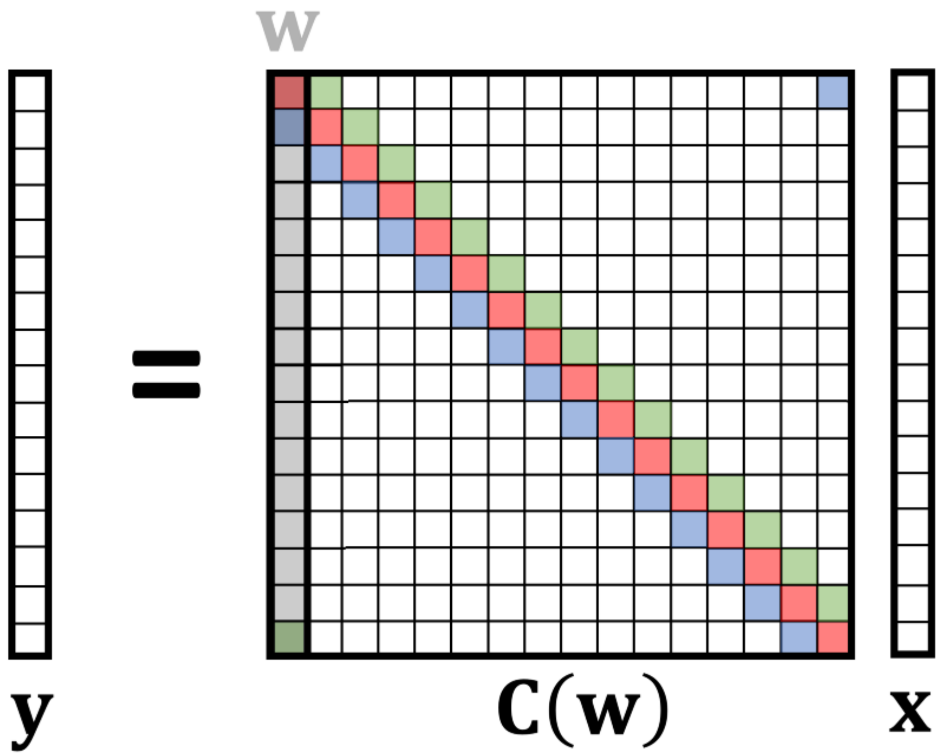
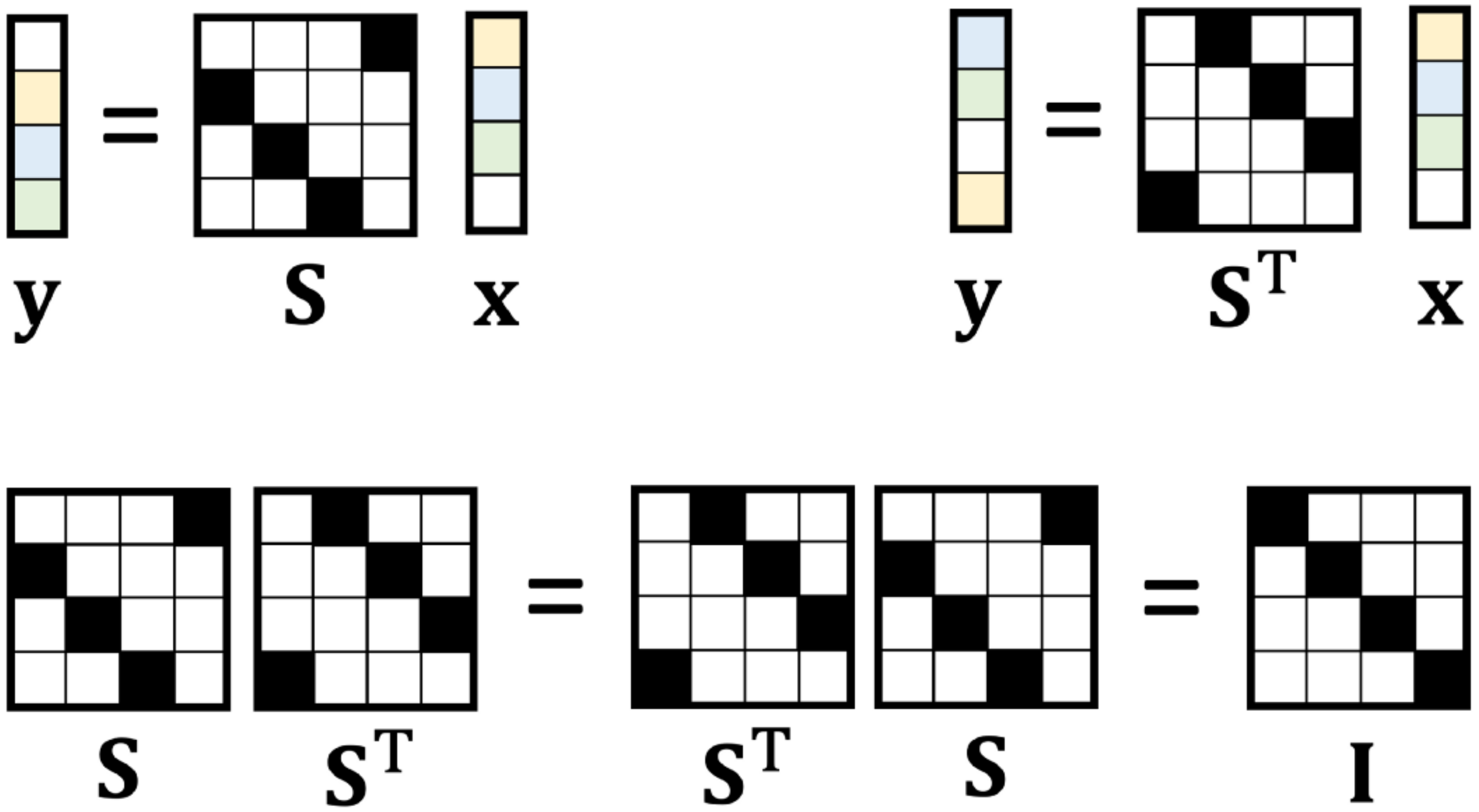


Image Credit: https://towardsdatascience.com/deriving-convolution-from-first-principles-4ff124888028

Translation/Shift Operator



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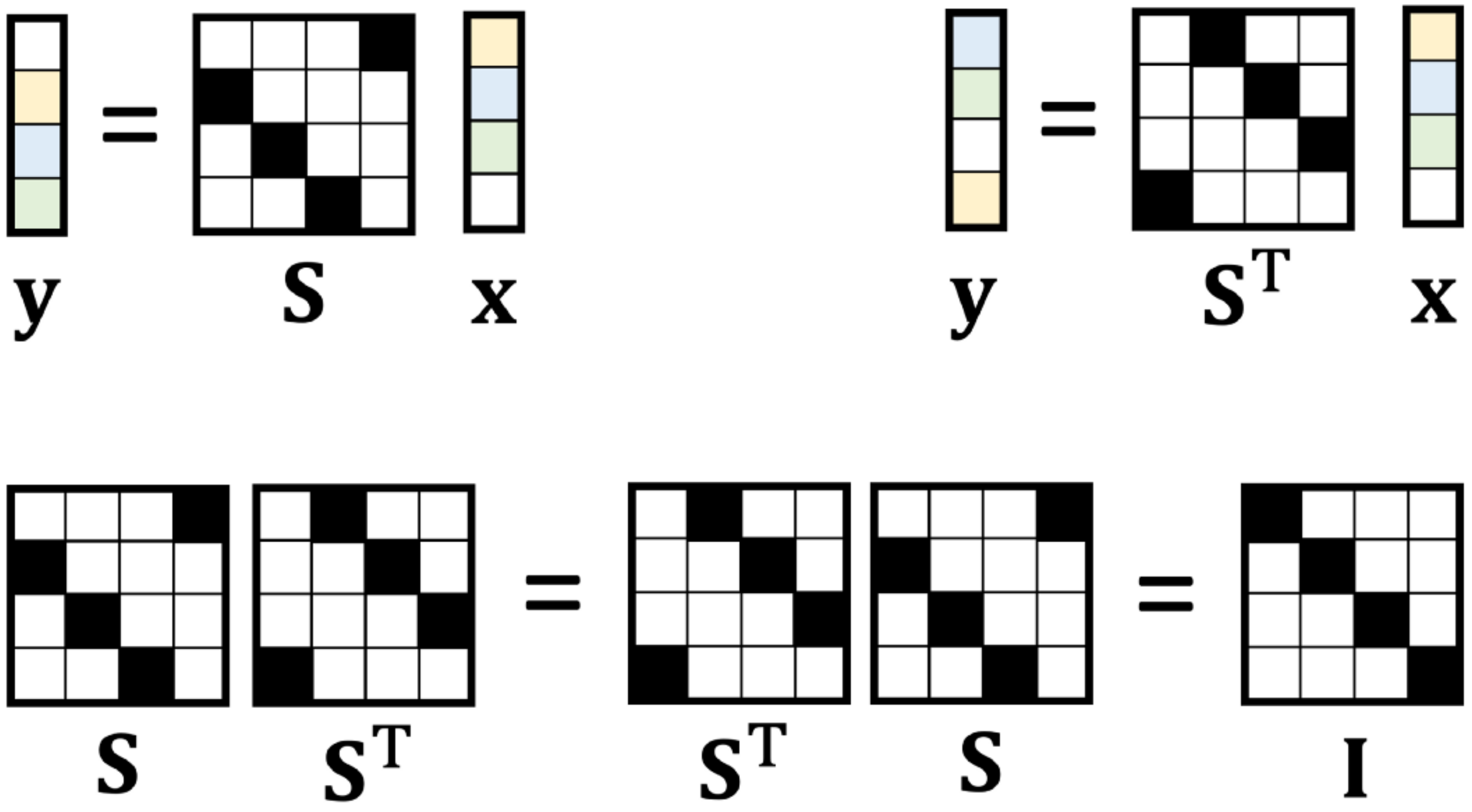
Translation/Shift Operator

Shift operator is also a circulant matrix!



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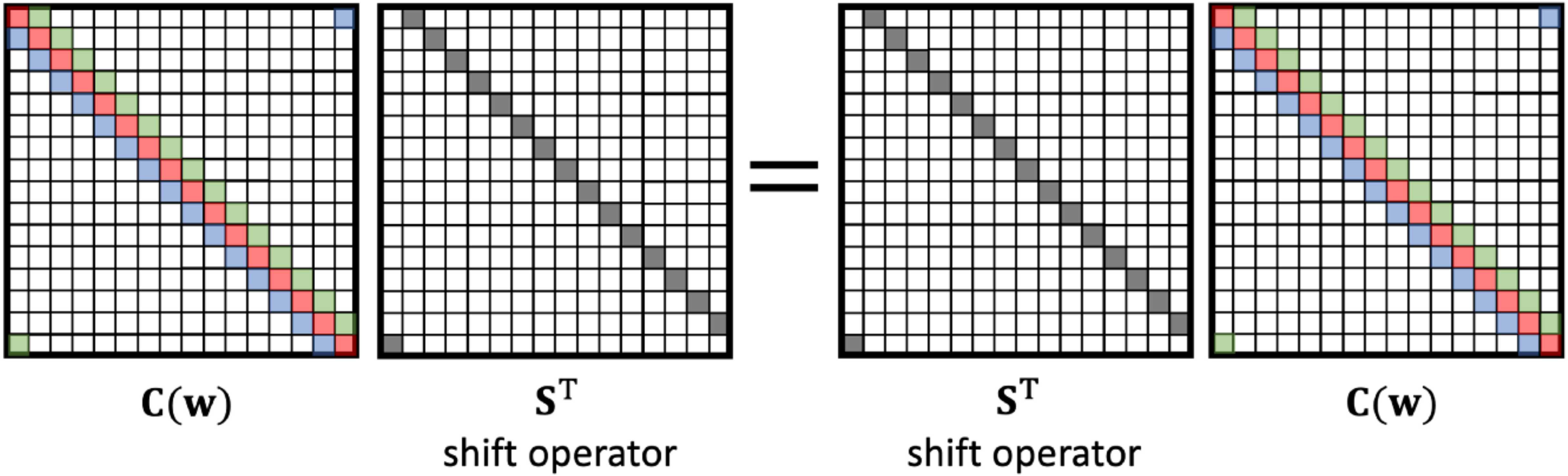
Translation/Shift Equivariance

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



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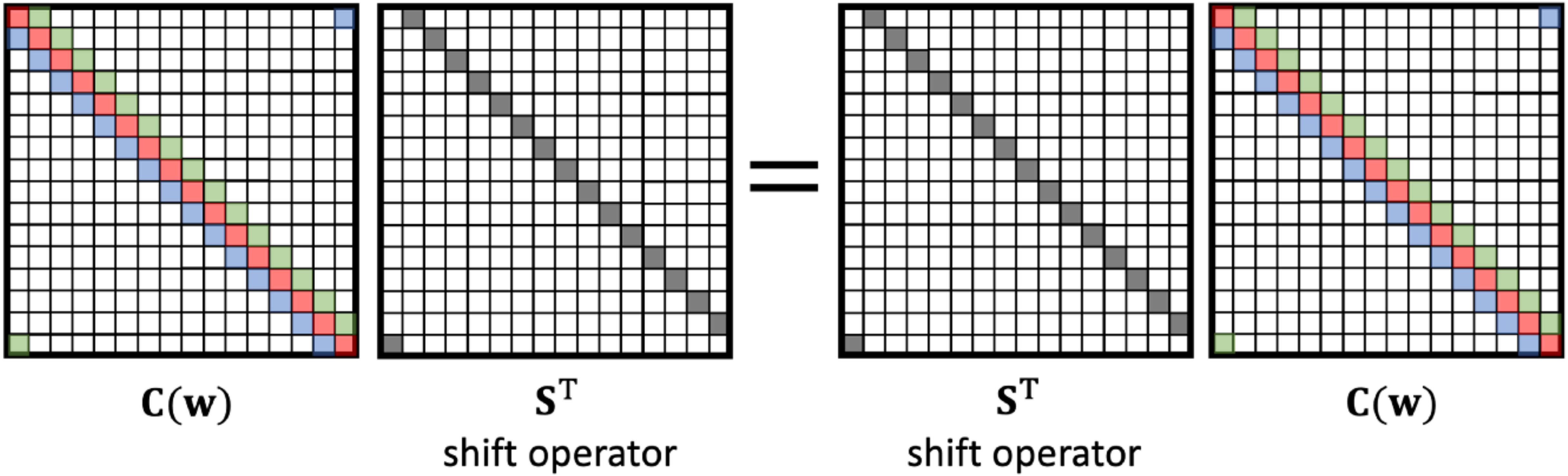

Convolution is translation equivariant, i.e., Conv(Shift(X)) = Shift(Conv(X))!

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Translation/Shift Invariance

Global pooling gives you shift-invariance!

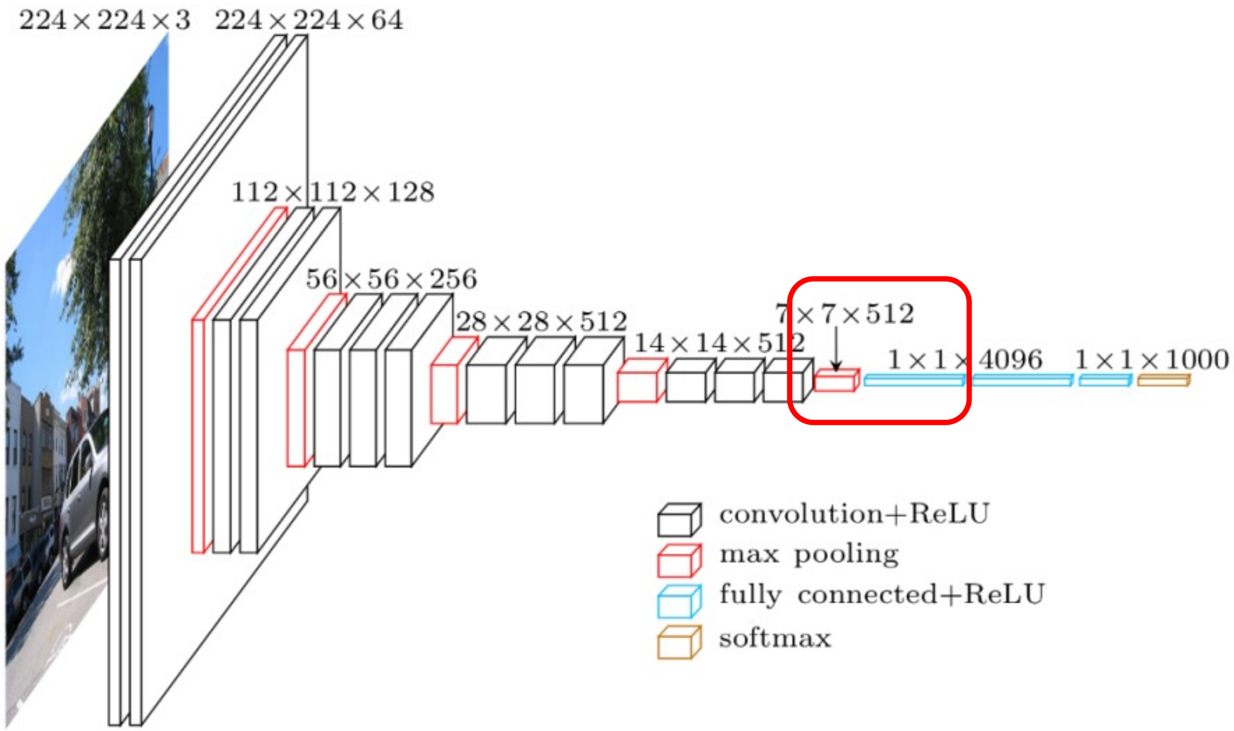
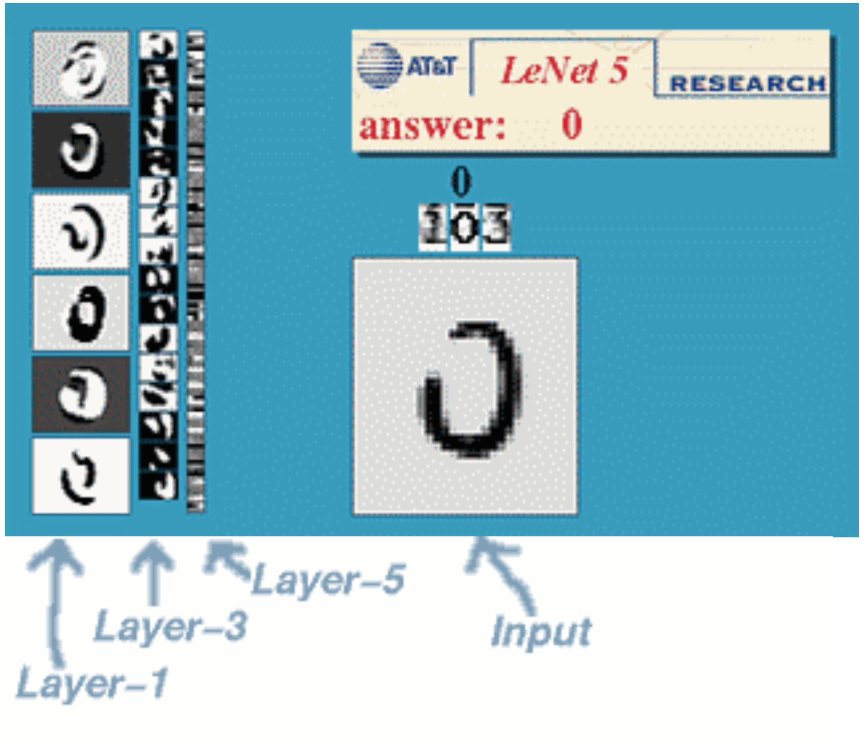
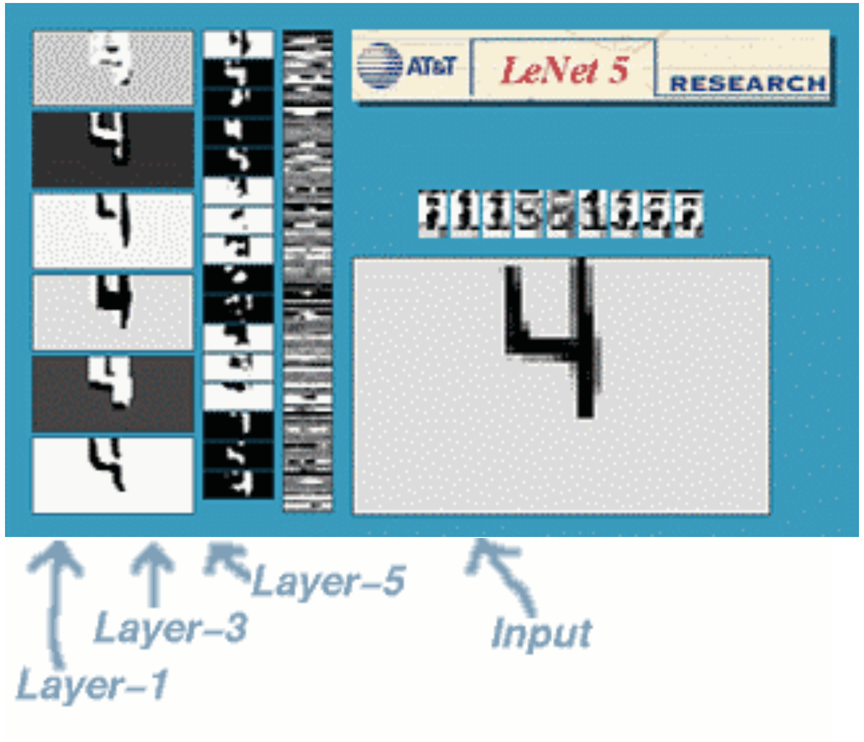


Image Credit: https://towardsdatascience.com/covolutional-neural-network-cb0883dd6529

Translation/Shift Equivariance Invariance

Yann LeCun's LeNet Demo:





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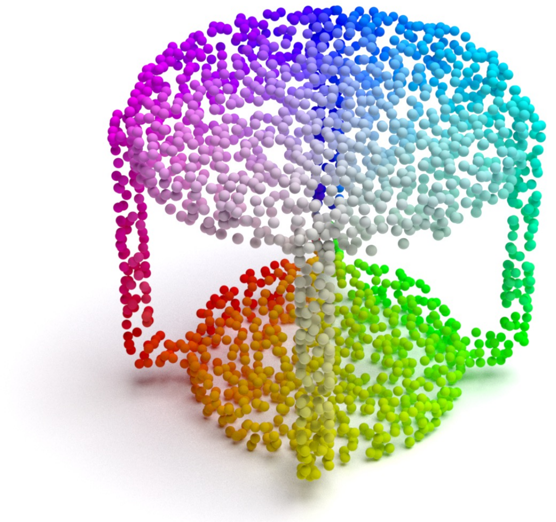
Permutation Invariance



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

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

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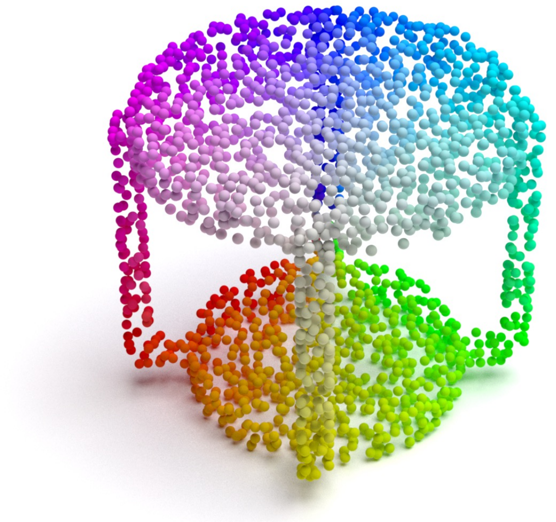

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$$\begin{bmatrix} 2 \\ 5 \\ 3 \\ 1 \\ 4 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{bmatrix}$$

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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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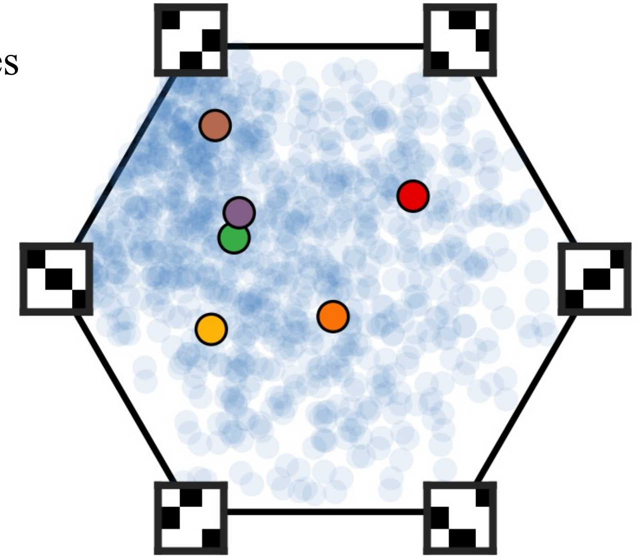
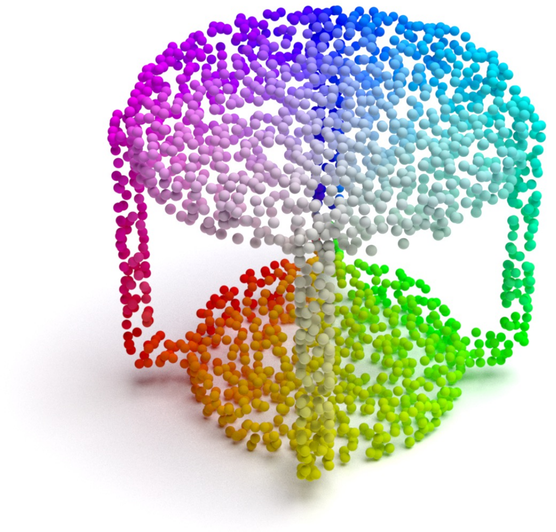


Image Credit: https://arxiv.org/pdf/1710.09508.pdf

Permutation Invariance



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

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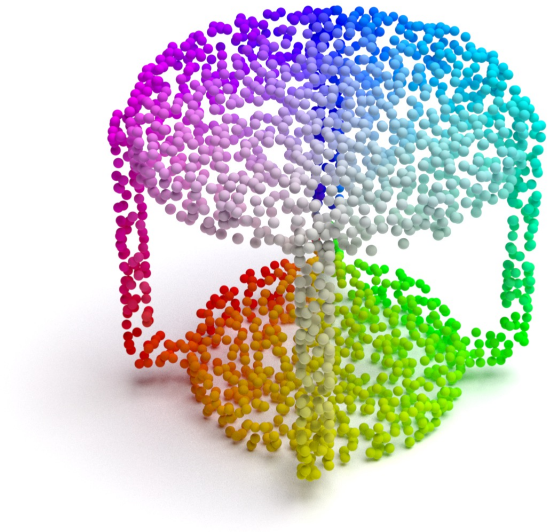
Permutation Equivariance



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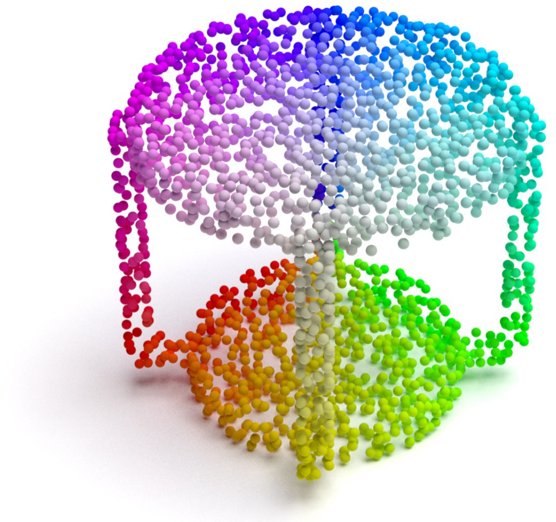

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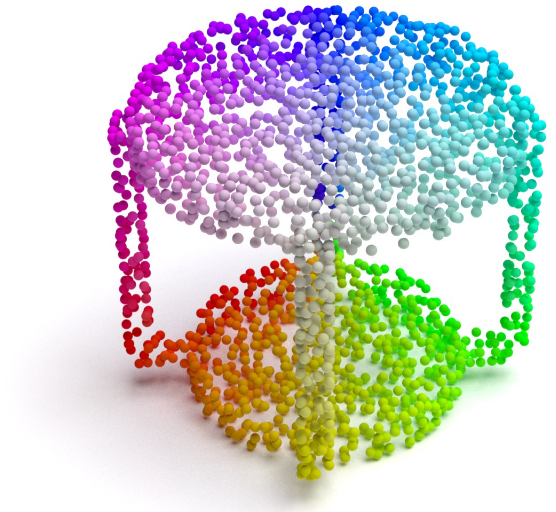

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More on Invariance & Equivariance

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

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

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

- 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

  Output: a label/vector per point

  Predictions of individual points are independent, e.g., image classification

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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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Sufficiency: summation is permutation invariant!

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2. Let $\phi(x) = 4^{-c(x)}$ Base 2 does not work! Why?
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Deep Learning for Sets

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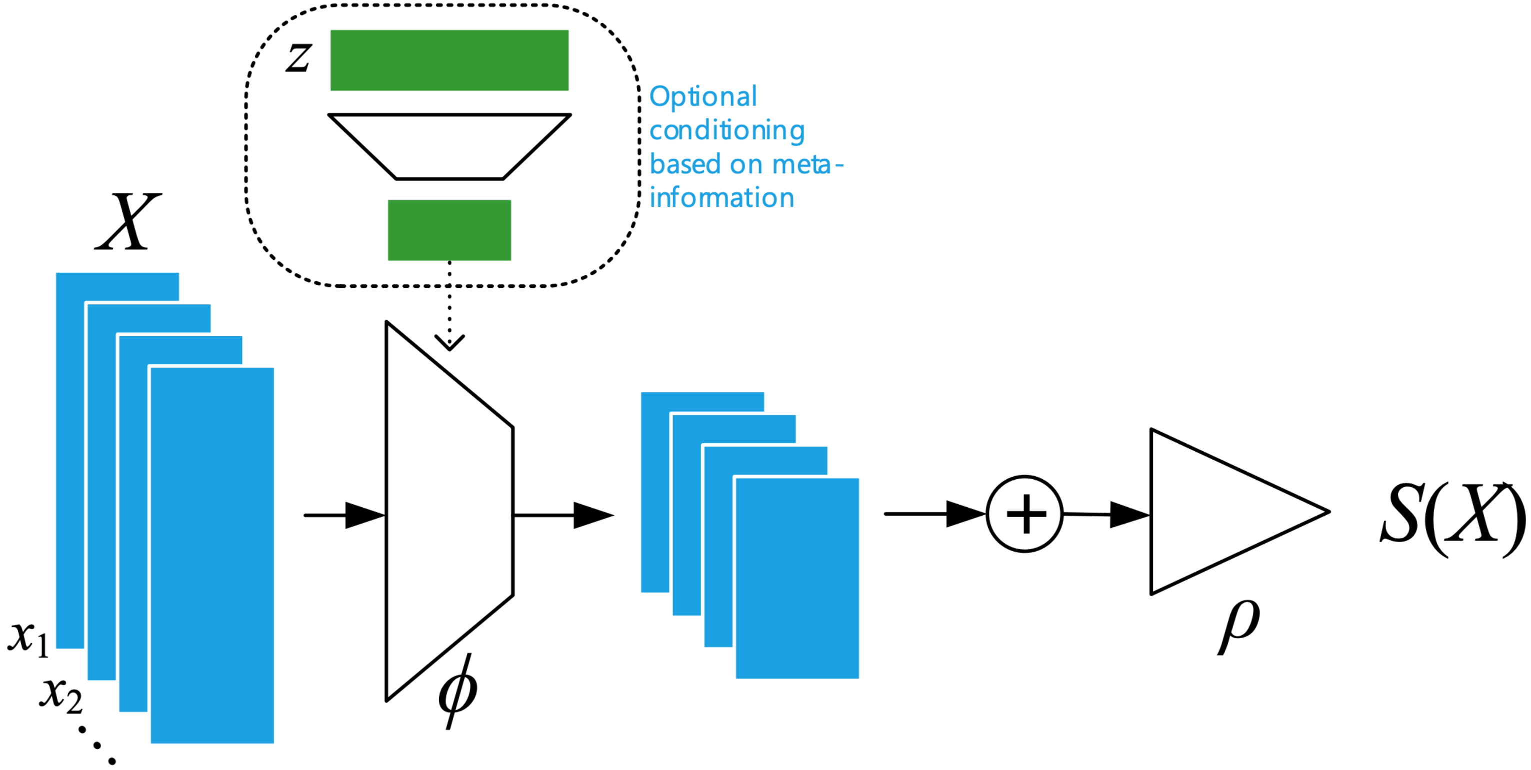
Invariant Architecture



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Deep Learning for Sets

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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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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

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

- Deep Sets [1]

Equivariant Architecture

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

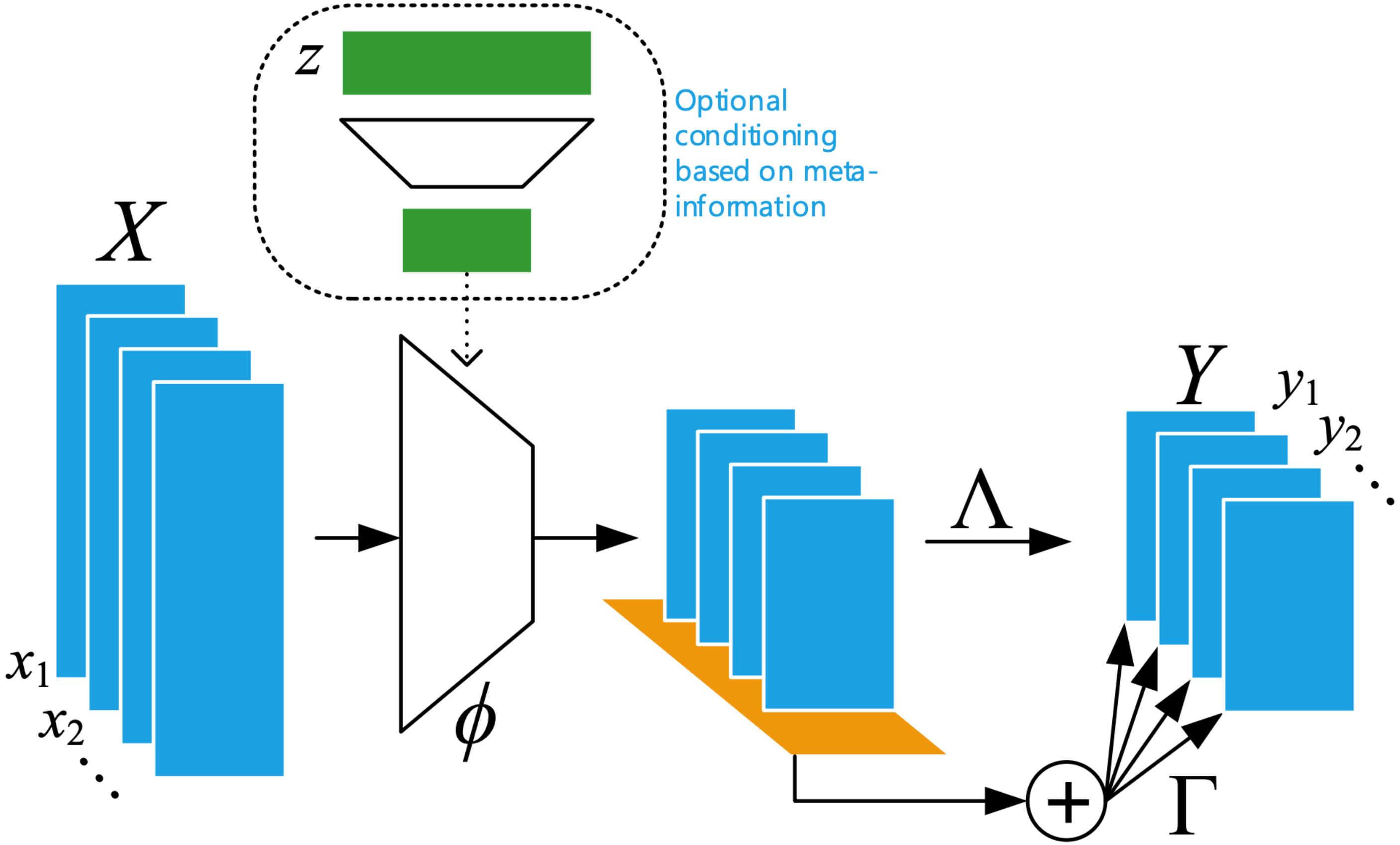


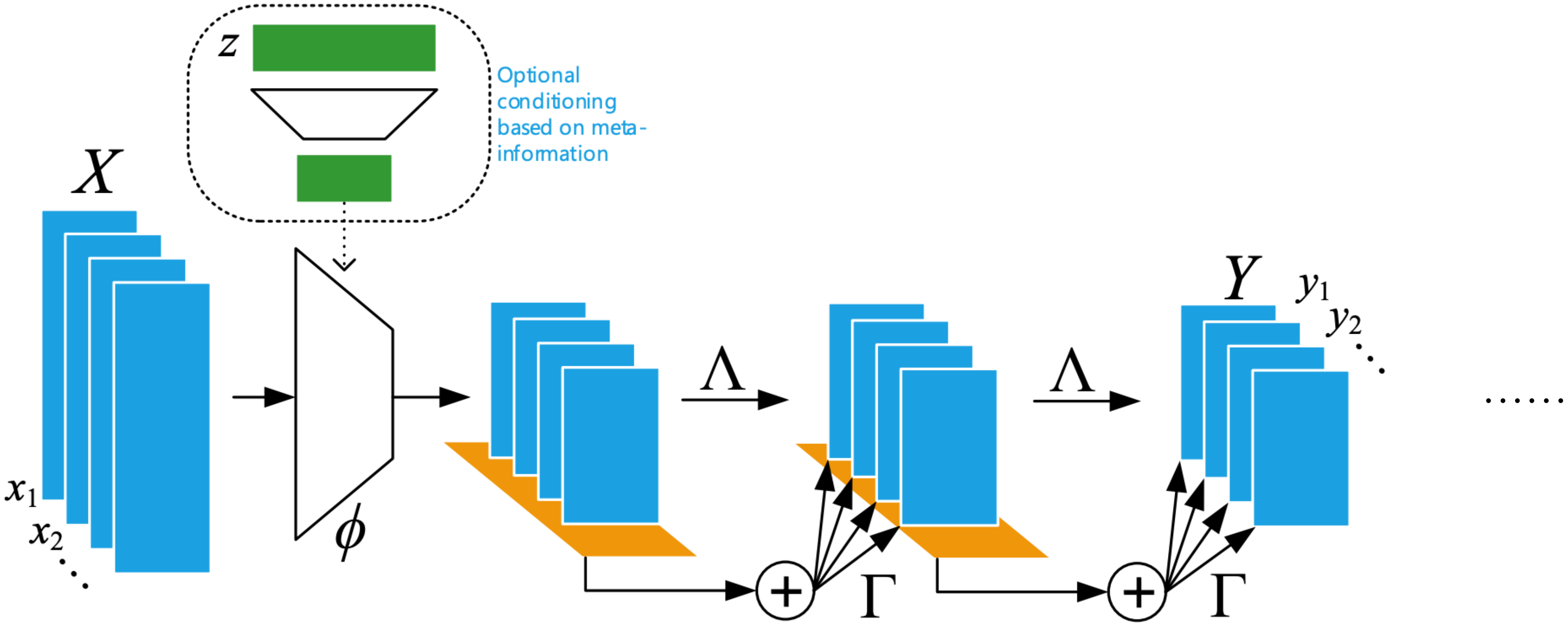
Image Credit: [1]

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

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

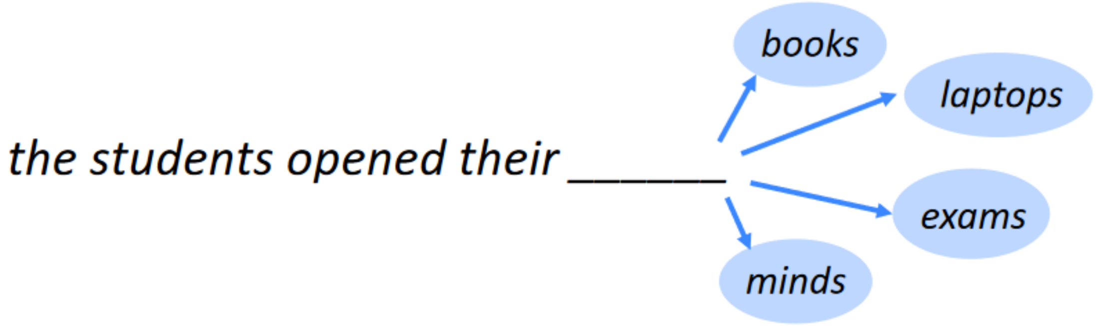

Image Credit: http://web.stanford.edu/class/cs224n/

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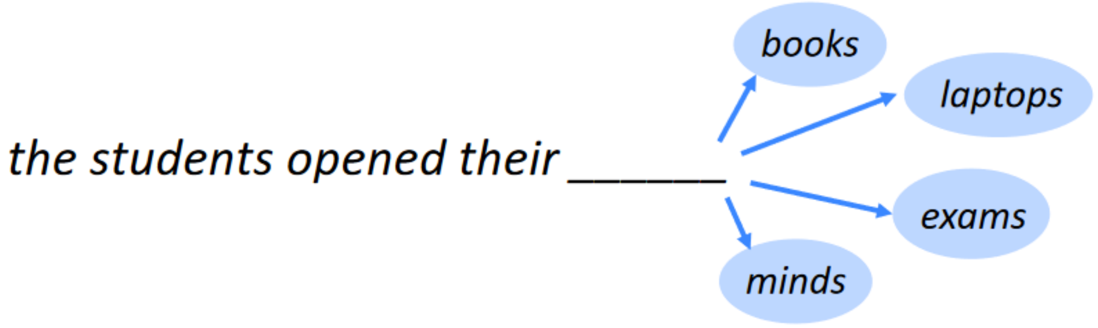

- Machine Translation

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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- Orders “may” be crucial for cognition

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

Deep Learning for Sequences

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https://towardsdatascience.com/illustrated-guide-to-transformers-step-by-step-explanation-f74876522bc0

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LSTM [3]
GRU [4]
Seq2Seq [5]
Transformer [6]

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Transformers

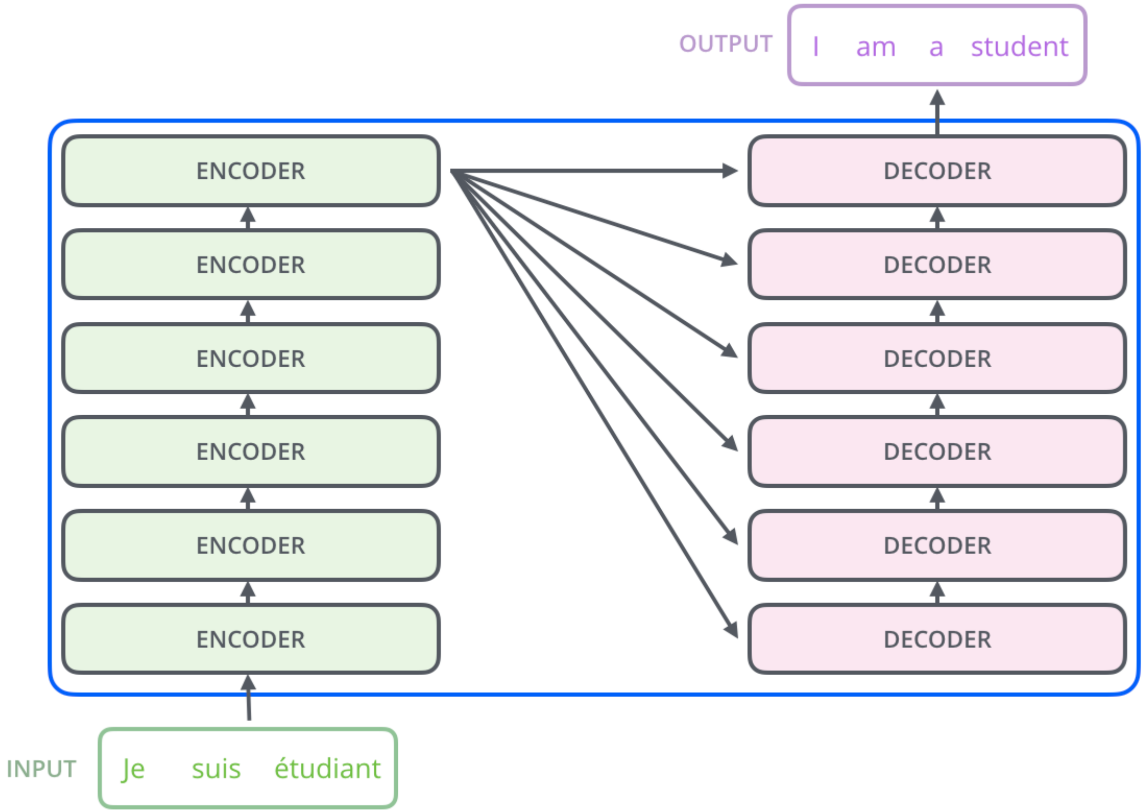
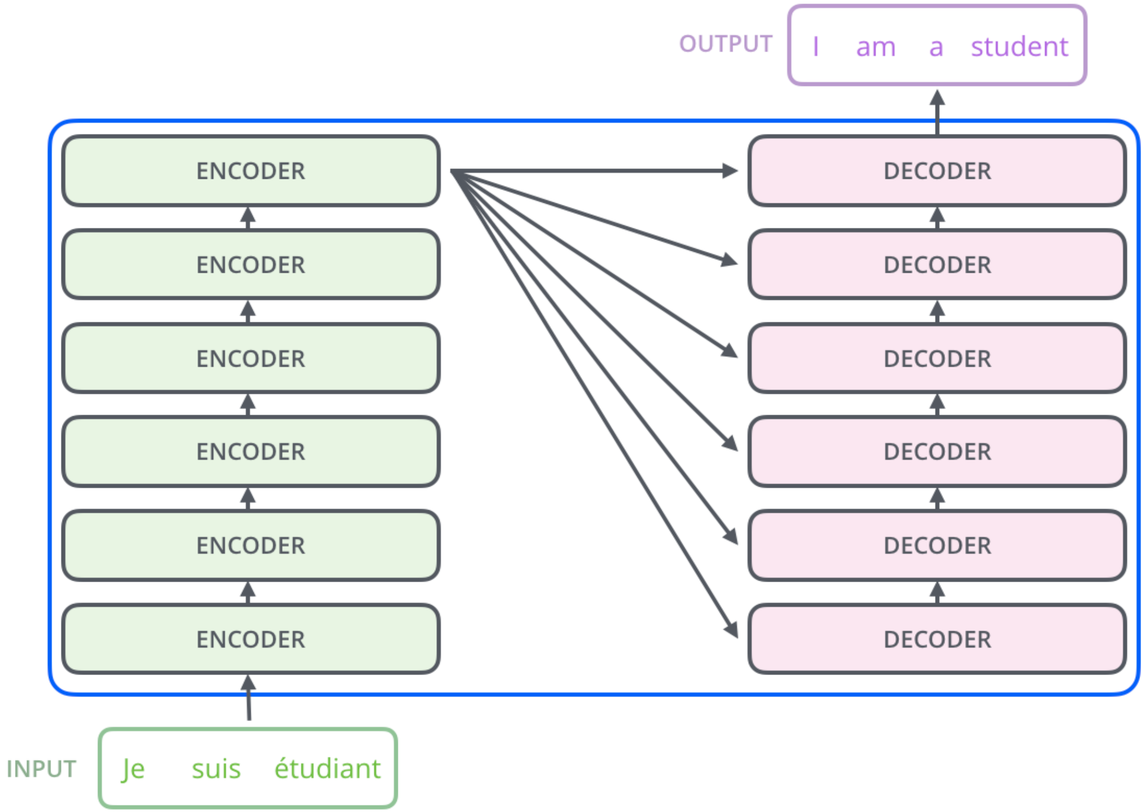
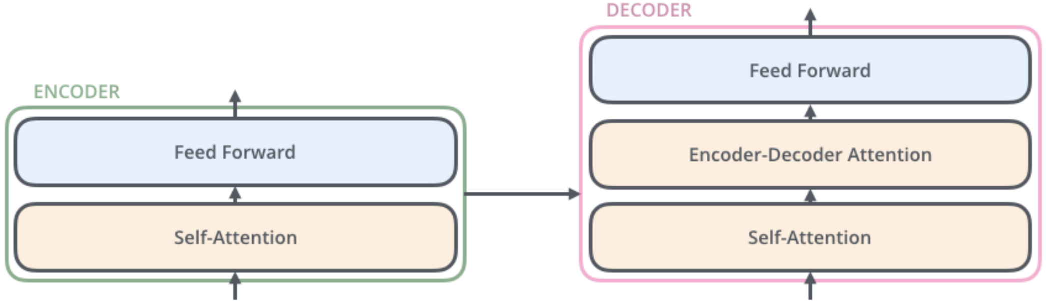


Image Credit: https://jalammar.github.io/illustrated-transformer/

Transformers





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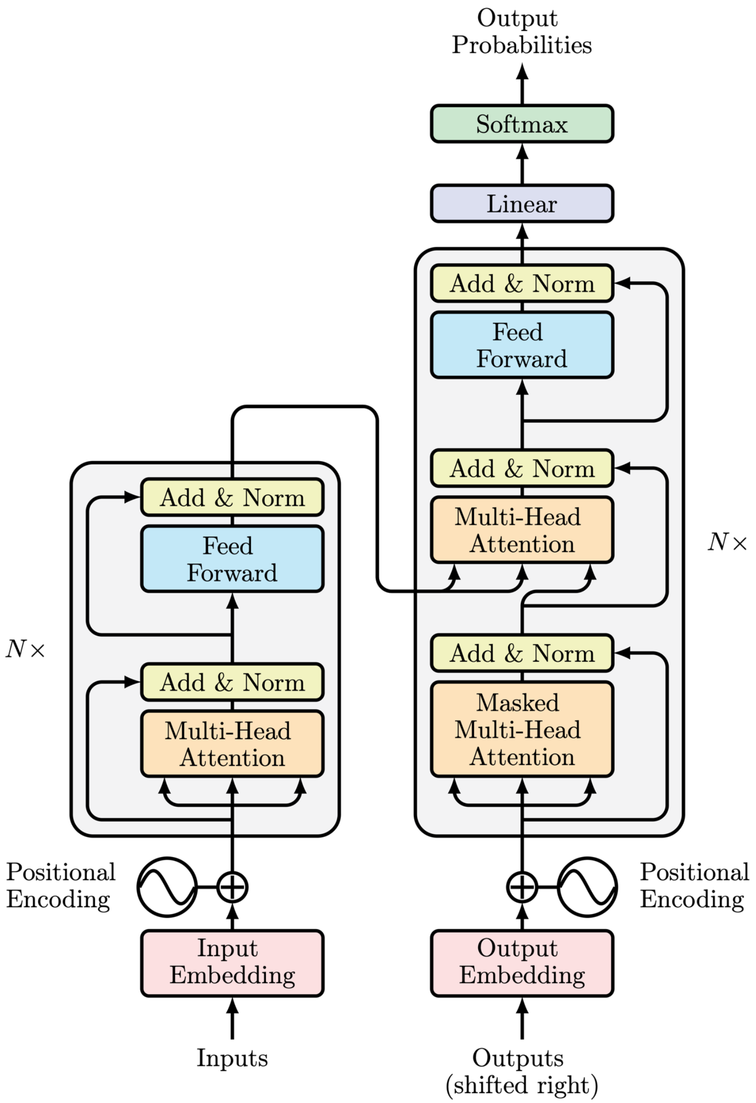


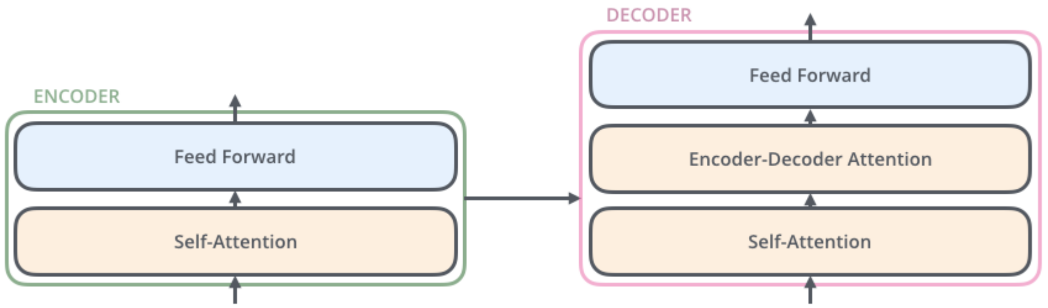
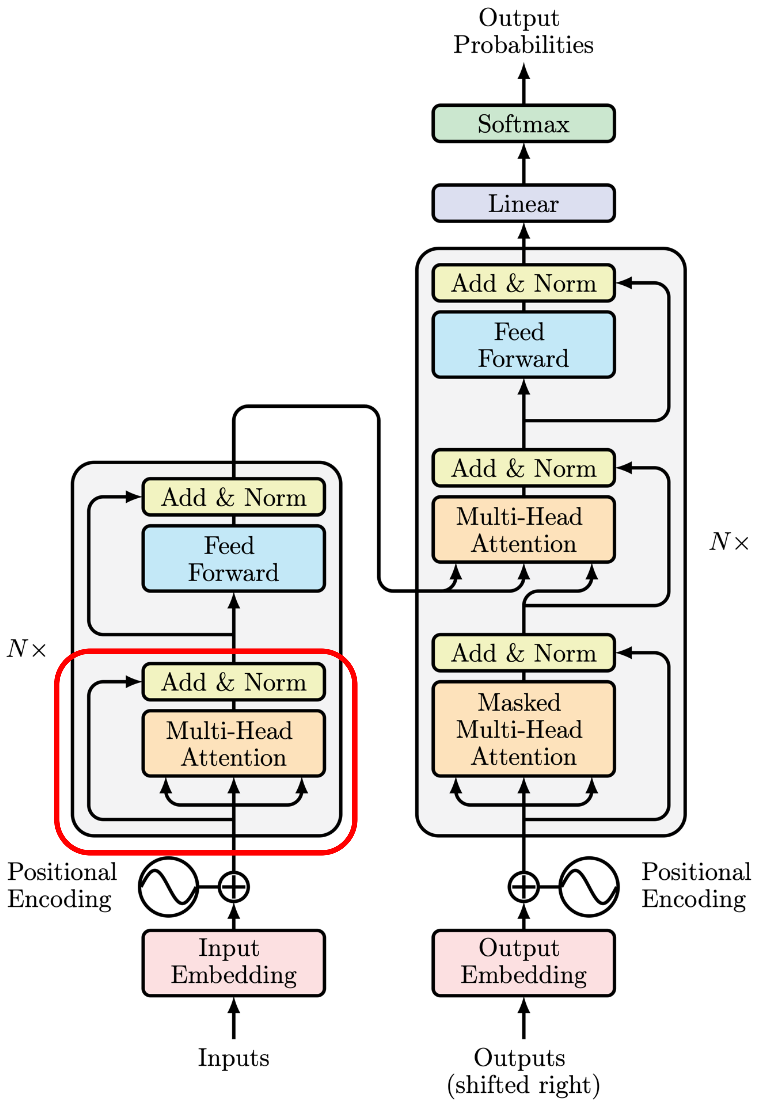
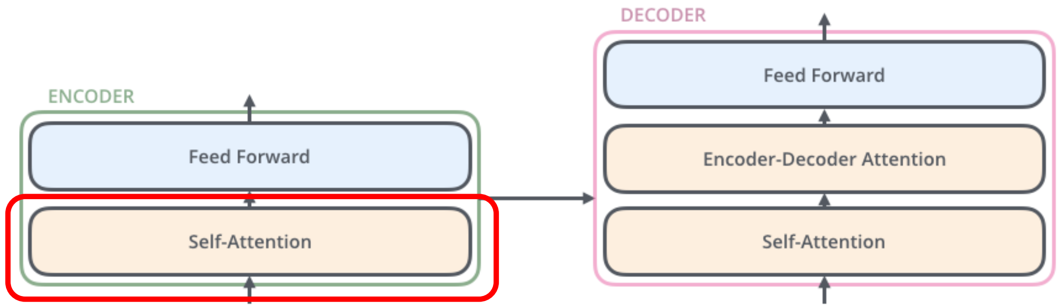


Image Credit: [6] & https://jalammar.github.io/illustrated-transformer/

Transformers





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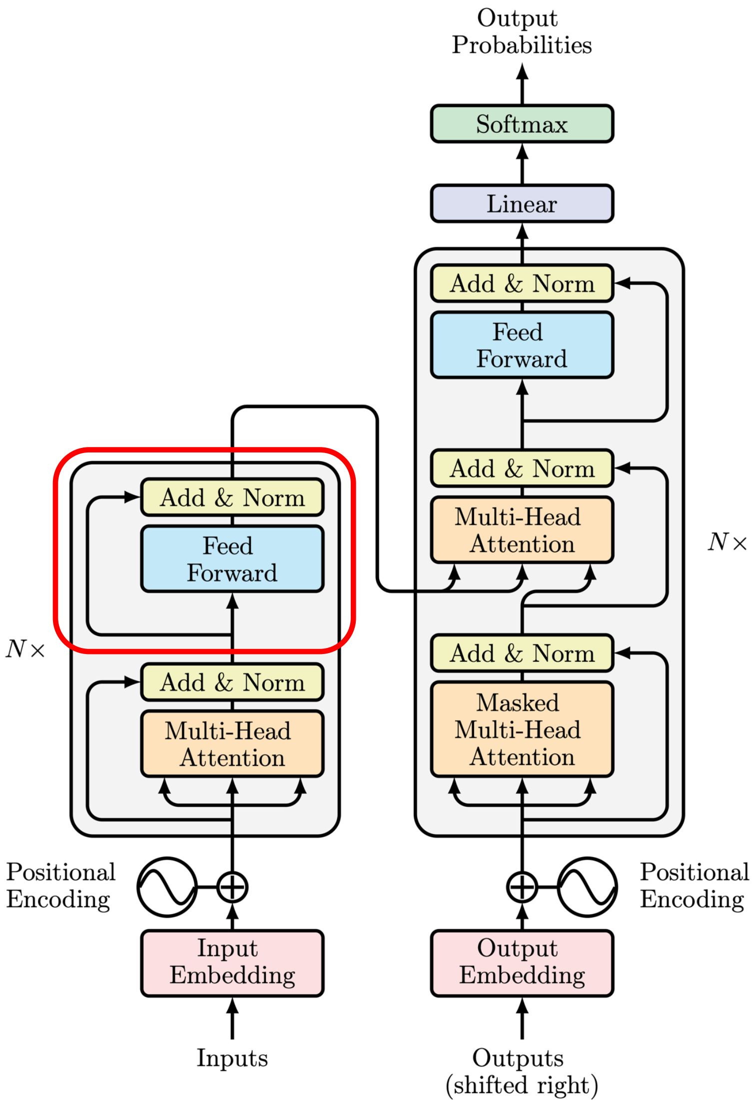
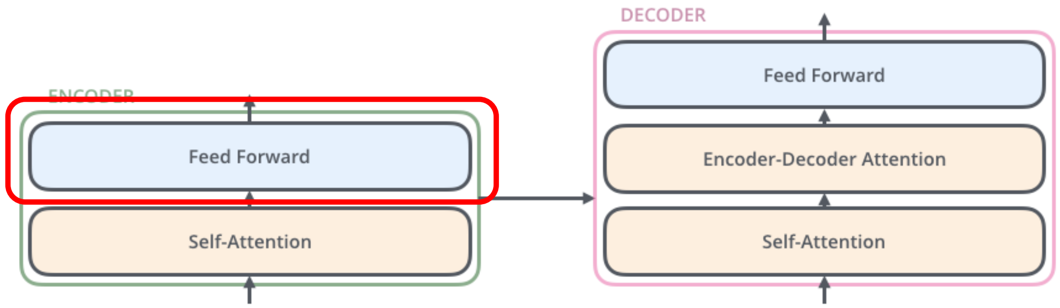
Transformers





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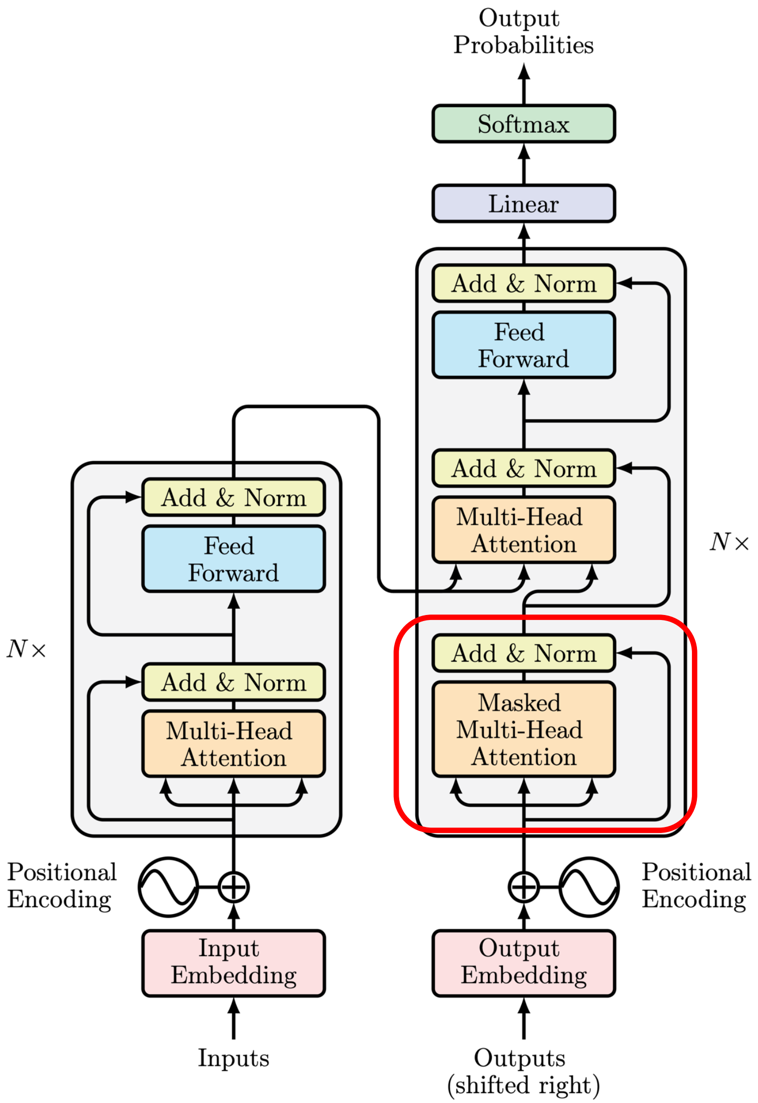
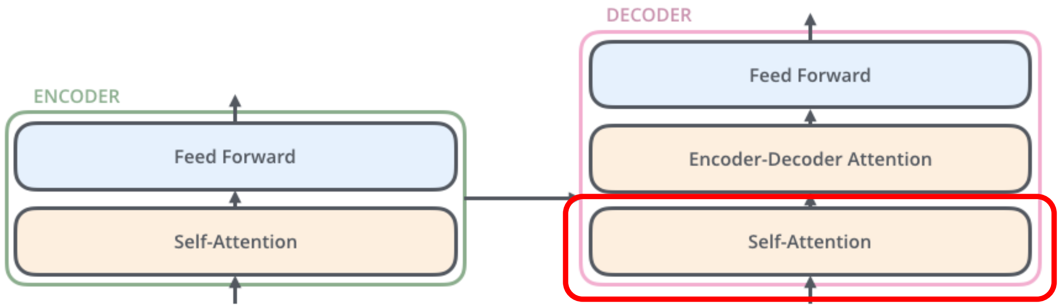
Transformers





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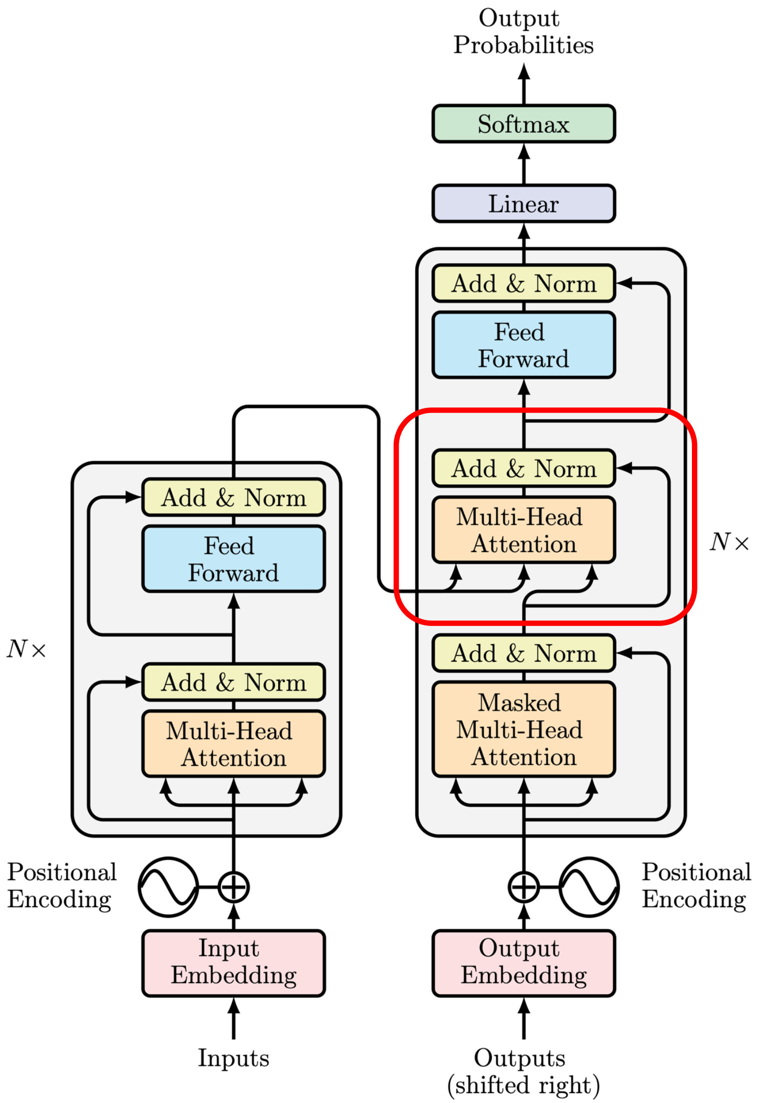

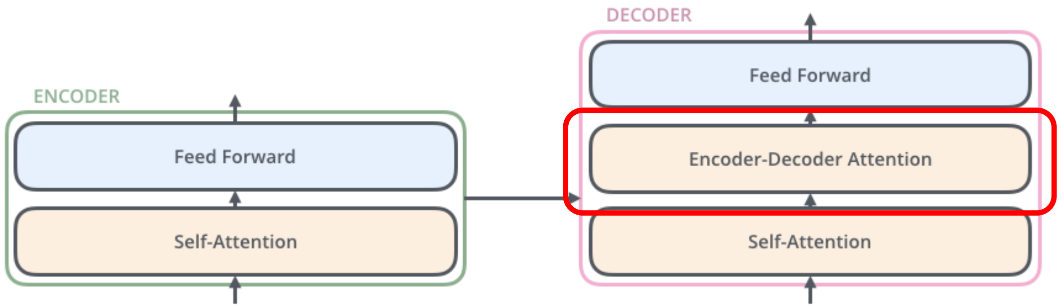

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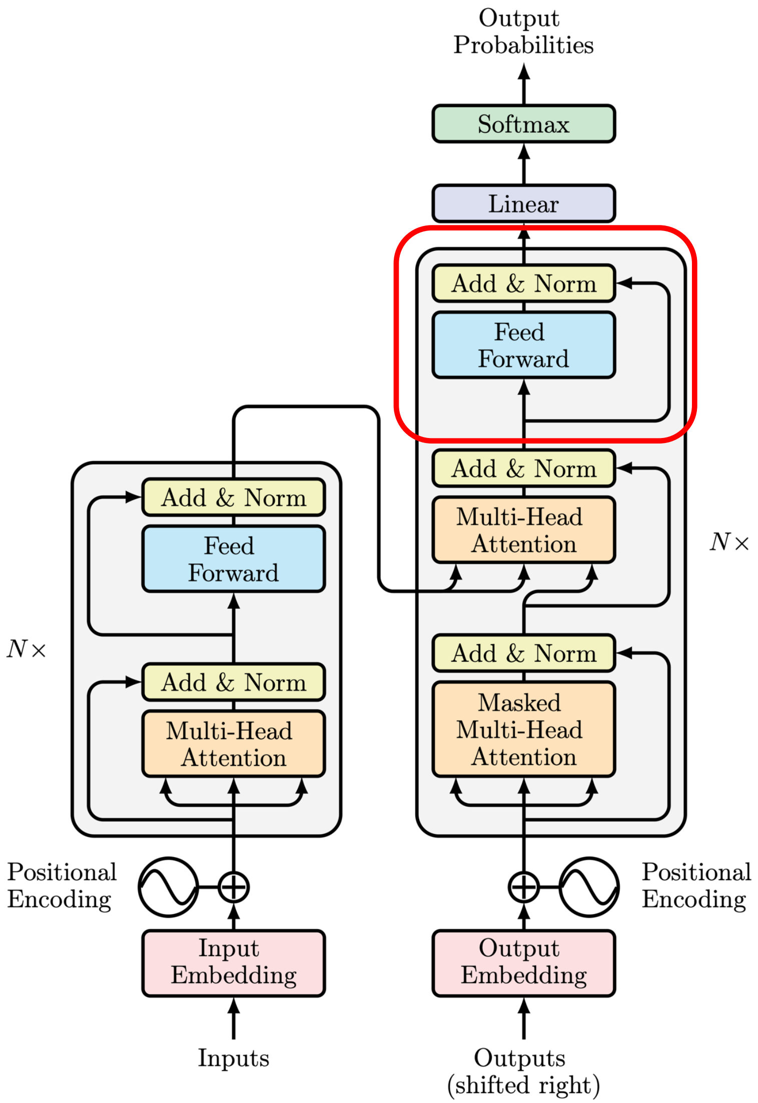


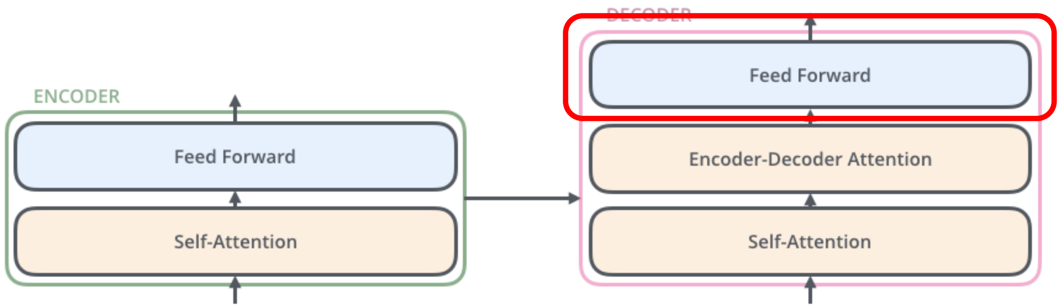


Image Credit: [6] & https://jalammar.github.io/illustrated-transformer/

Input Encoding

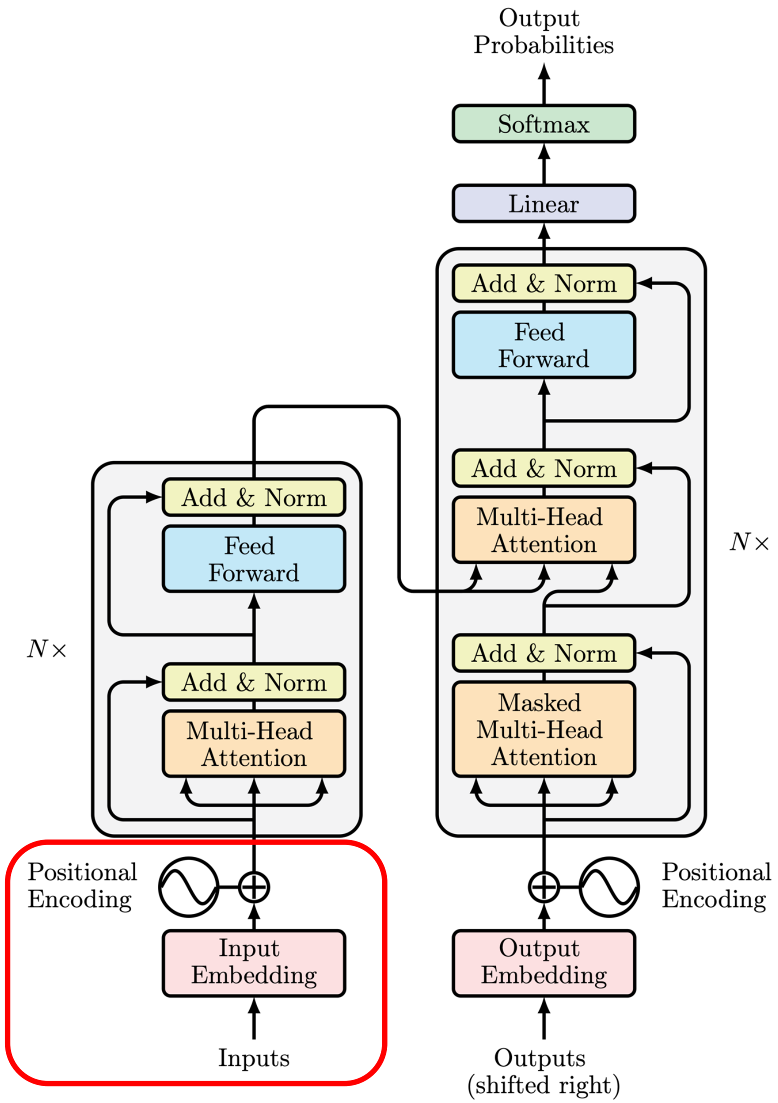
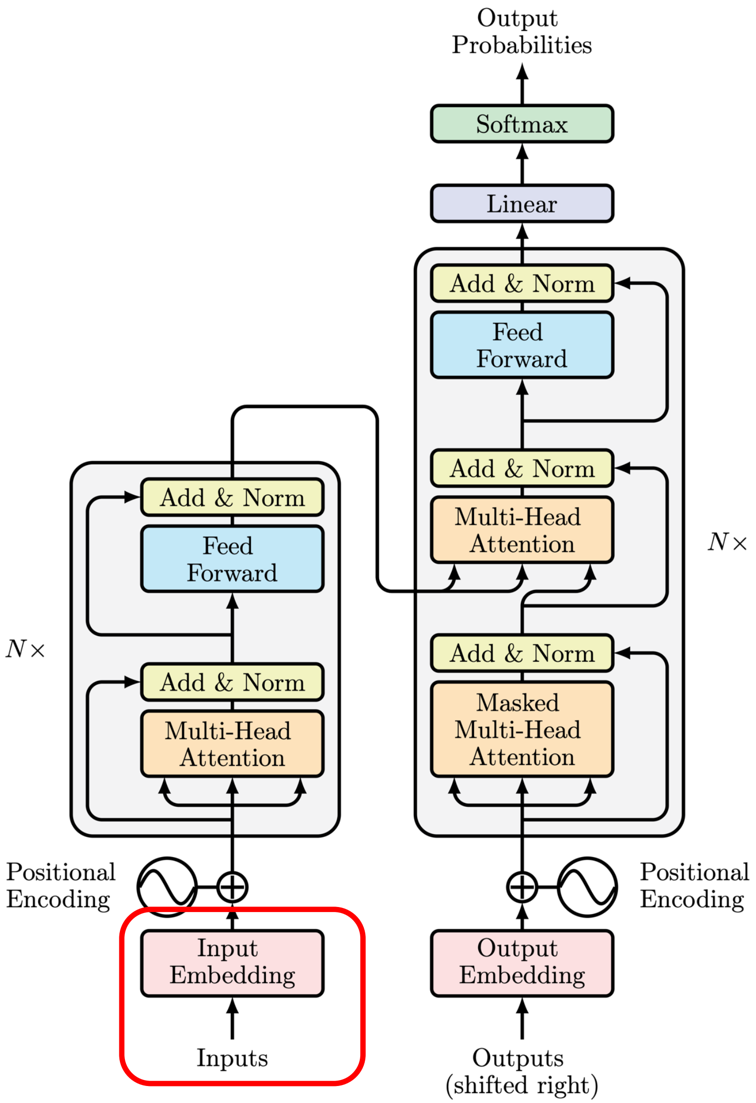


Image Credit: [6]

Input Embedding



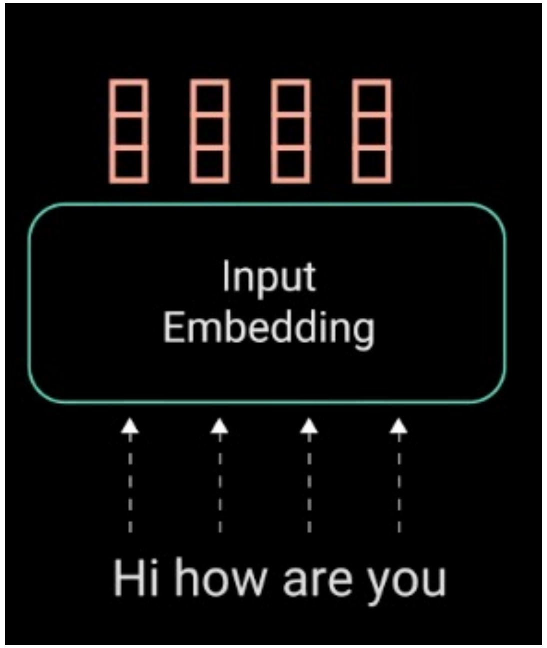
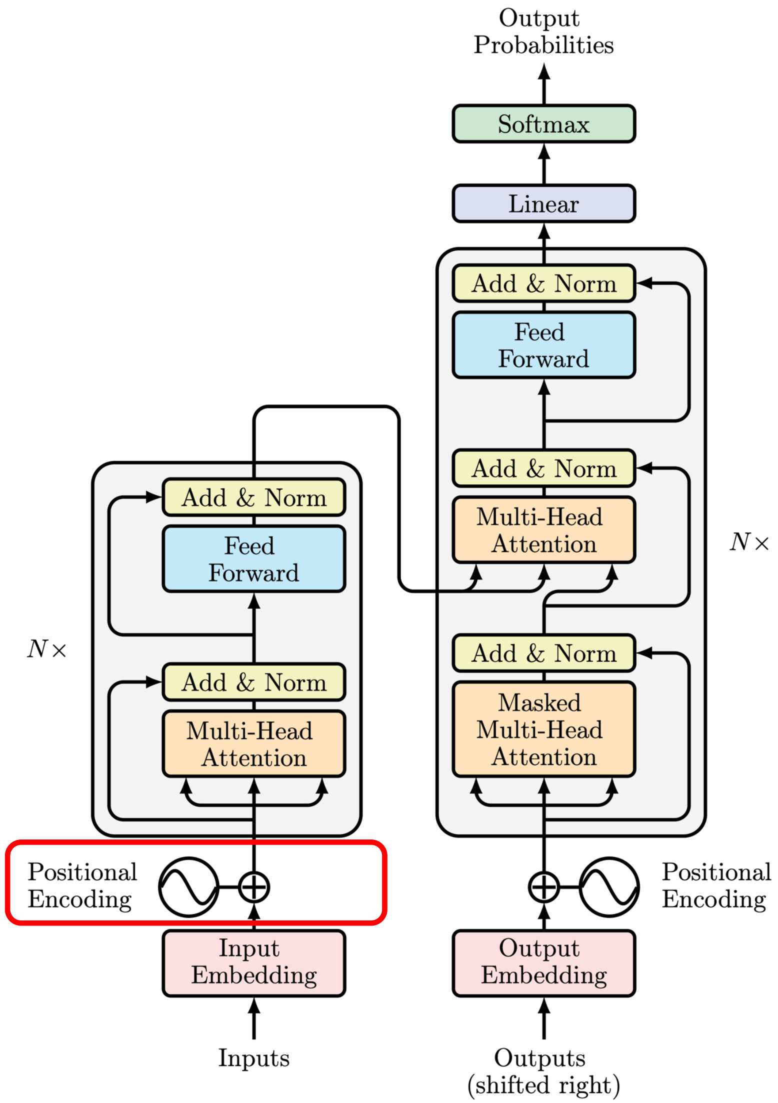
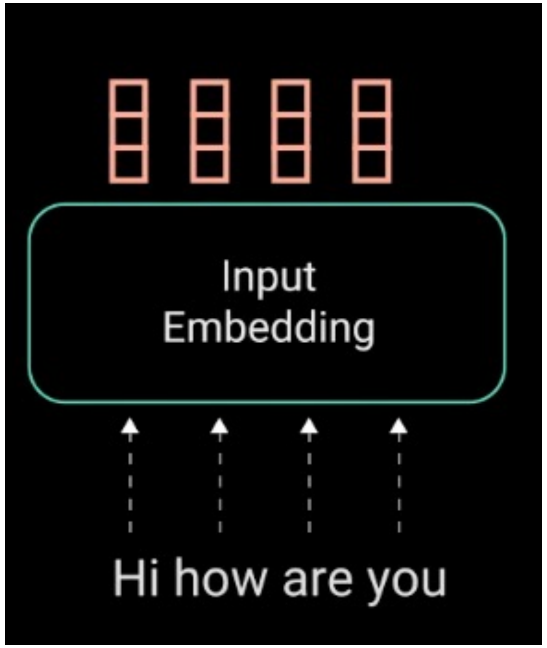


Image Credit: [6] & https://towardsdatascience.com/illustrated-guide-to-transformers-step-by-step-explanation-f74876522bc0

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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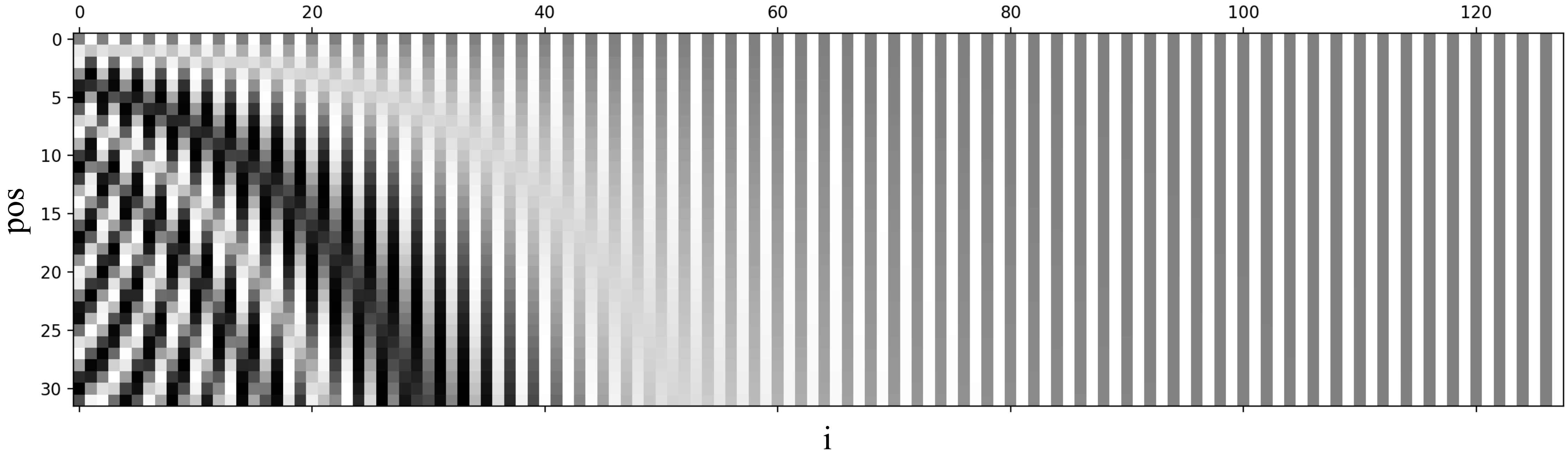

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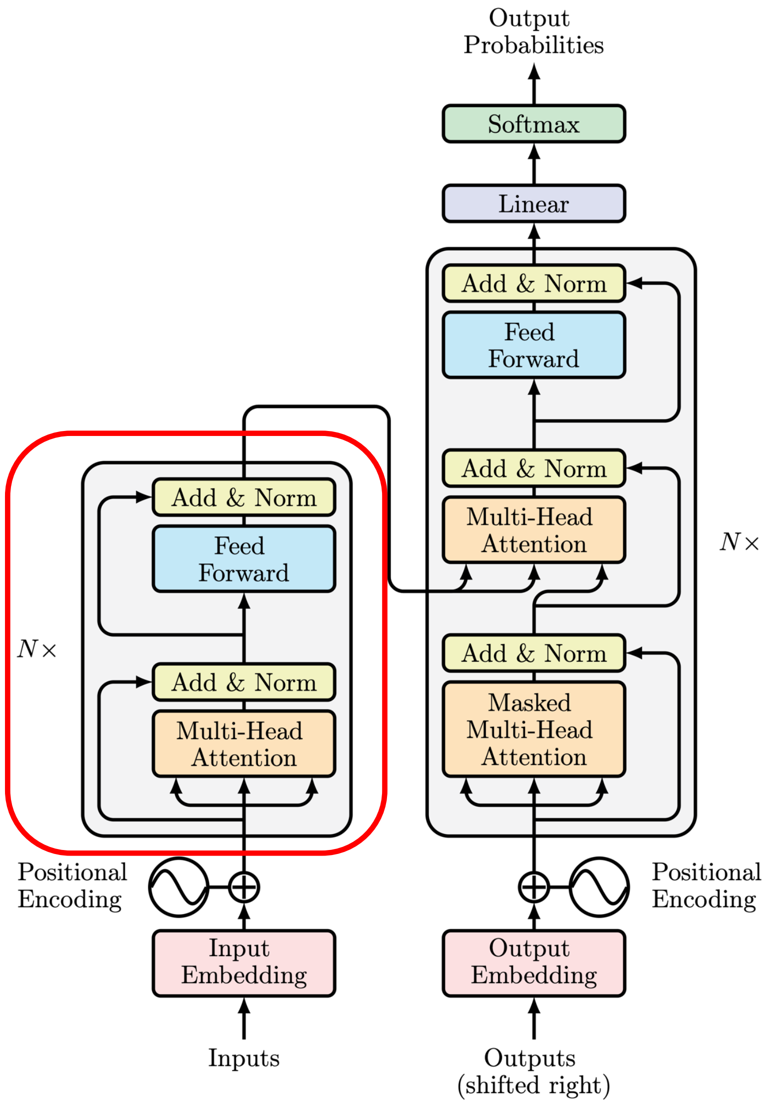
Image Credit: https://lilianweng.github.io/lil-log/2020/04/07/the-transformer-family.html

Encoder



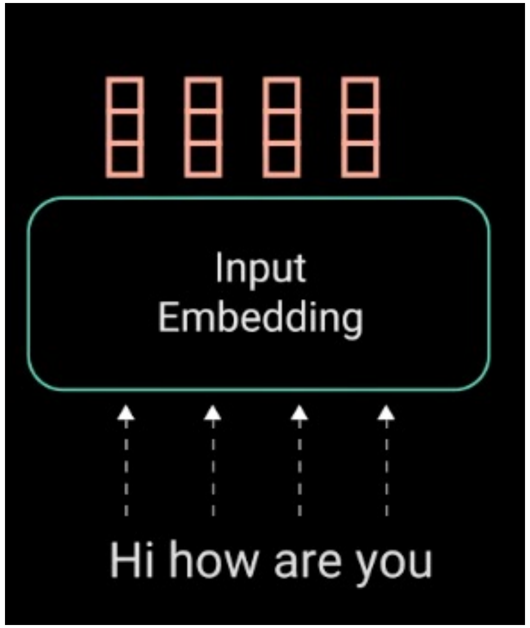
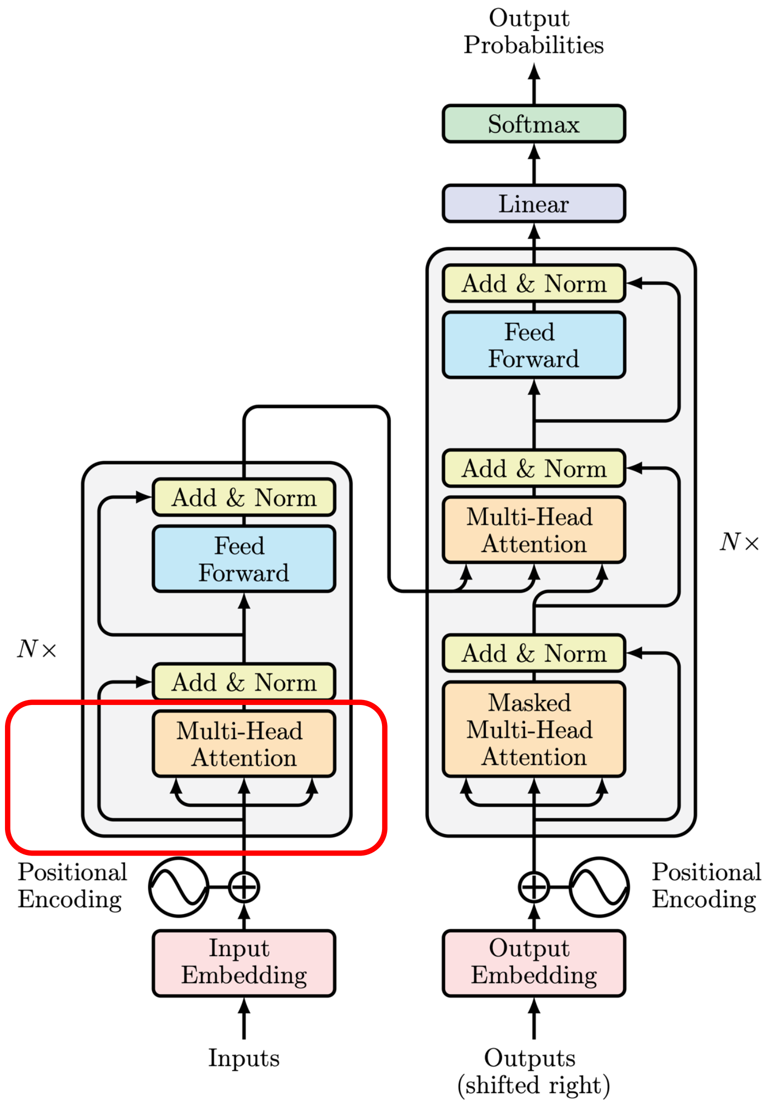


Image Credit: [6] & https://towardsdatascience.com/illustrated-guide-to-transformers-step-by-step-explanation-f74876522bc0

Multi-Head Attention



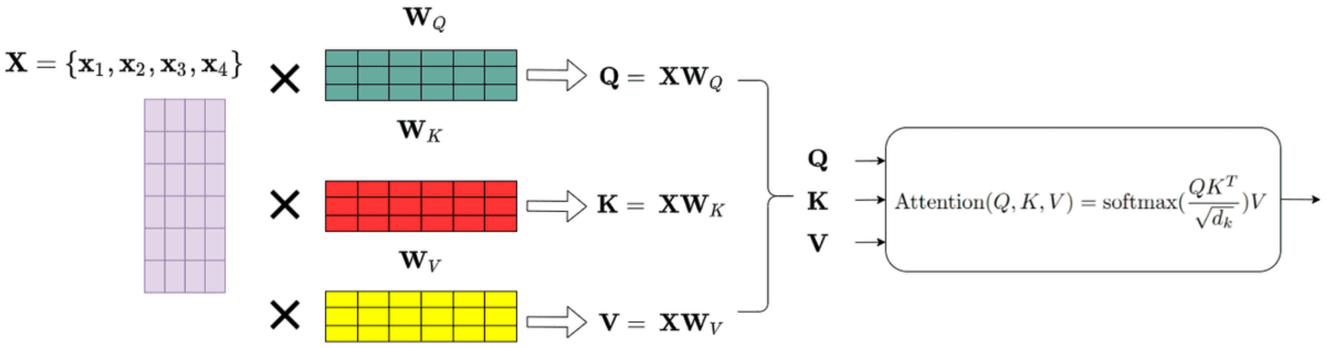


Image Credit: [6] & https://theaisummer.com/transformer/

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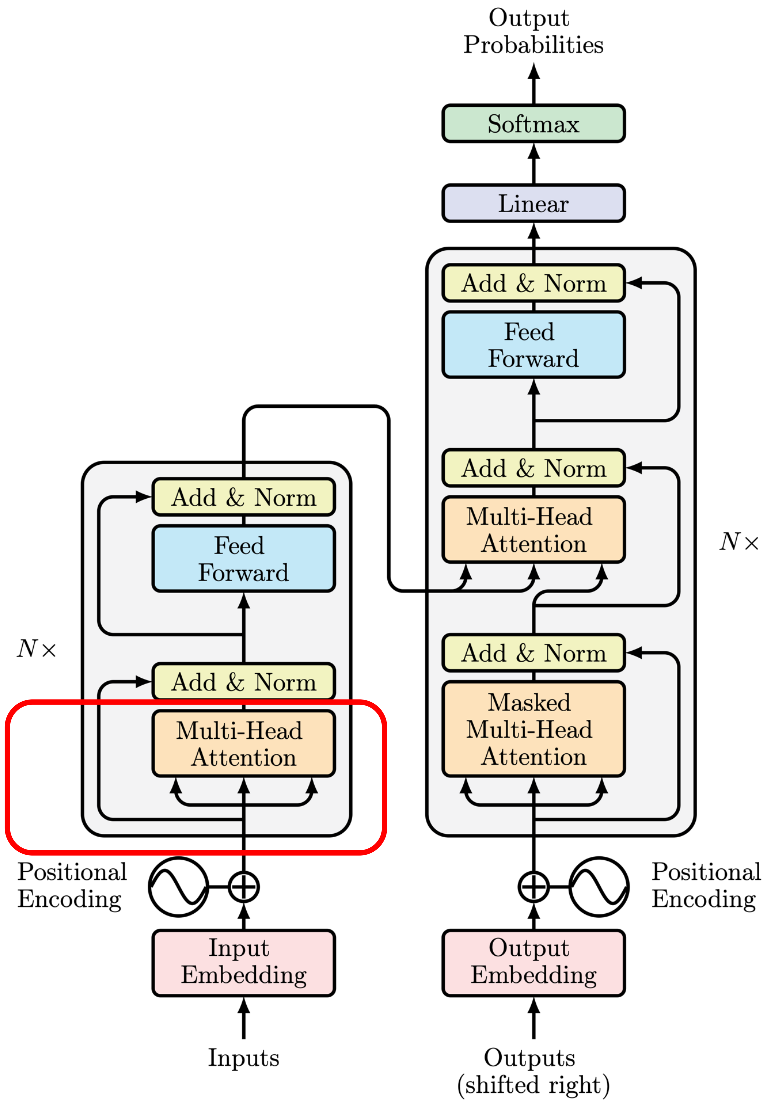

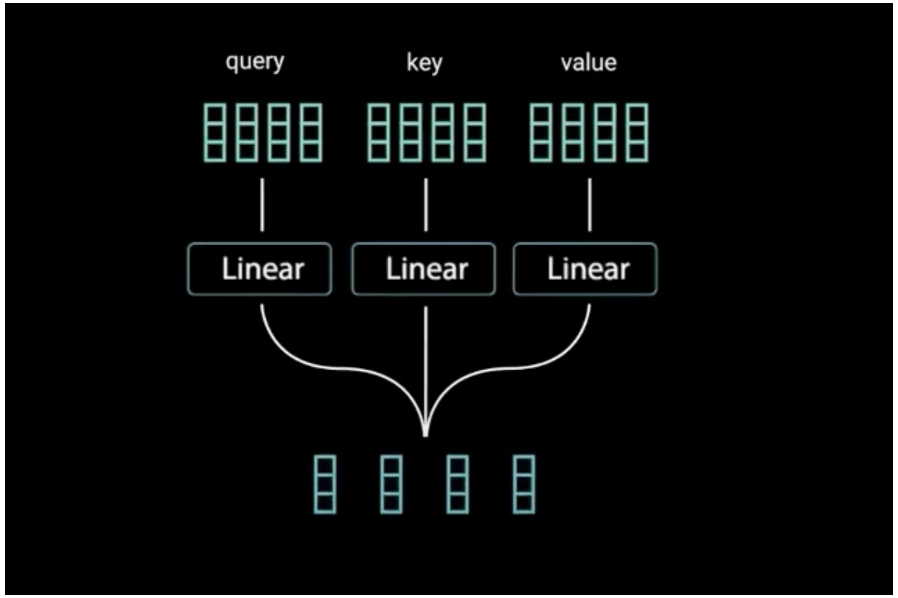

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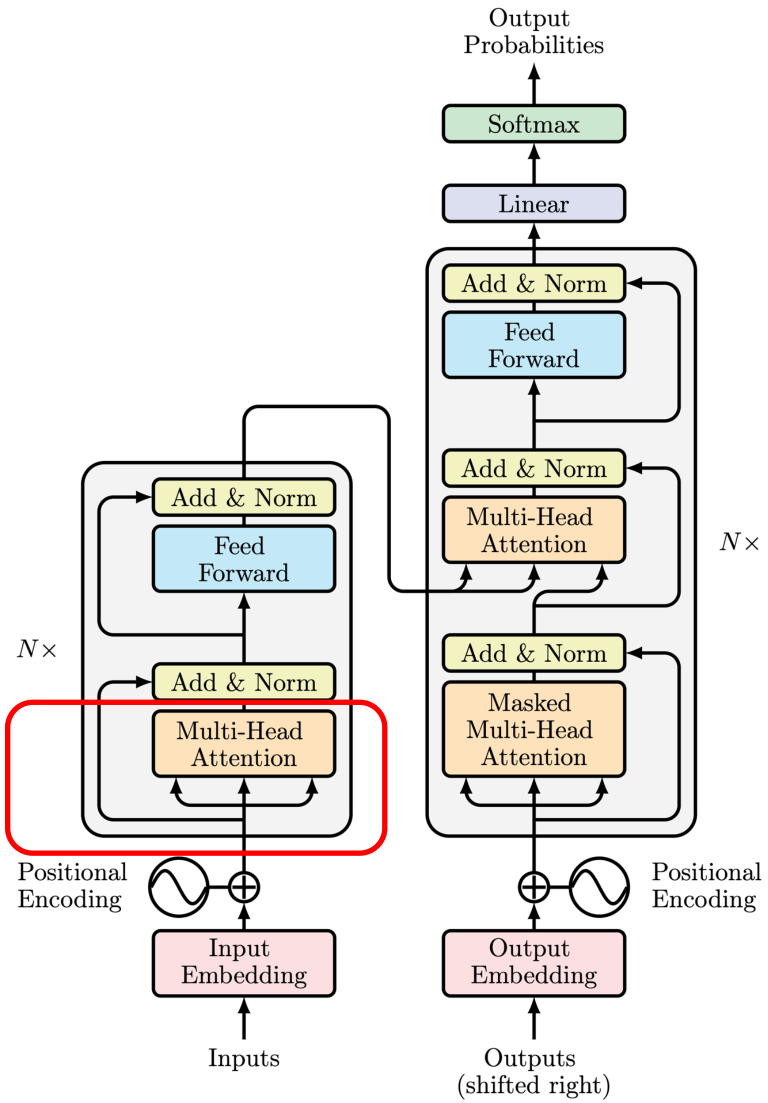

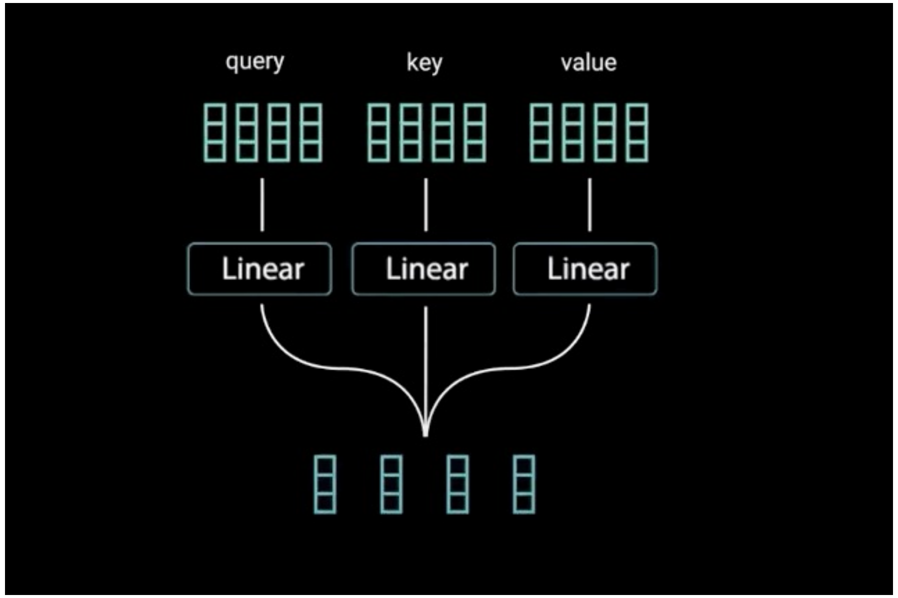

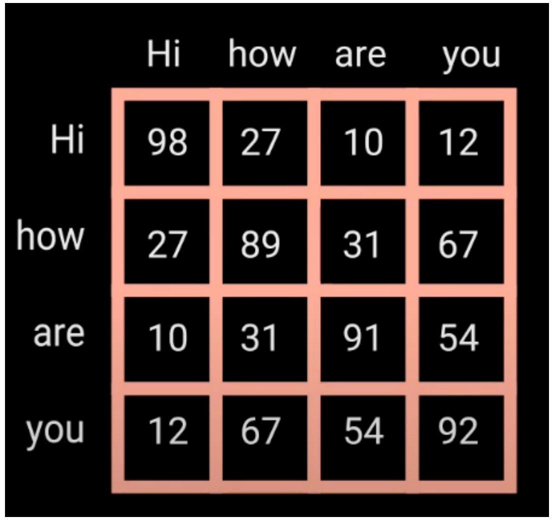

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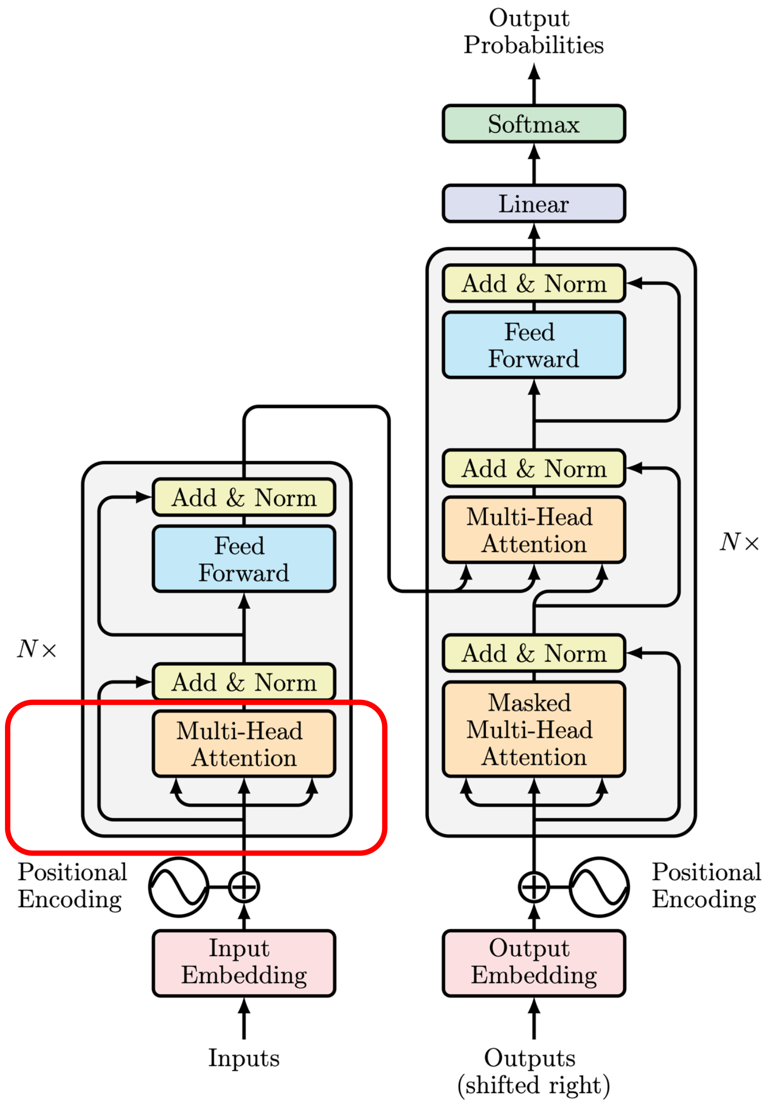

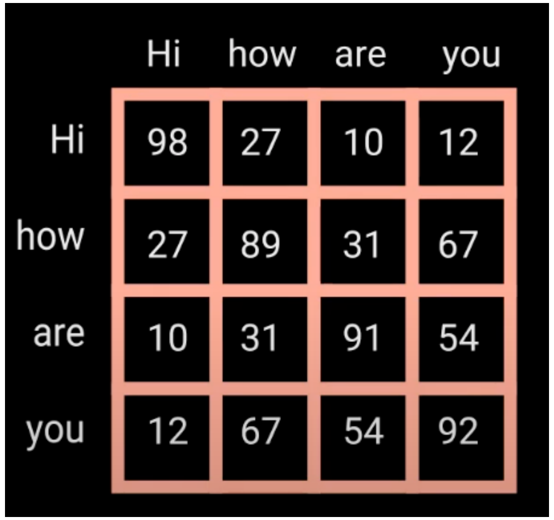

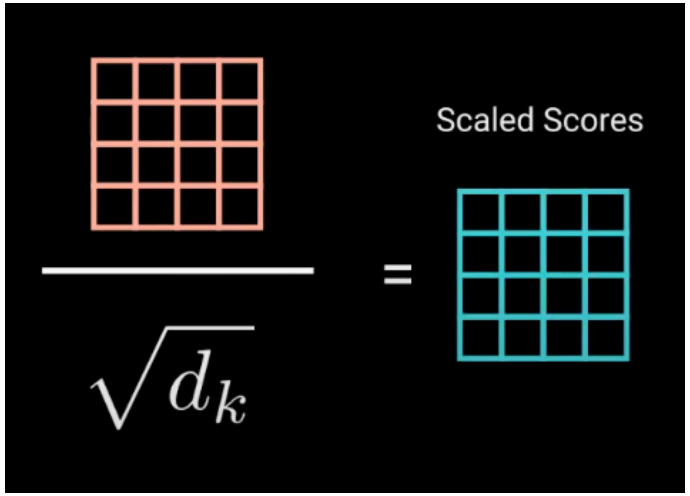

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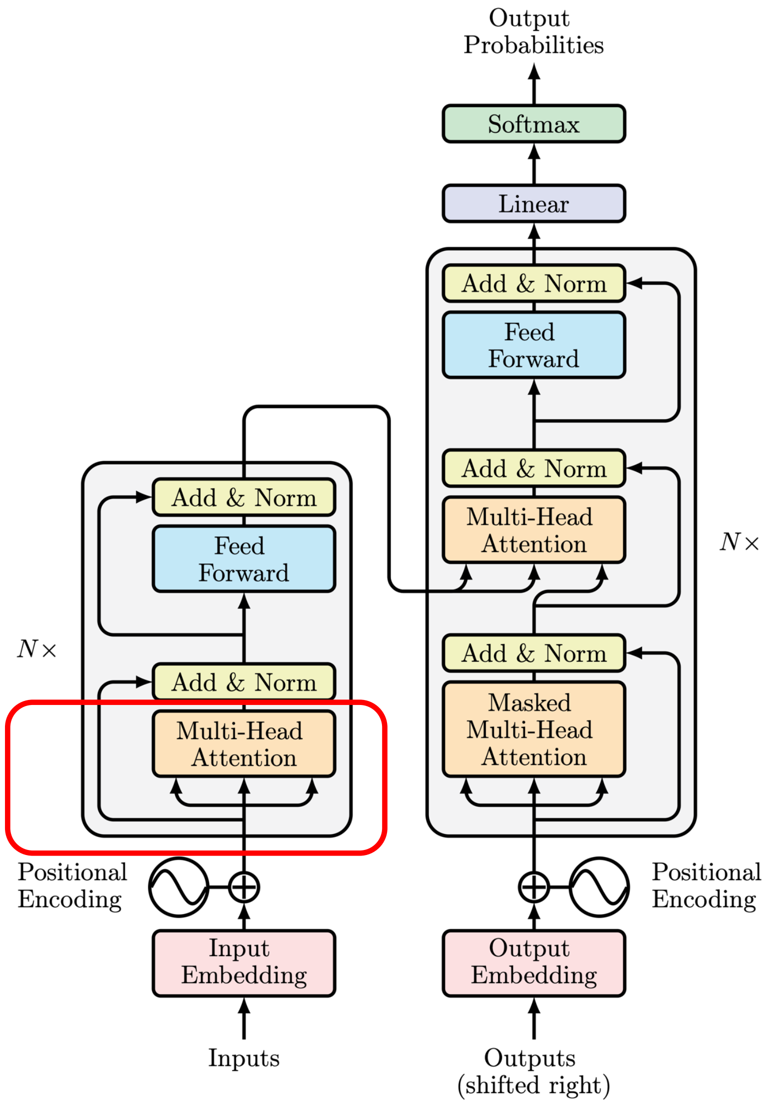

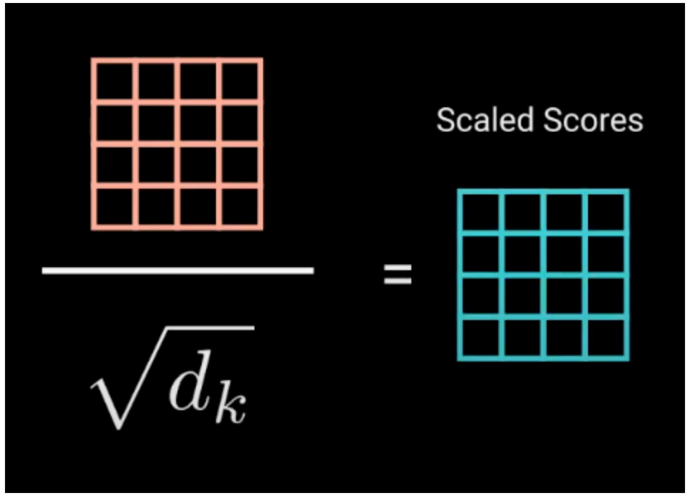

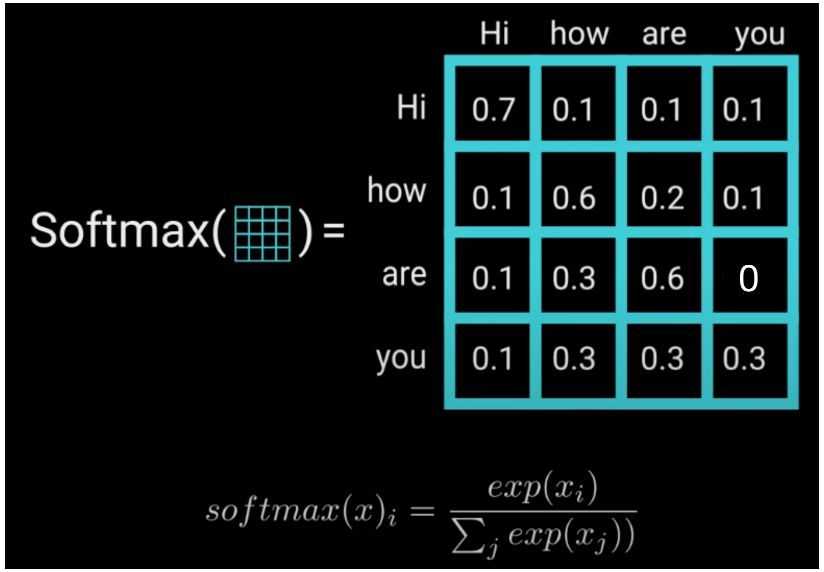

Image Credit: [6] & https://towardsdatascience.com/illustrated-guide-to-transformers-step-by-step-explanation-f74876522bc0

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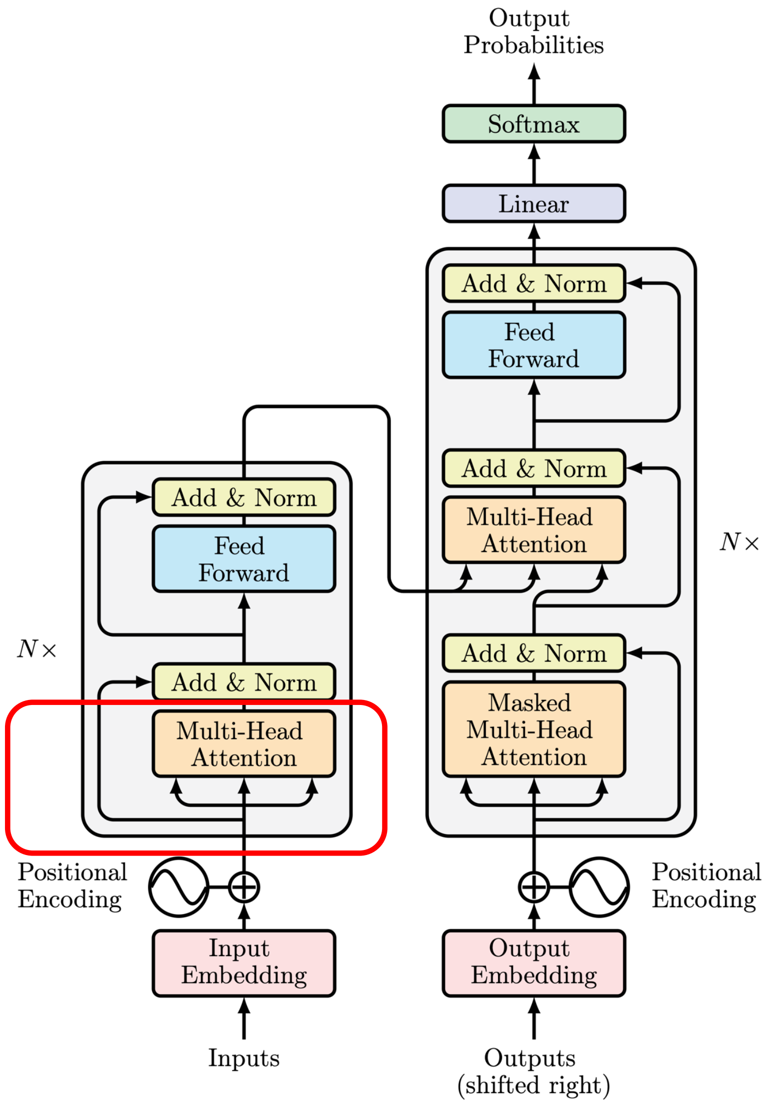
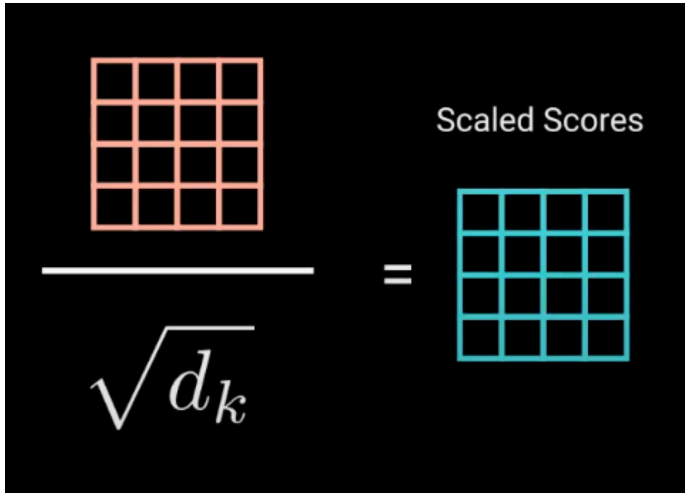
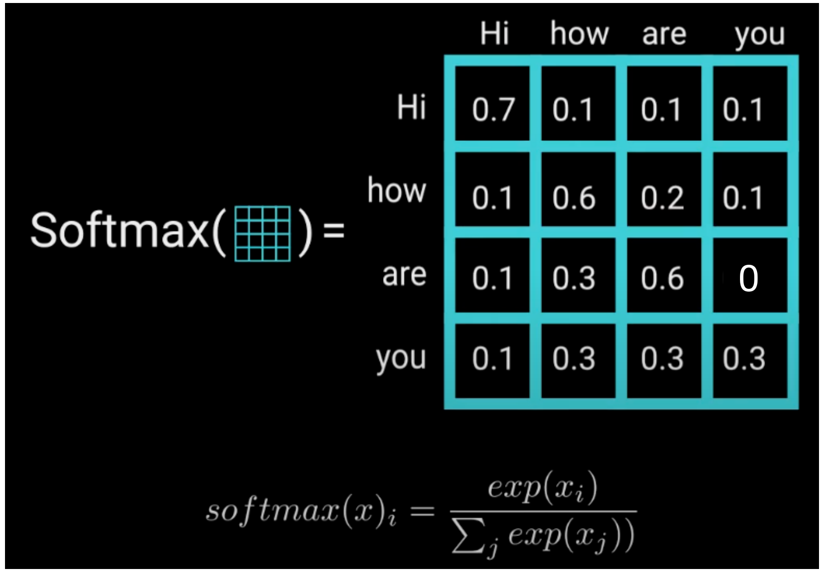




Why square root?



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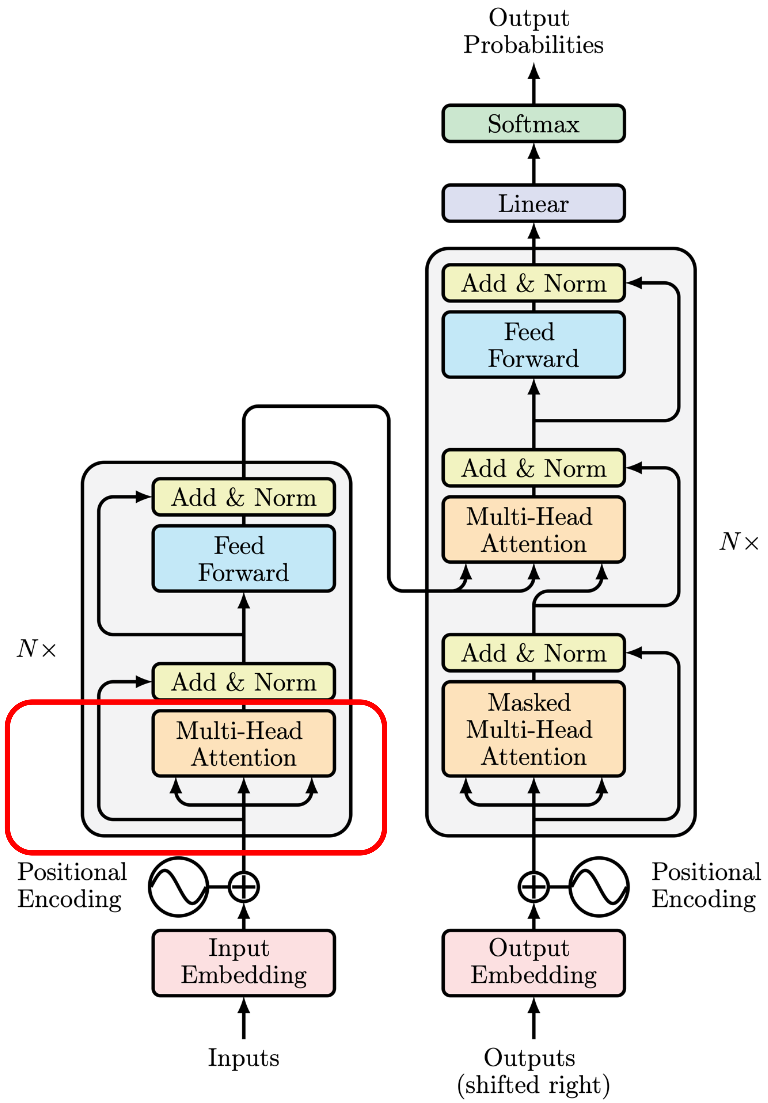

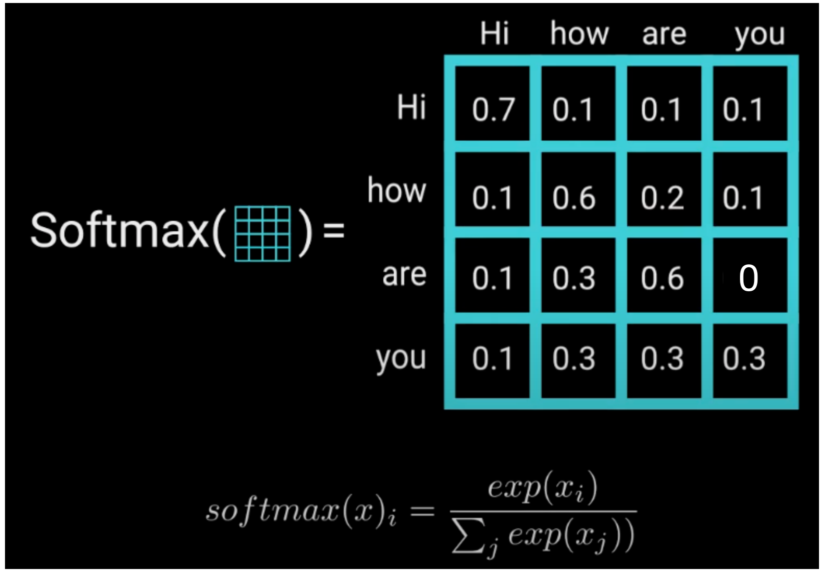

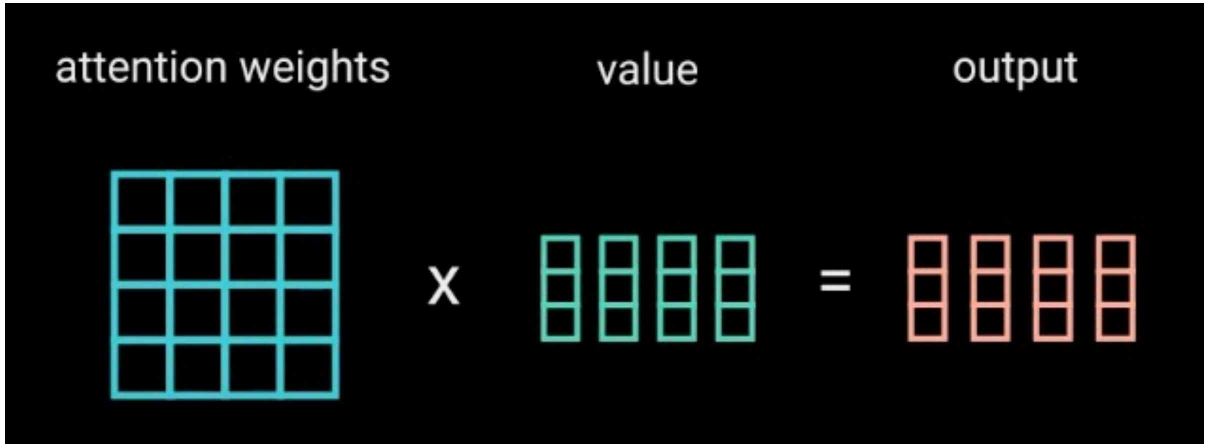

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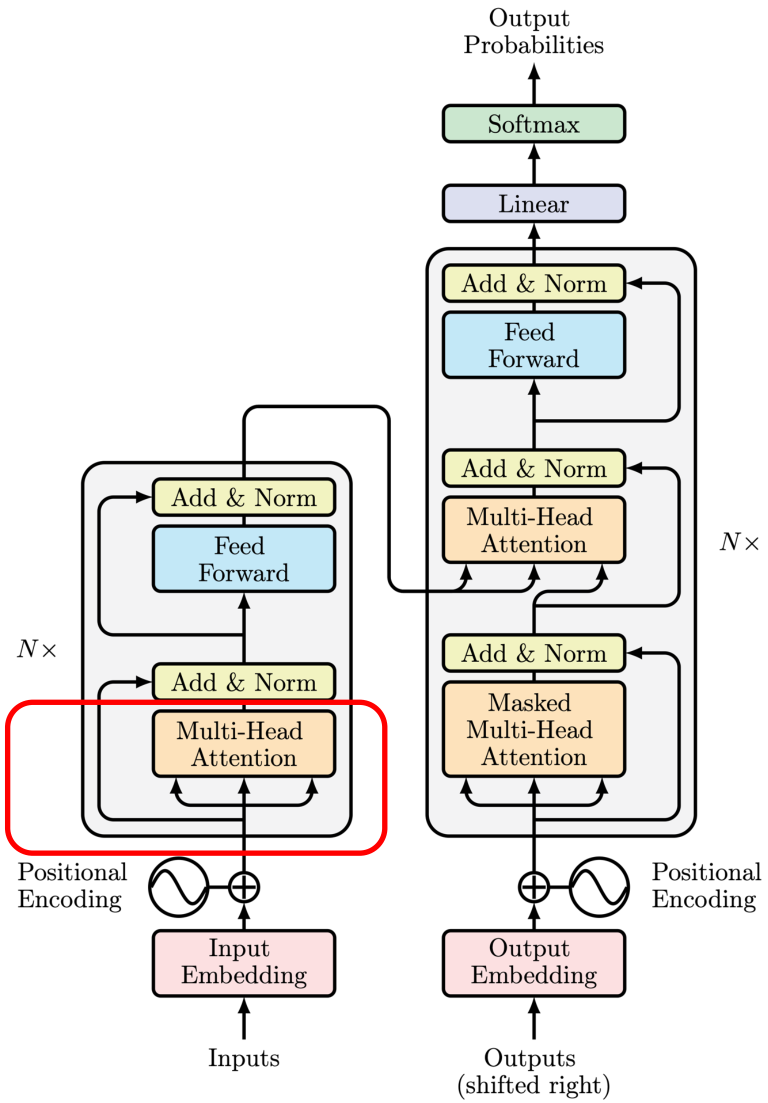


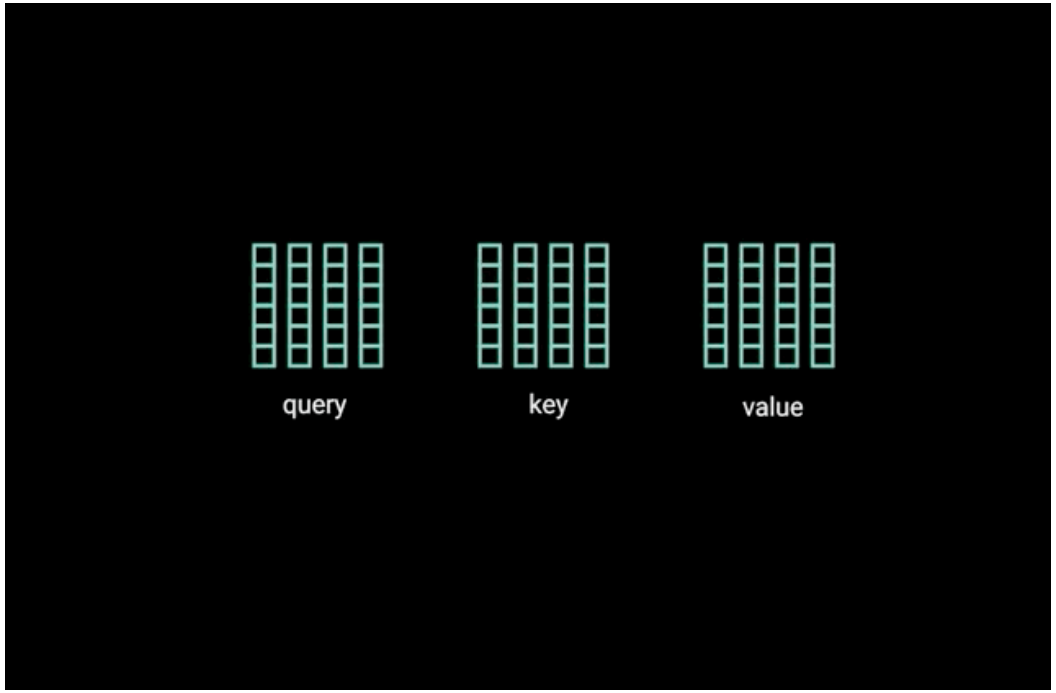
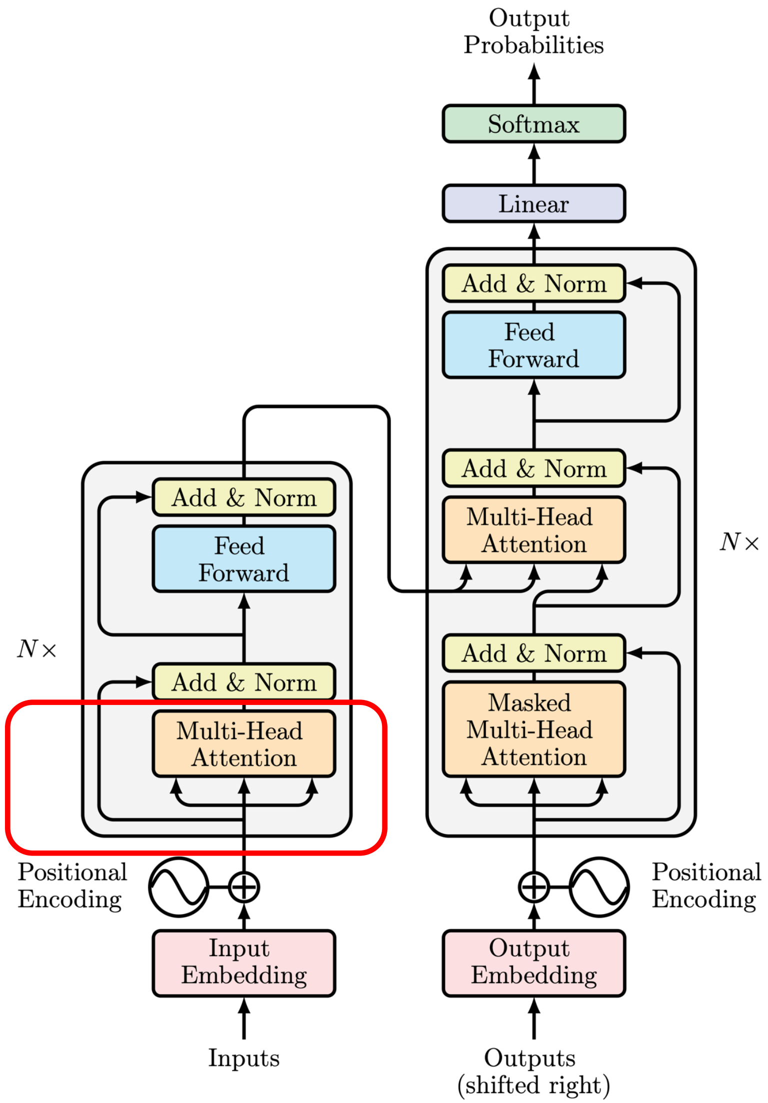
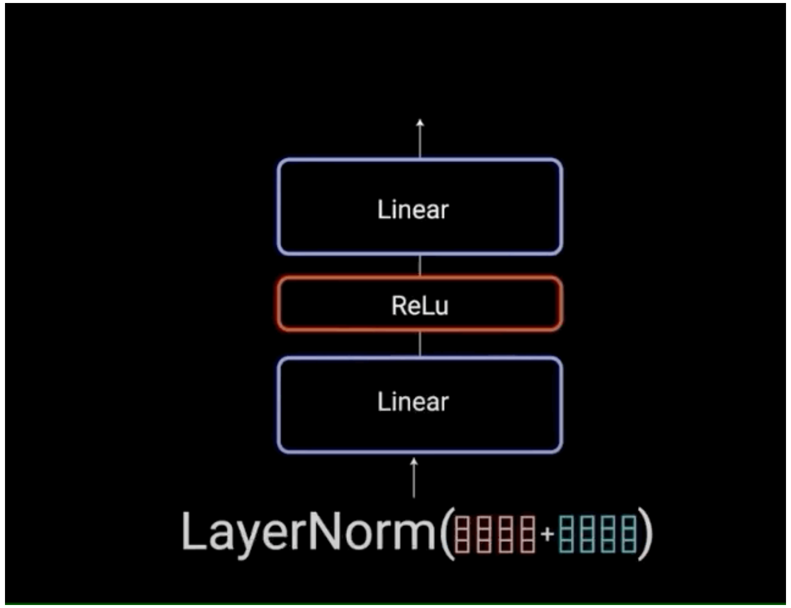


Image Credit: [6] & https://towardsdatascience.com/illustrated-guide-to-transformers-step-by-step-explanation-f74876522bc0

Layer Norm & Residual Connection





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

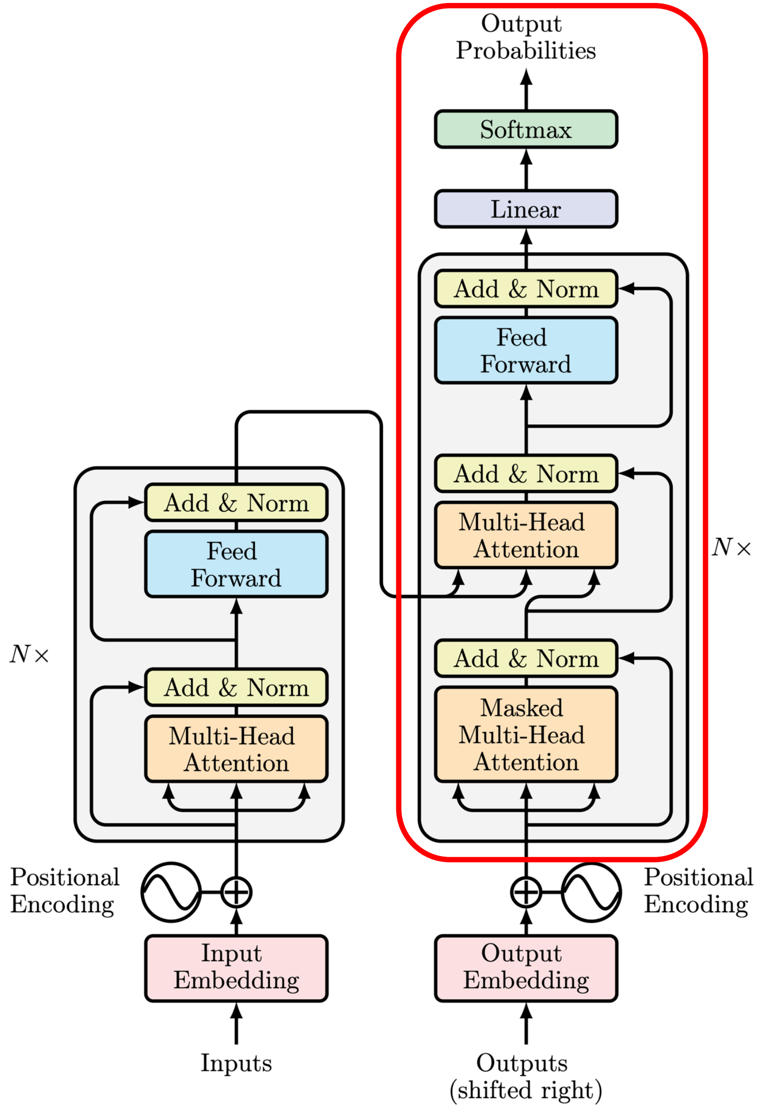
$$\sigma_i^2 = \frac{1}{K}\sum_{k=1}^{K} (x_{i,k} - \mu_i)^2$$

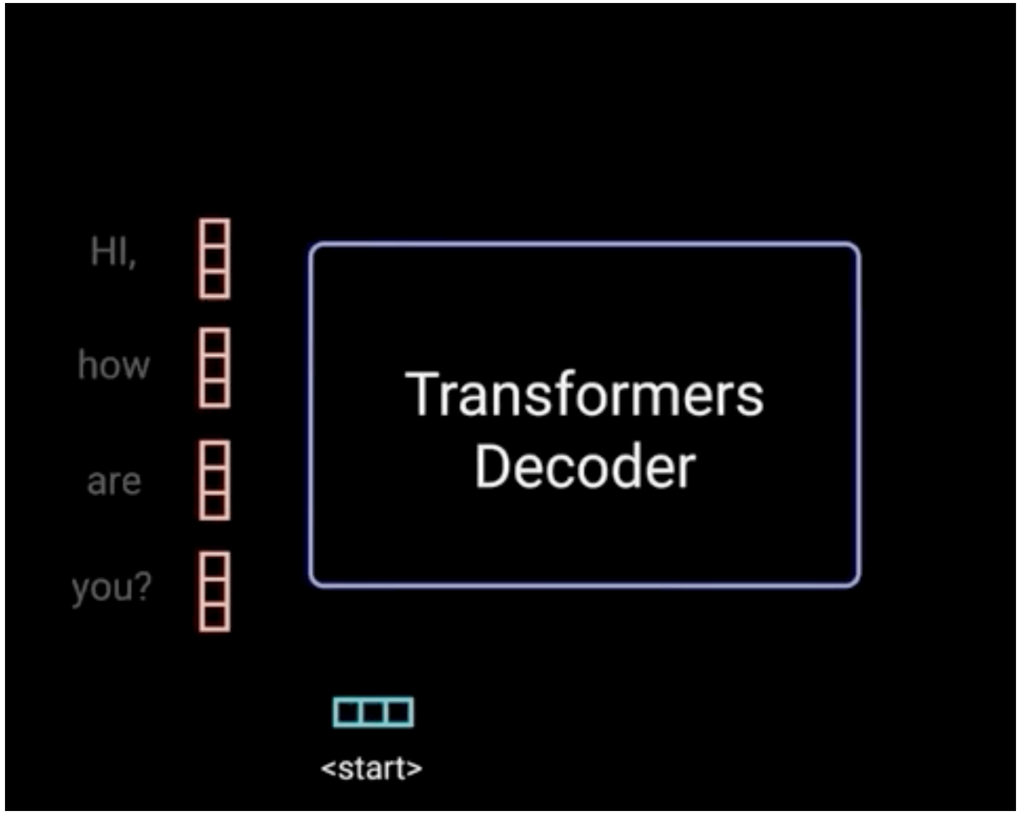
$$\hat{x}_{i,k} = \frac{x_{i,k} - \mu_i}{\sqrt{\sigma_i^2 + \epsilon}}$$

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

Image Credit: [6] & [7] & https://towardsdatascience.com/illustrated-guide-to-transformers-step-by-step-explanation-f74876522bc0

Decoder

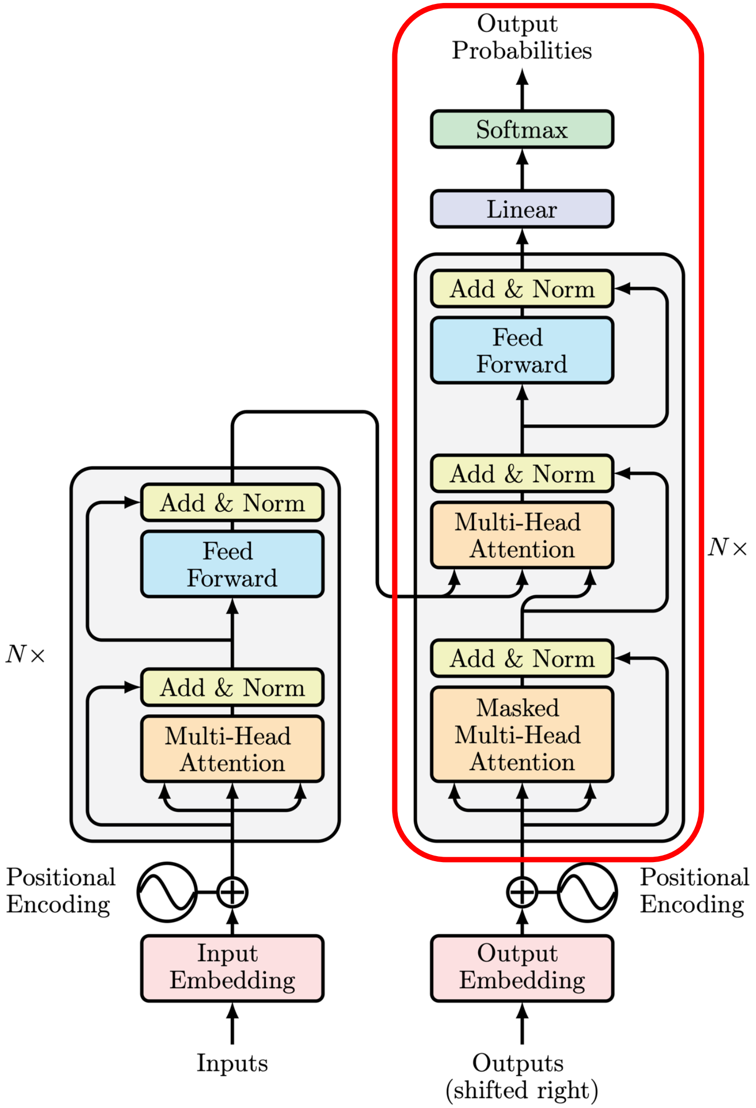


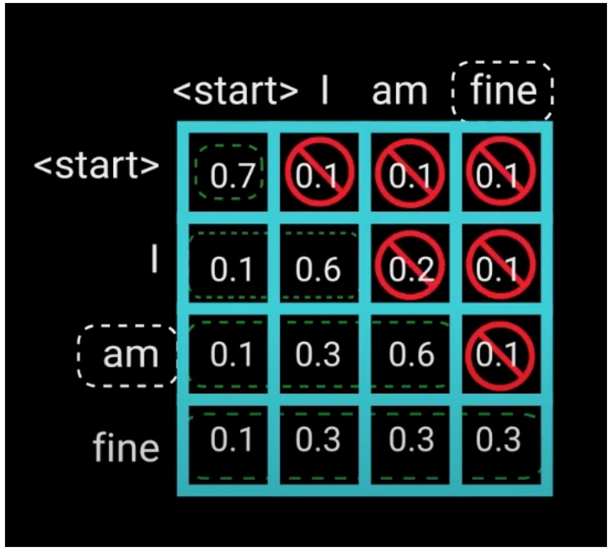


For certain applications like language models, decoder should be autoregressive!

Image Credit: [6] & https://towardsdatascience.com/illustrated-guide-to-transformers-step-by-step-explanation-f74876522bc0

Masked Multi-Head Attention

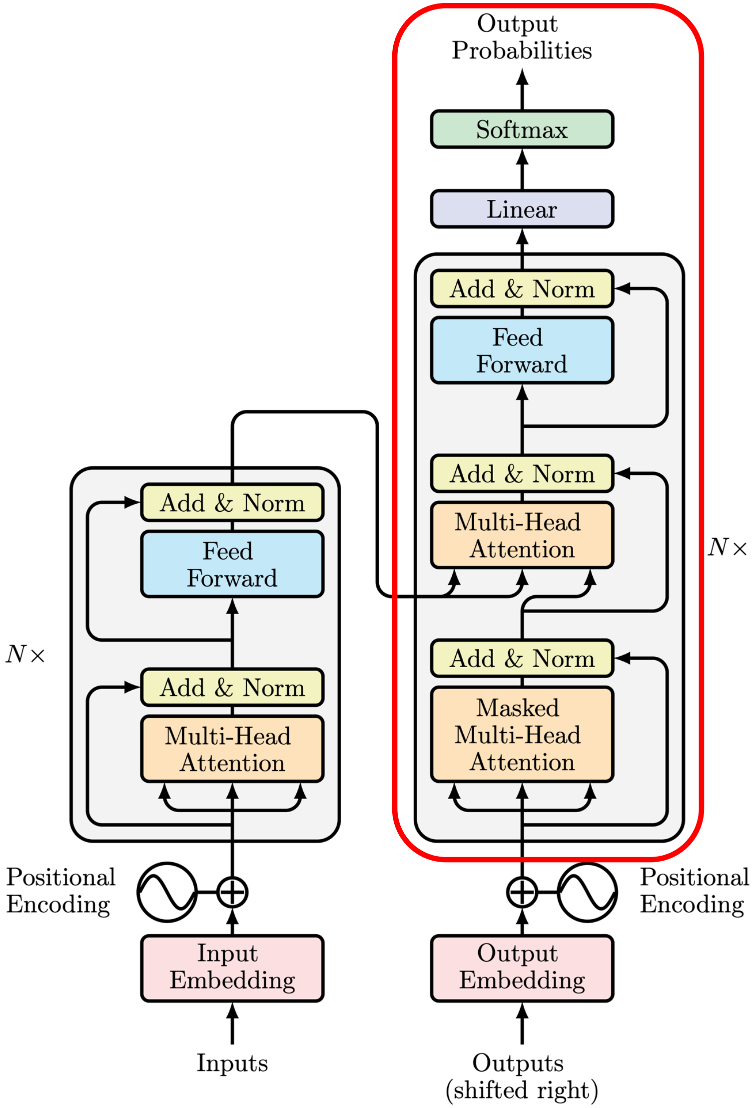


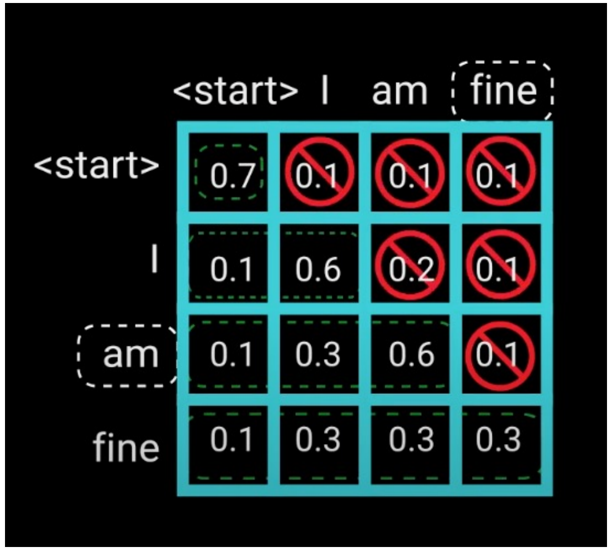


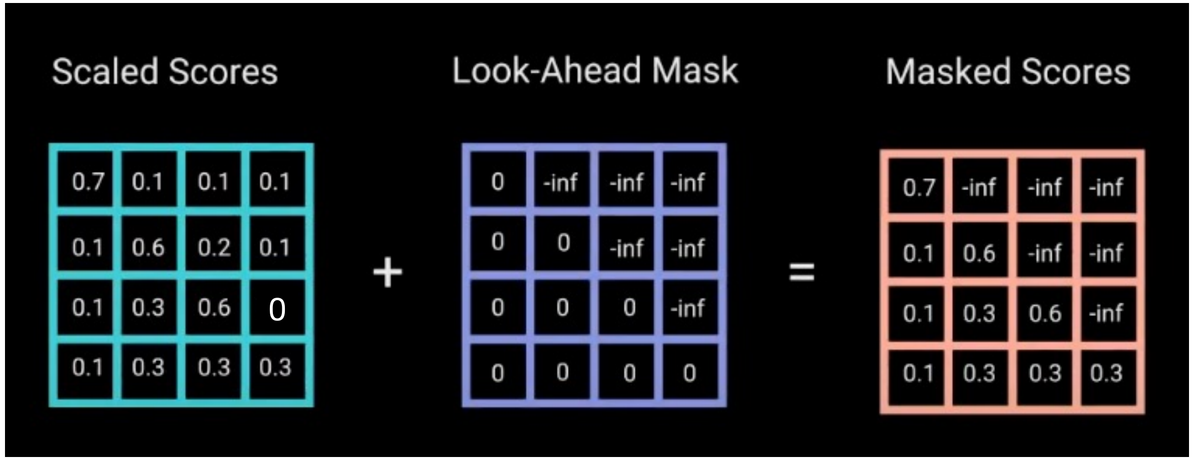
Prevent attending from future!

Image Credit: [6] & https://towardsdatascience.com/illustrated-guide-to-transformers-step-by-step-explanation-f74876522bc0

Masked Multi-Head Attention







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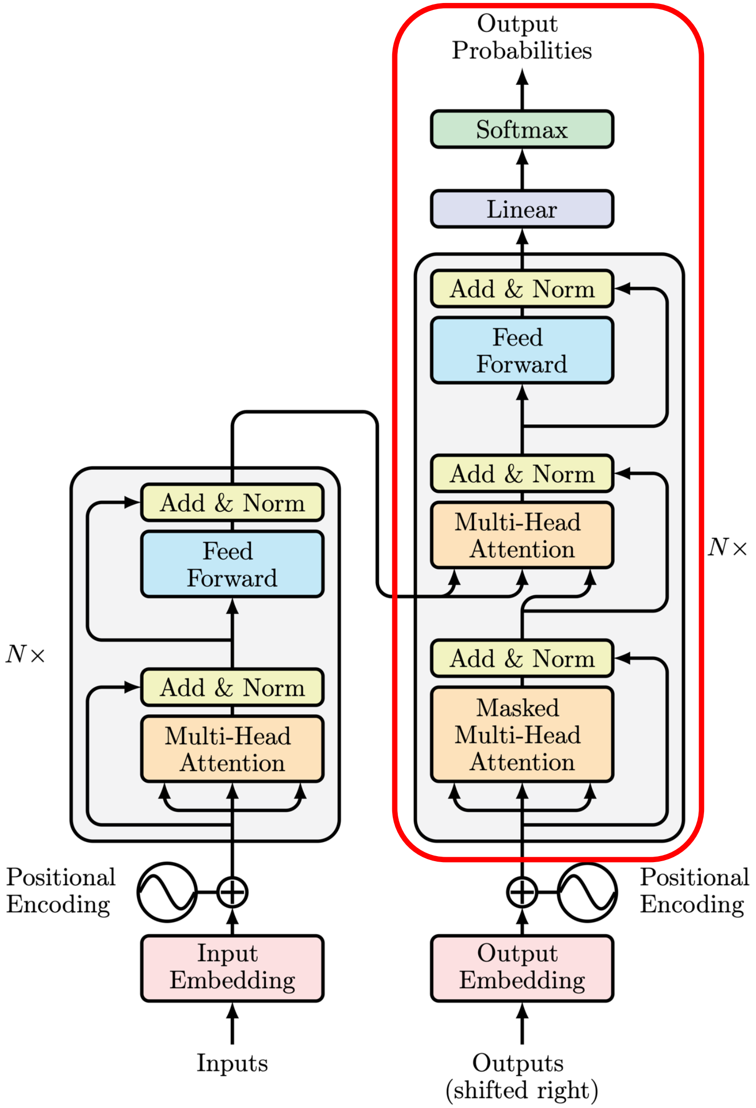
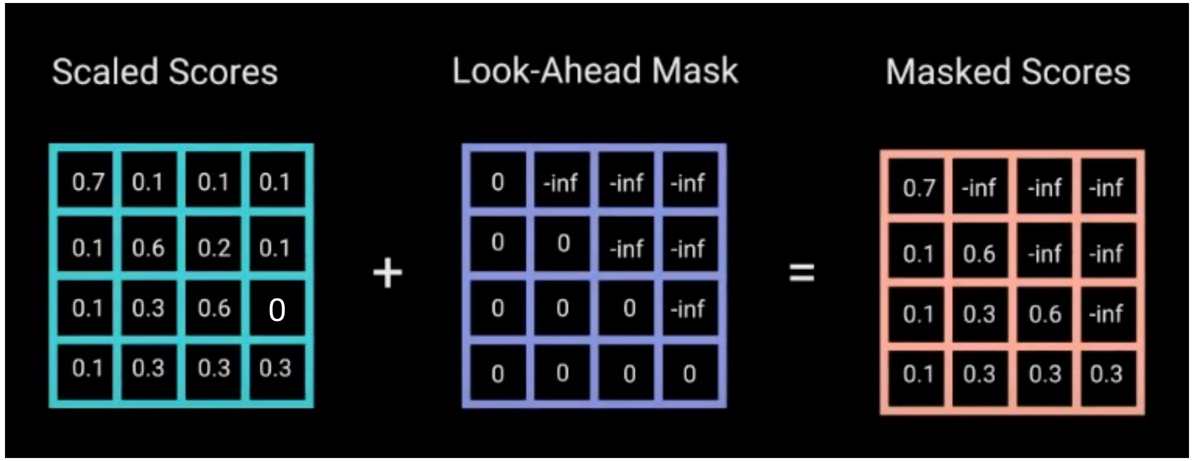




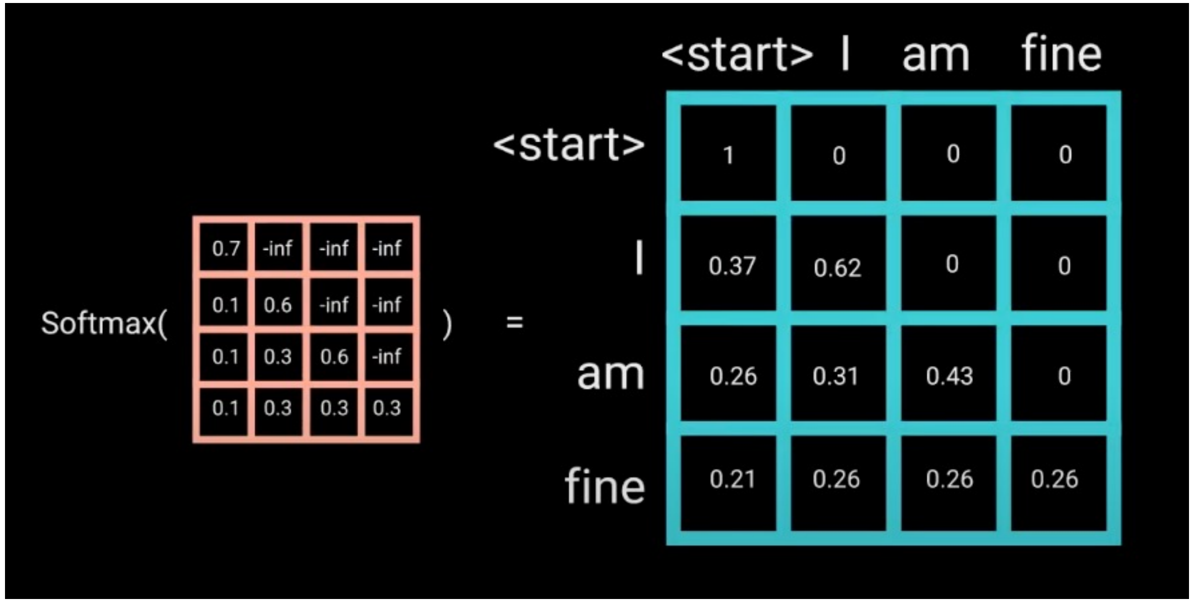


Image Credit: [6] & https://towardsdatascience.com/illustrated-guide-to-transformers-step-by-step-explanation-f74876522bc0

Hugging Face Demos

https://transformer.huggingface.co/

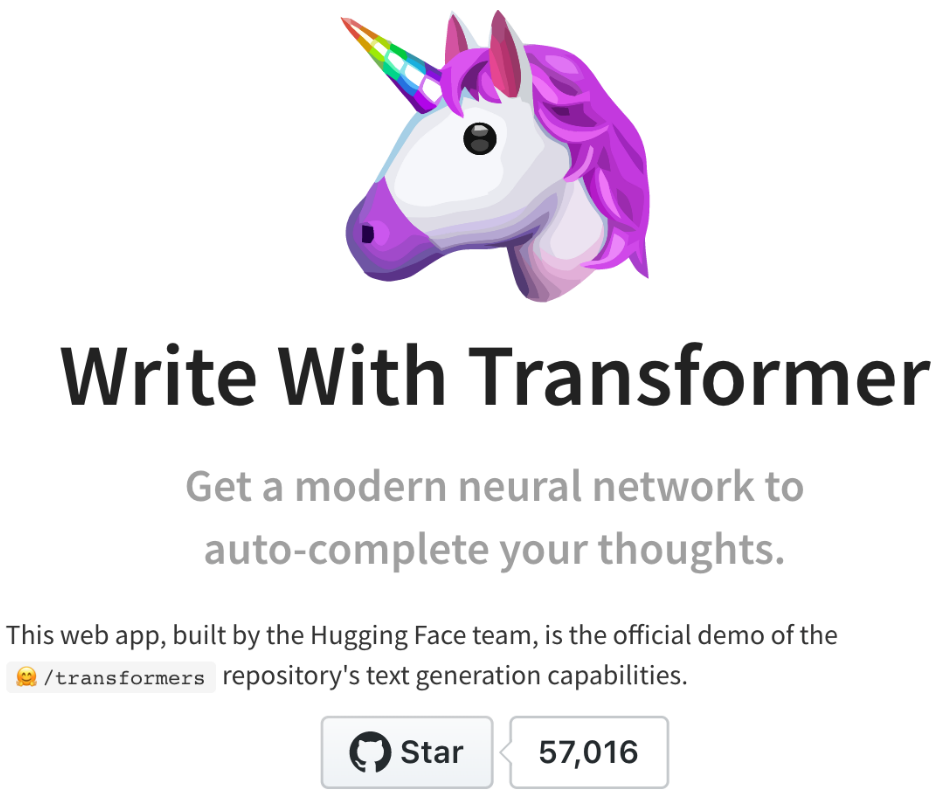
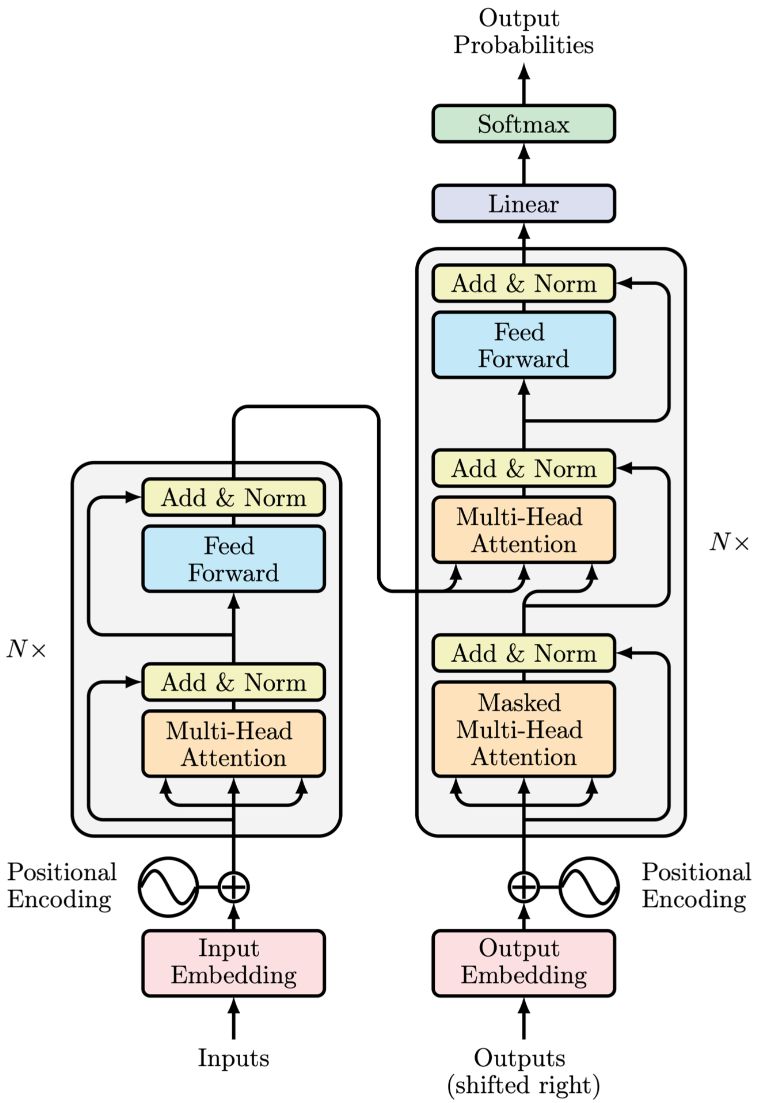


Image Credit: https://transformer.huggingface.co/

Limitations

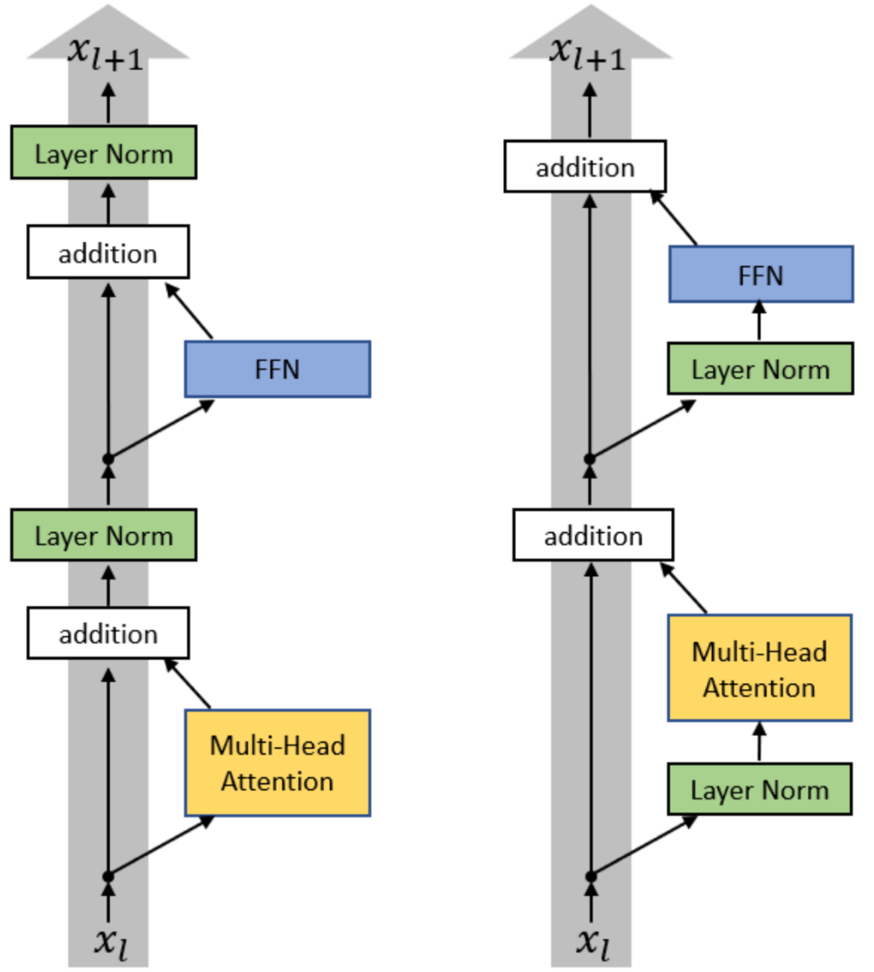


- O(L^2) time/memory cost for self-attention
- How can we incorporate prior knowledge into attention rather than having a fully connected attention?
  - Encourage sparse attention
  - Inject known graph structures
  - ……

Image Credit: [6]

Pre-Norm vs. Post-Norm

Where to place the Layer Normalization?



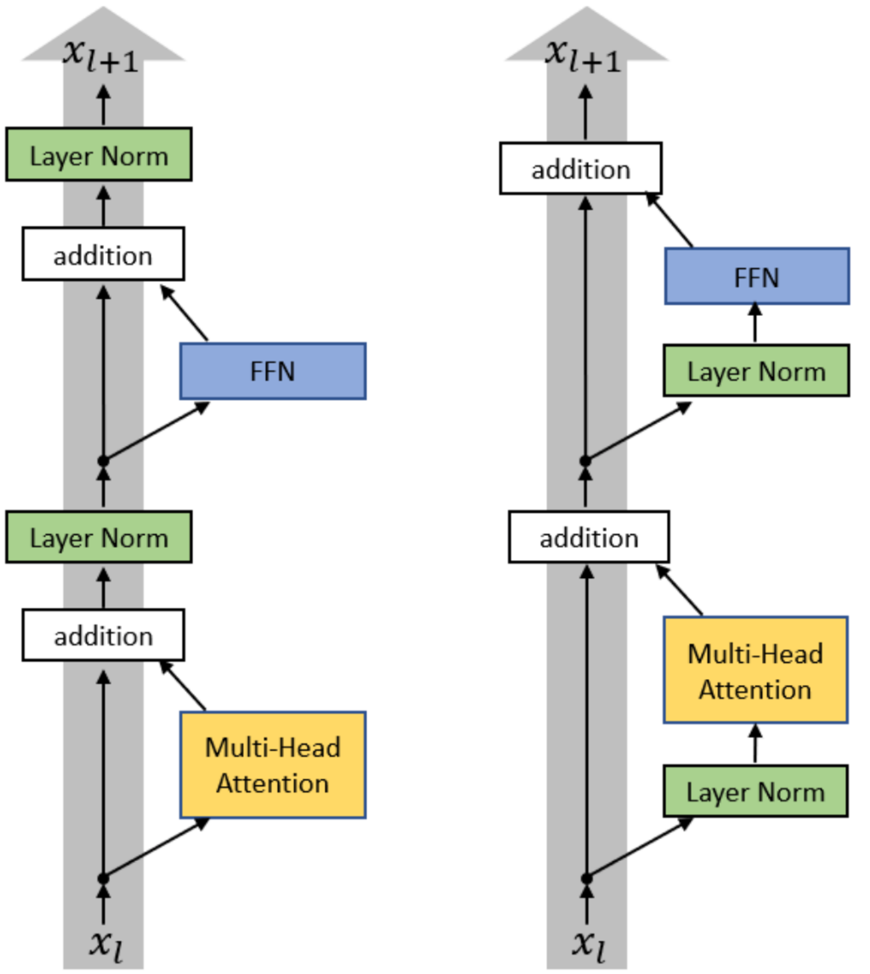
Post-Norm Pre-Norm

Image Credit: [8]

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

Image Credit: [8]

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

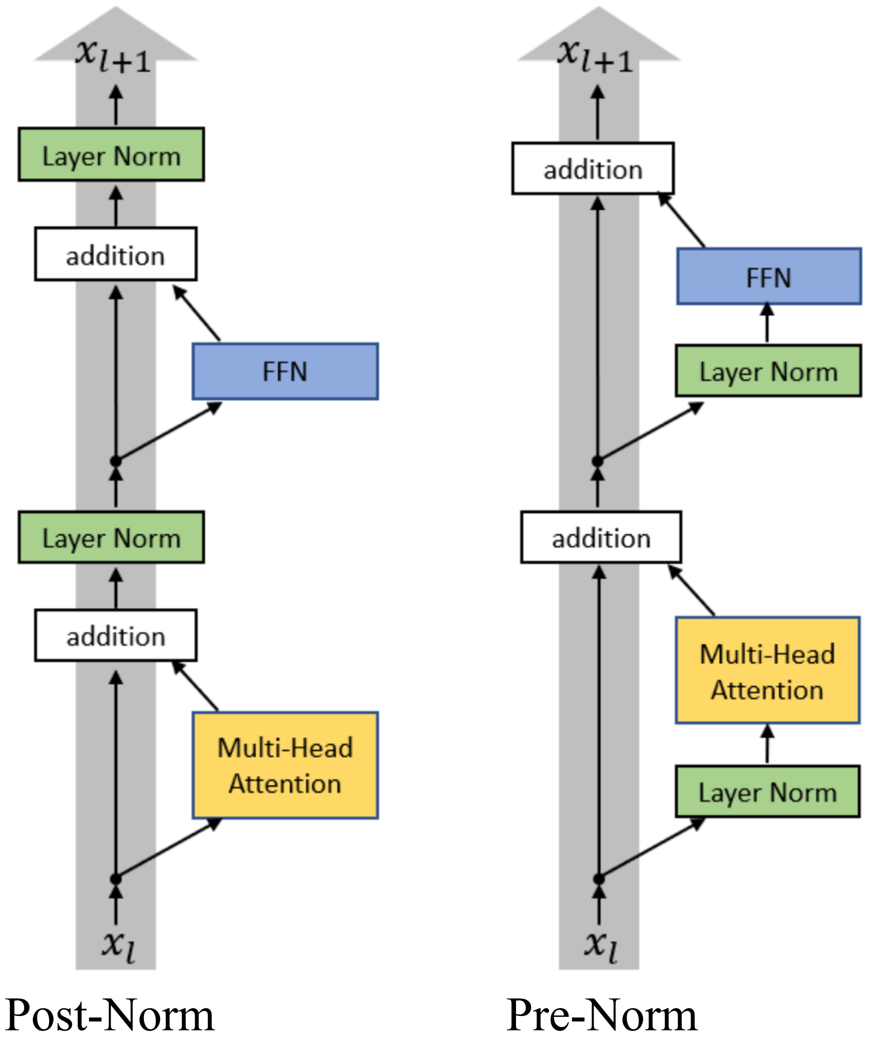


Image Credit: [8]

Extensions: Vision Transformer

Image Credit: [9] & https://github.com/lucidrains/vit-pytorch

Extensions: Swin Transformer

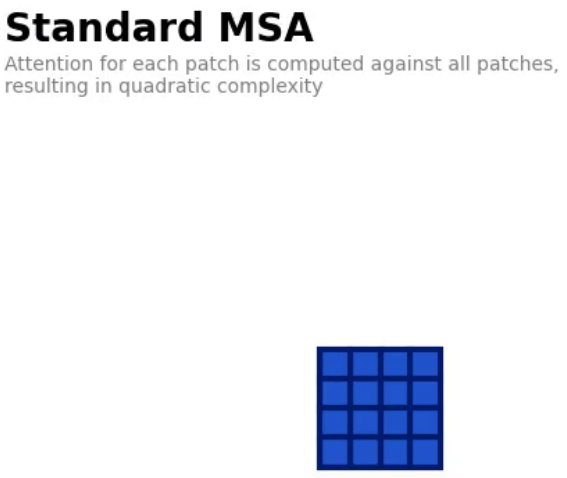
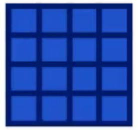


Image Credit: https://towardsdatascience.com/a-comprehensive-guide-to-swin-transformer-64965f89d14c

Extensions: Swin Transformer

Standard MSA

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

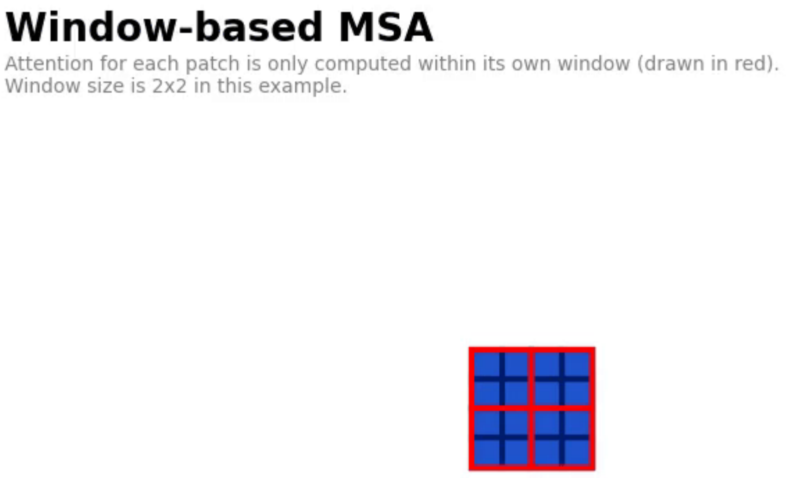


Window-based MSA

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 Transformer



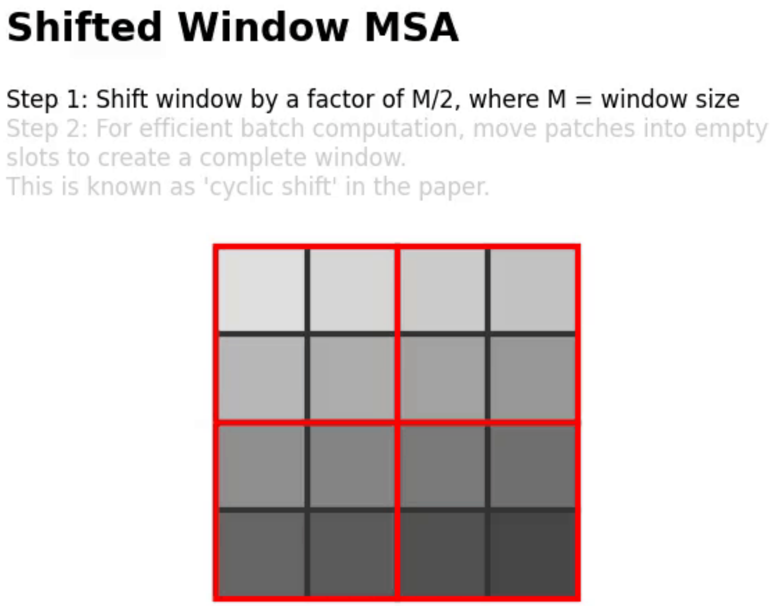
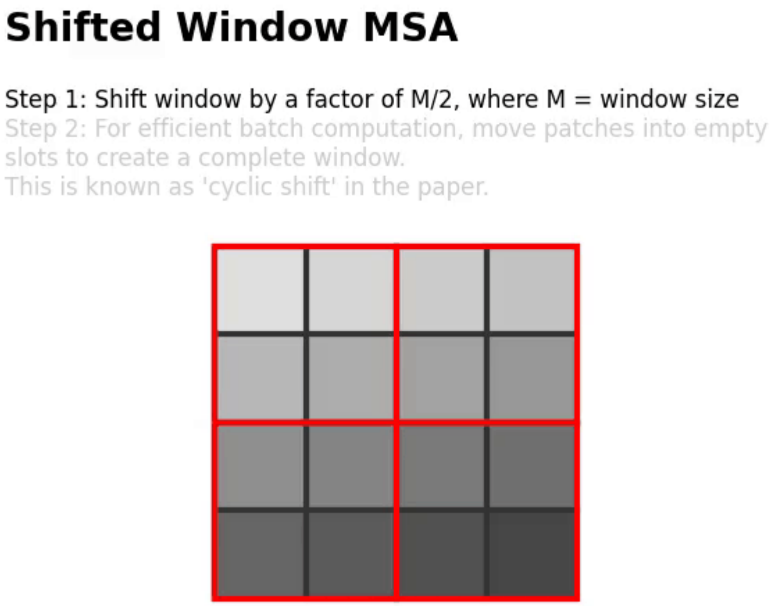


Image Credit: https://towardsdatascience.com/a-comprehensive-guide-to-swin-transformer-64965f89d14c

Extensions: Swin Transformer



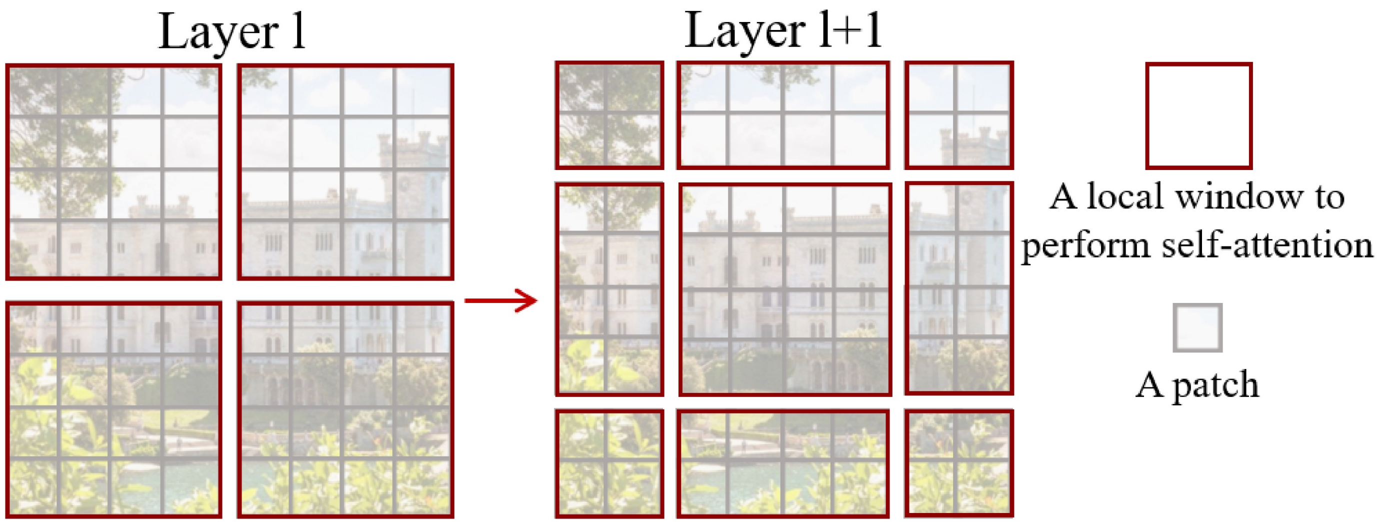


Image Credit: https://towardsdatascience.com/a-comprehensive-guide-to-swin-transformer-64965f89d14c, [10]

Extensions: Swin Transformer

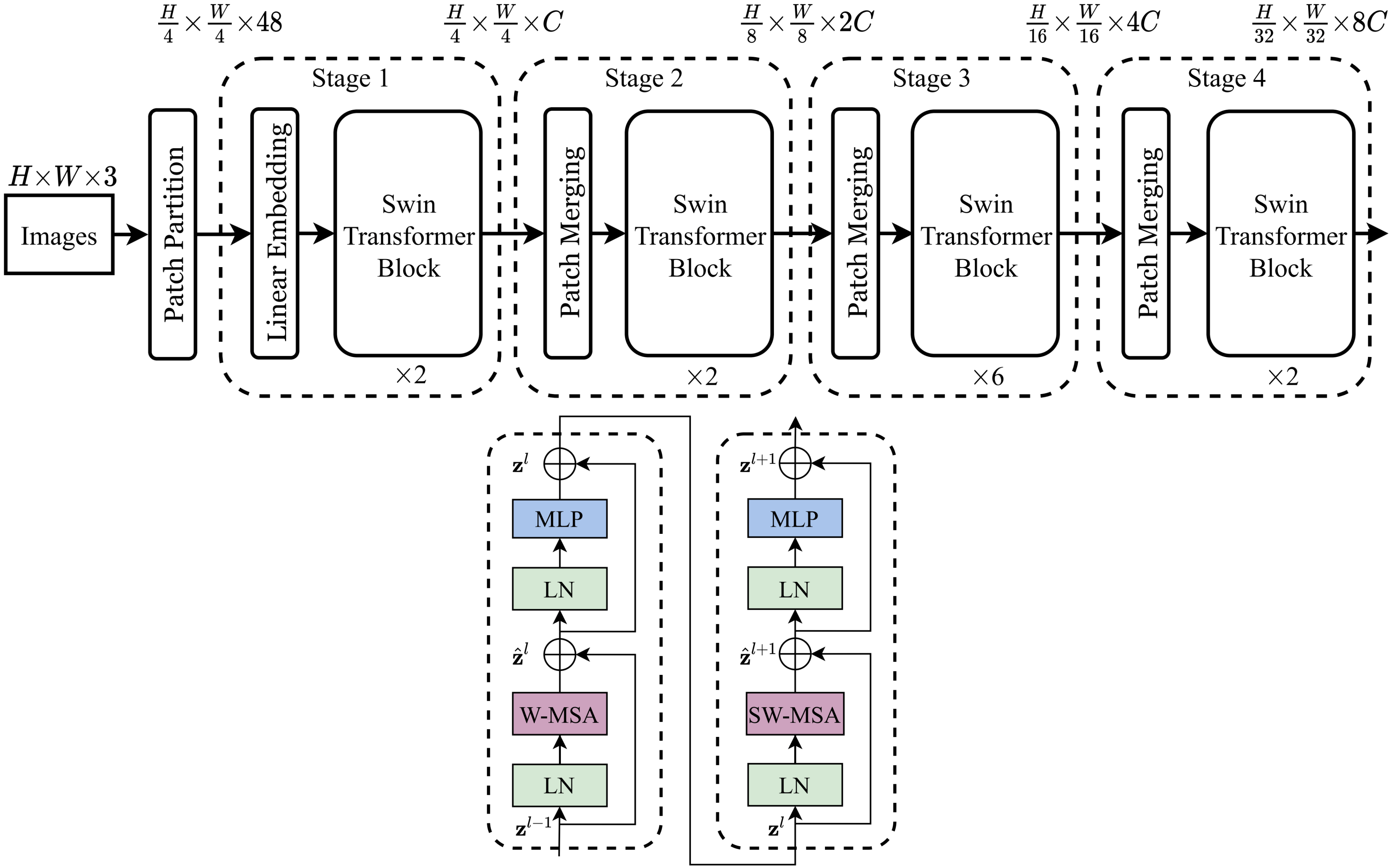


Image Credit: [10]

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Questions?