

Machine Learning in Particle Theory

- MITP Summer School 2023

Eilam Gross

Particle Flow with Deep Learning

- ✓ Lecture 1: GNN+Attention
- ✓ Lecture 2: Transformers + Set Generation
(with the help of **N. Kakati** and **N. Soybelman**)
- Lecture 3: Hyper Graphs + TSPN Particle Flow
(with the help of **N. Kakati**)

Syllabus

✓ Graph Neural Nets

✓ Set to Graph

✓ Attention is all you need

✓ Transformers, ✓ Slot Attention (SA)

✓ Set Prediction Networks with a Transformer and SA (TSPN-SA)

✓ Constrained Variational Auto Encoder (cVAE)

- Particle Flow
(Reconstructing Particles in Jets using TSPN-SA,
Hyper-Graph PFlow [HGPflow])

✓ Simulation of PF Objects (Using TSPN-SA, cVAE)

Attention Is All You Need

<https://arxiv.org/abs/1706.03762>

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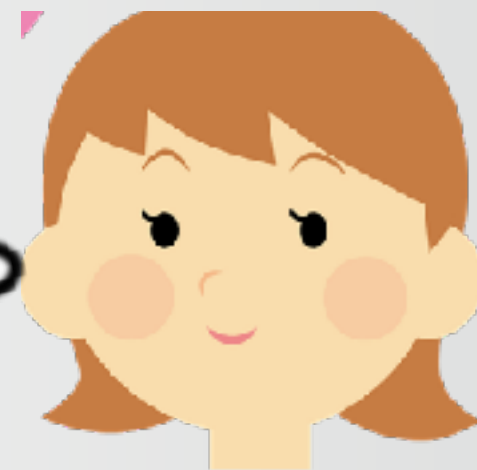
Attention is All You Need

Level 1 N. Kakati

Once upon a time, people in AI were working in peace..



AI will change the world in 50 years



The field was making good progress

One bright summer morning, a paper showed up

Attention Is All You Need

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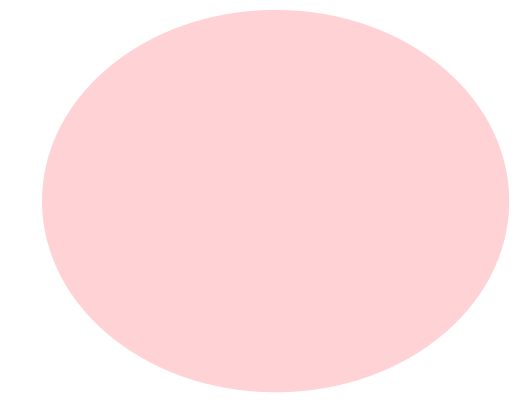
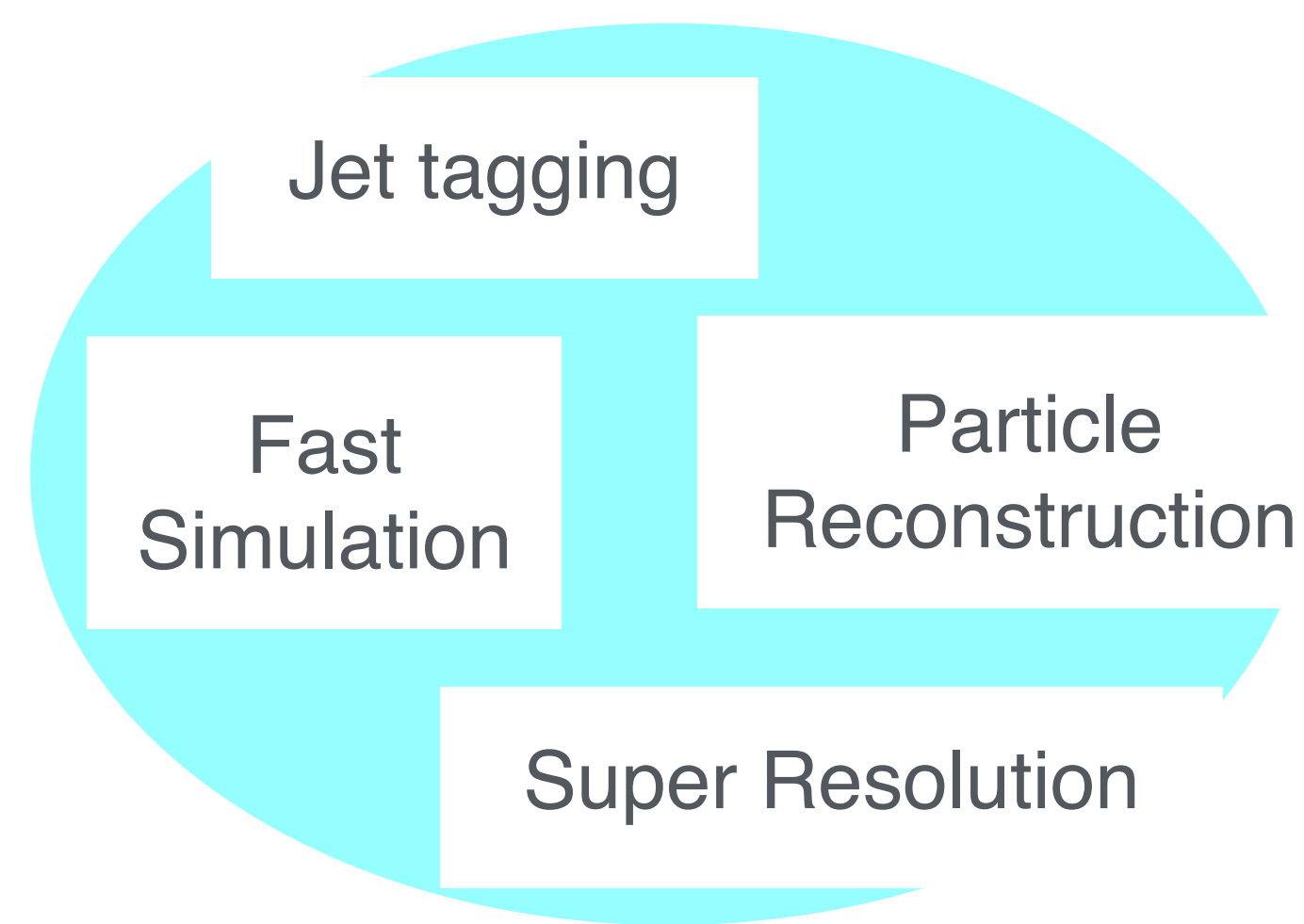
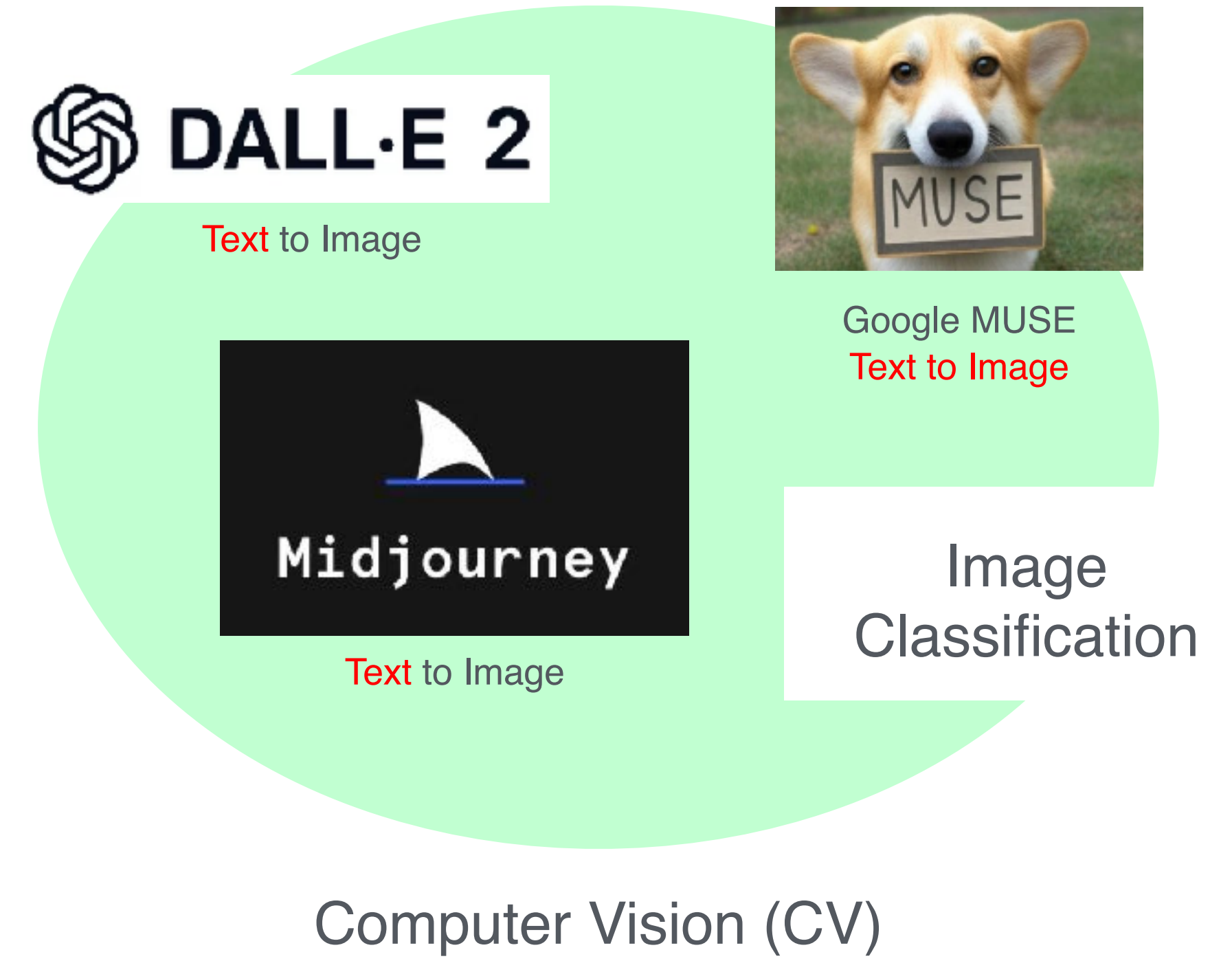
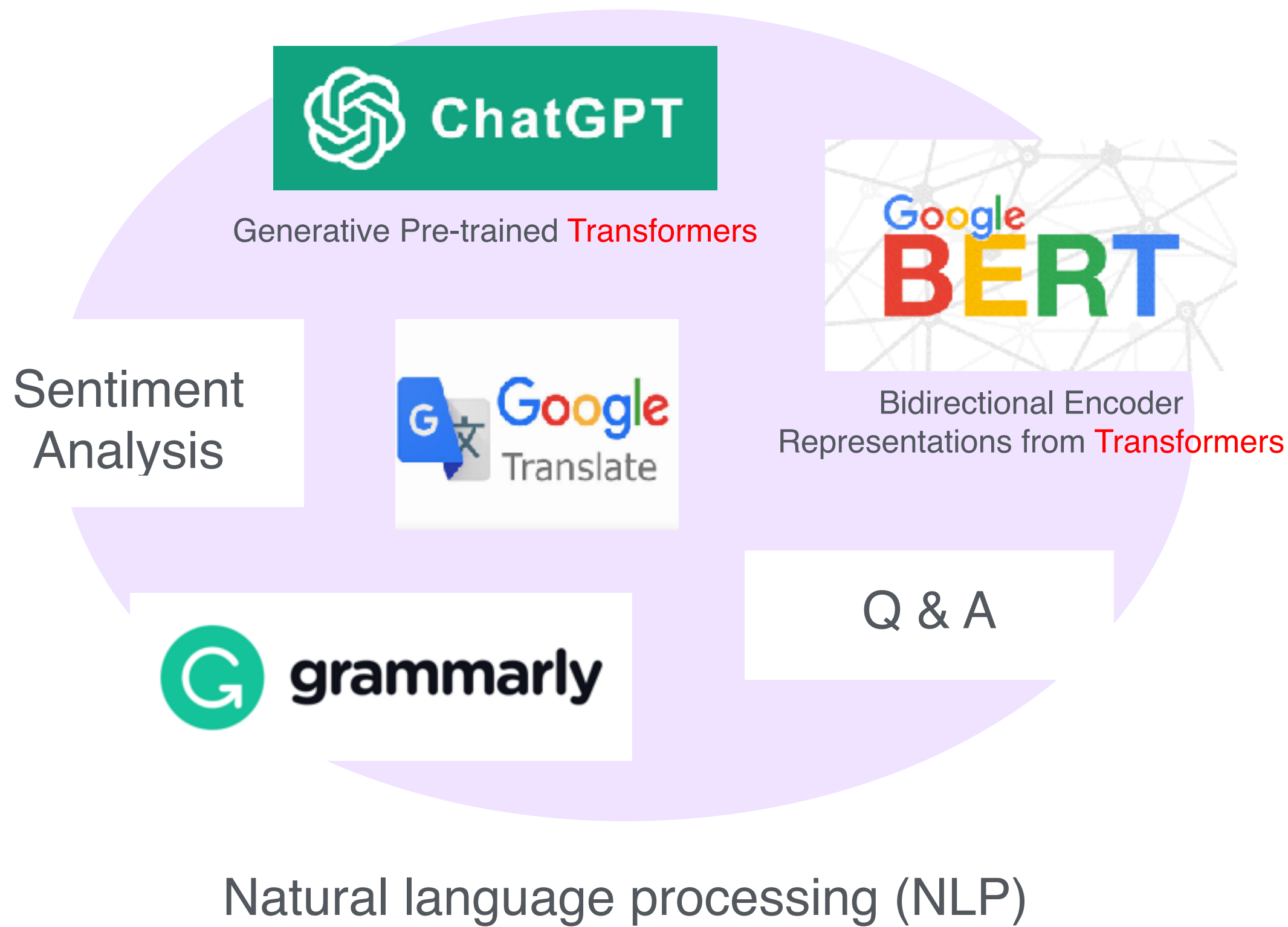
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AND THEN EVERYTHING CHANGED!

Where is Transformer?

It's everywhere...



What is a Transformer?

- ◆ Looks very complicated
- ◆ It'll make sense once we understand the components

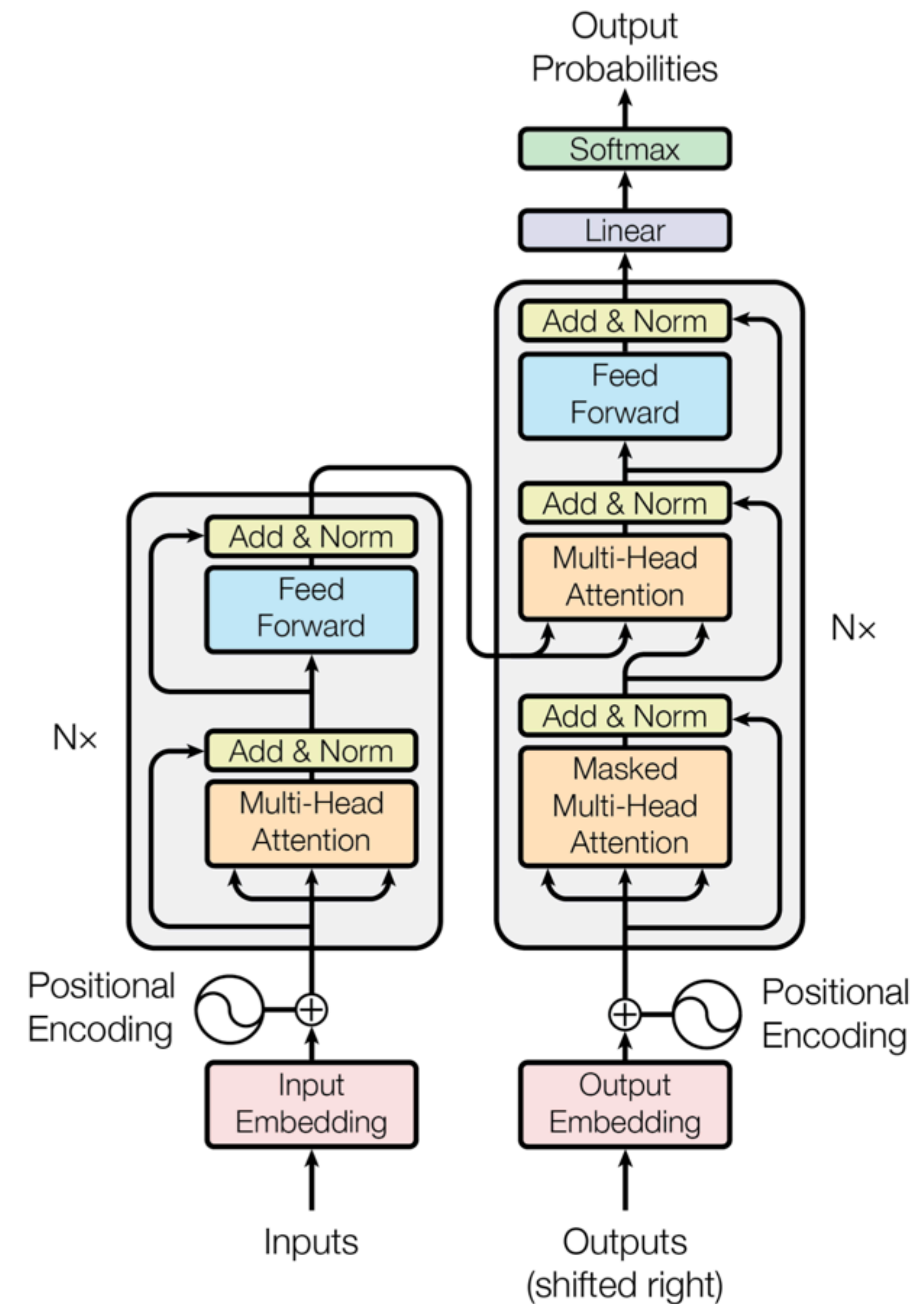
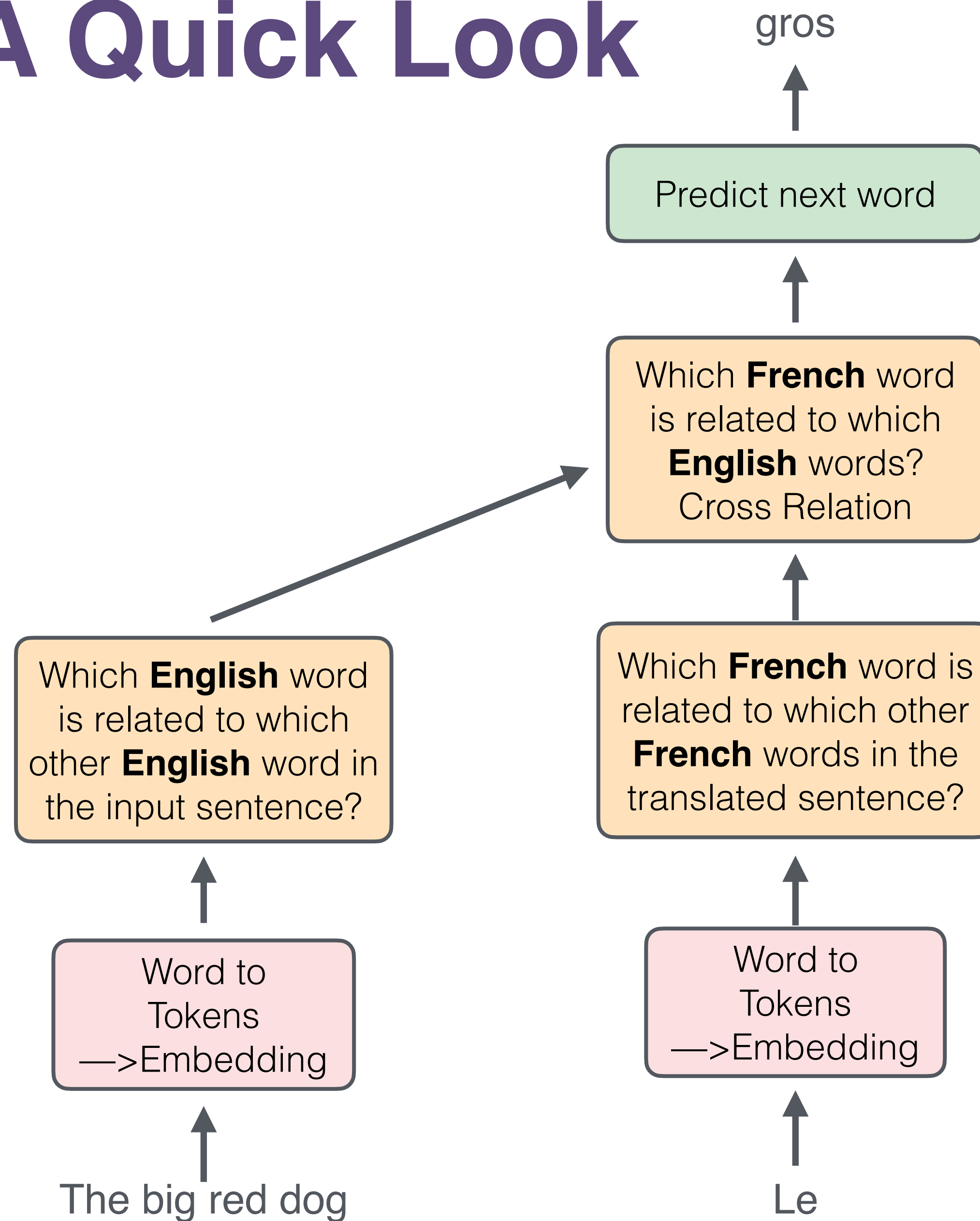


Figure 1: The Transformer - model architecture.

A Quick Look



- ◆ We are doing translation
 - ➔ English to French
- ◆ English sentence
 - ➔ The big red dog
- ◆ Someone told you that the first word in French is “Le”
 - ➔ You need to predict the next words one by one and complete the sentence

A Quick Look

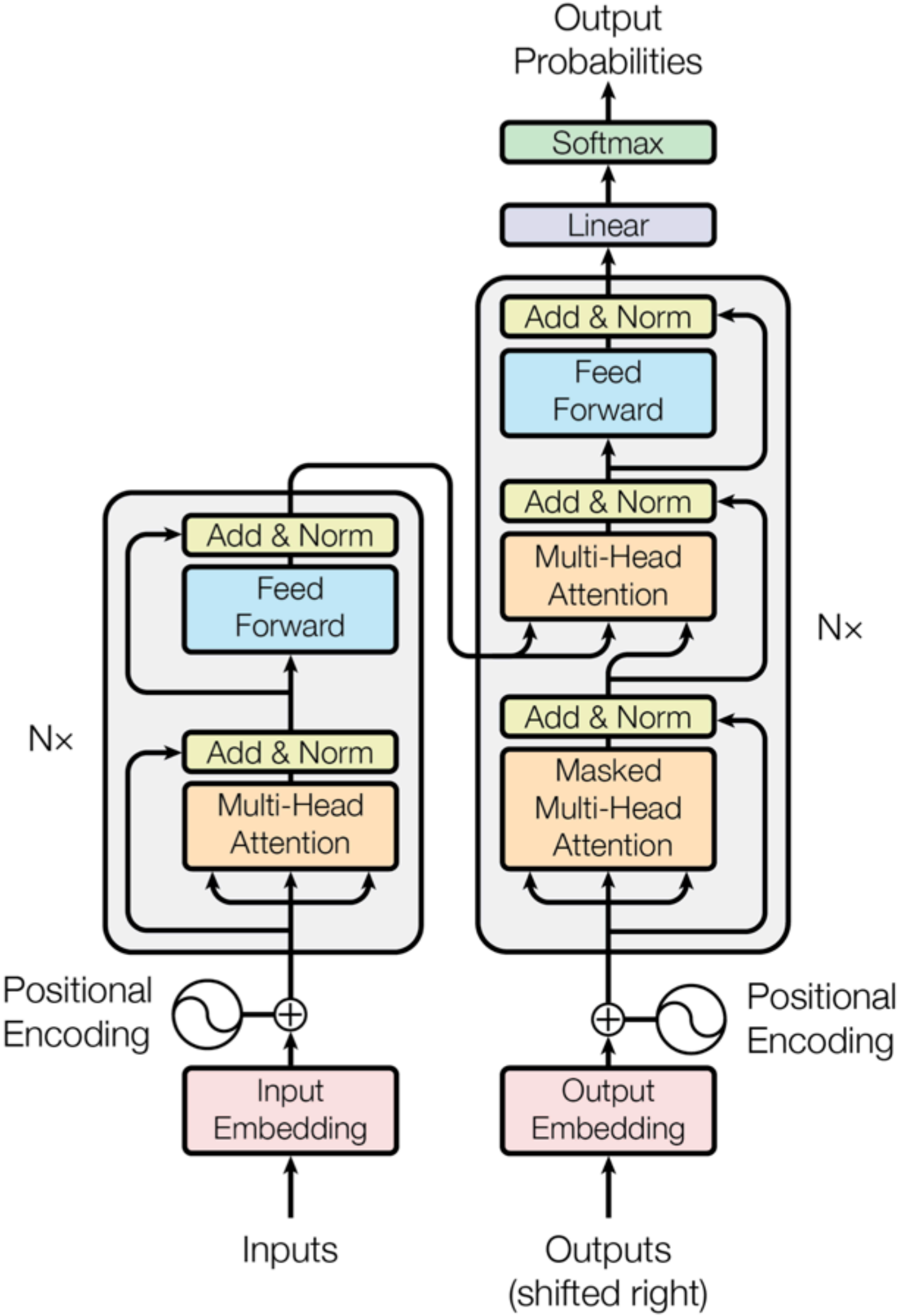
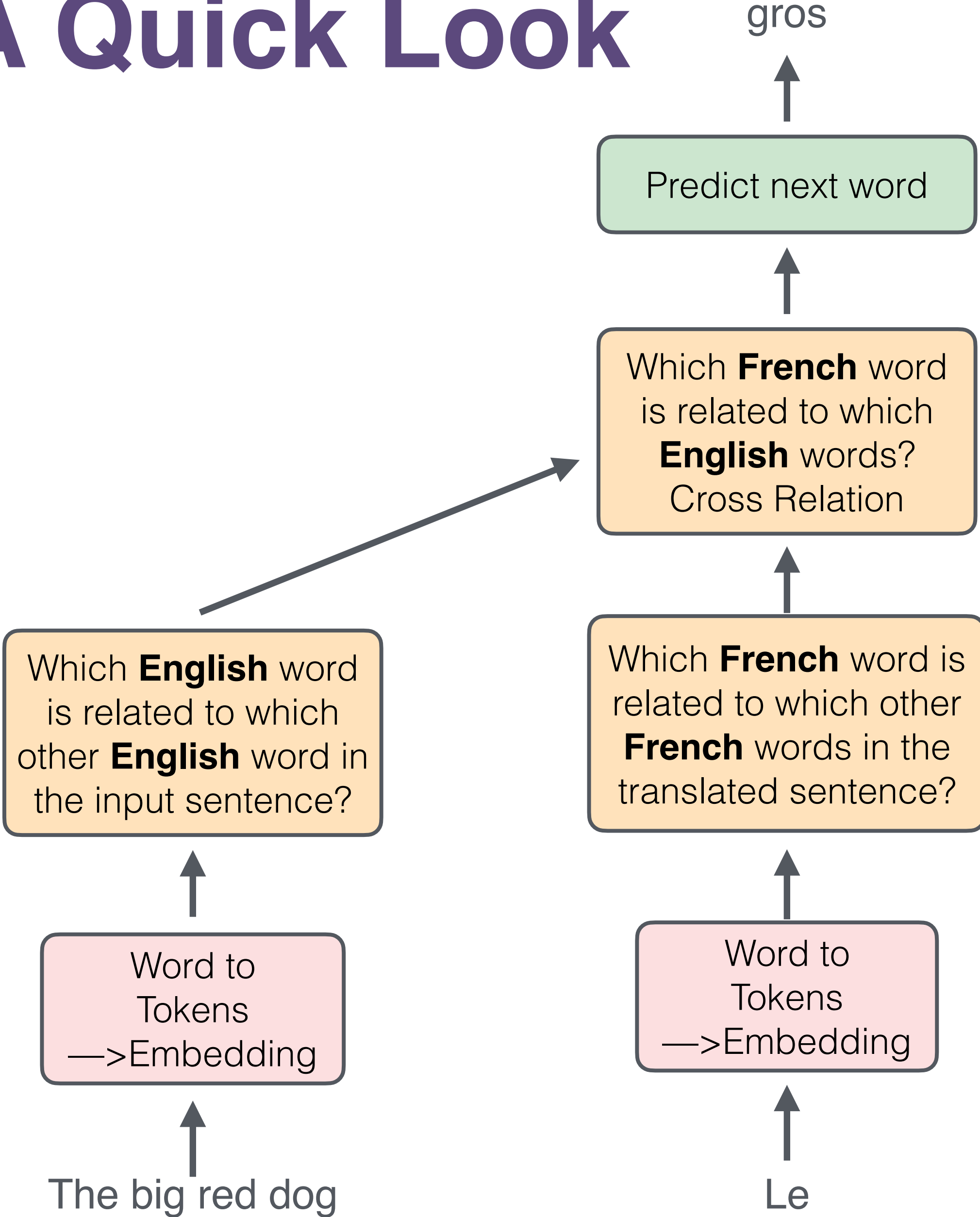


Figure 1: The Transformer - model architecture.

Attention is All You Need

Level 2 N. Kakati

- ◆ Pretty good explanation here
 - <https://www.youtube.com/watch?v=TQQIZhbC5ps>
 - [YouTube channel link](#)
- ◆ This part of the lecture is mainly based on that video

Embedding

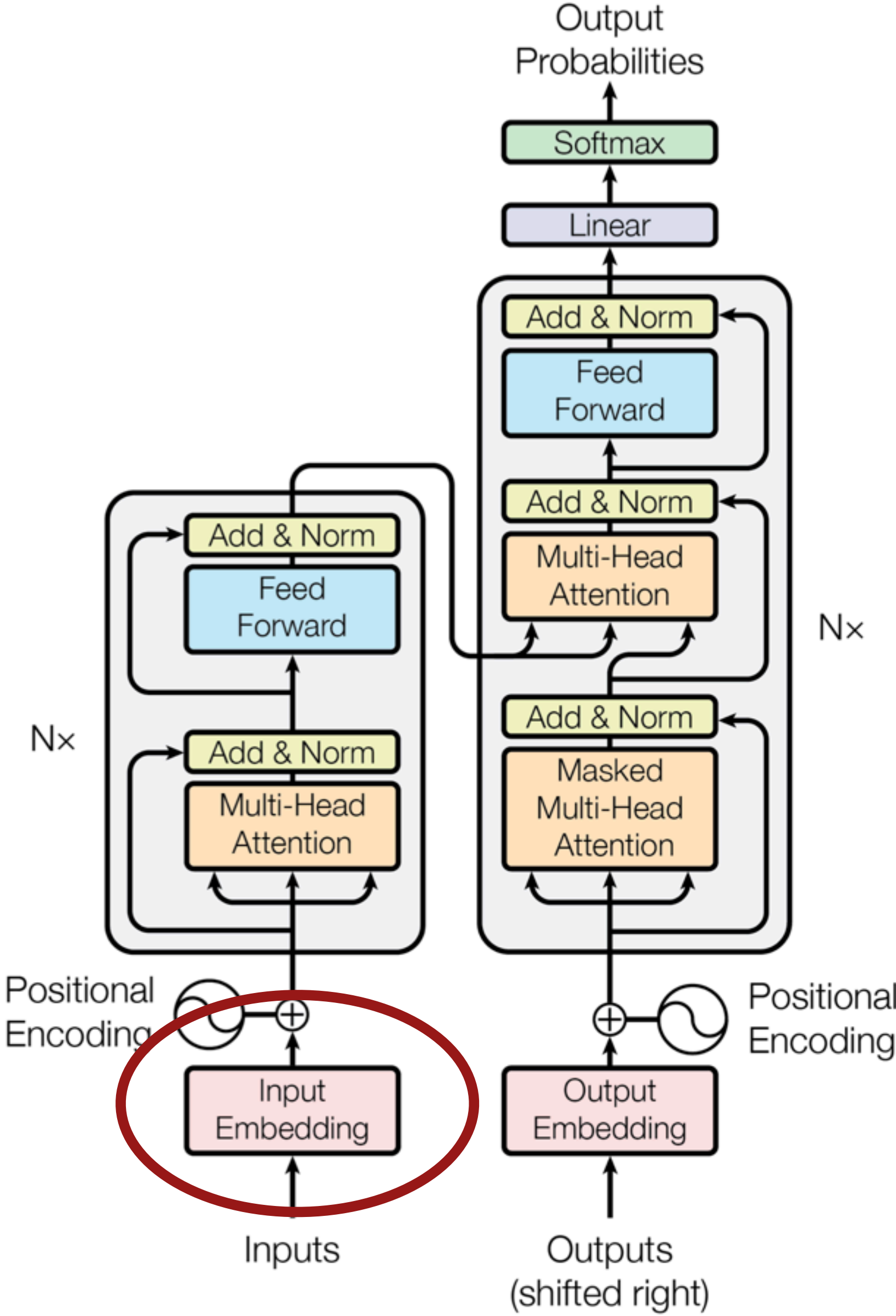
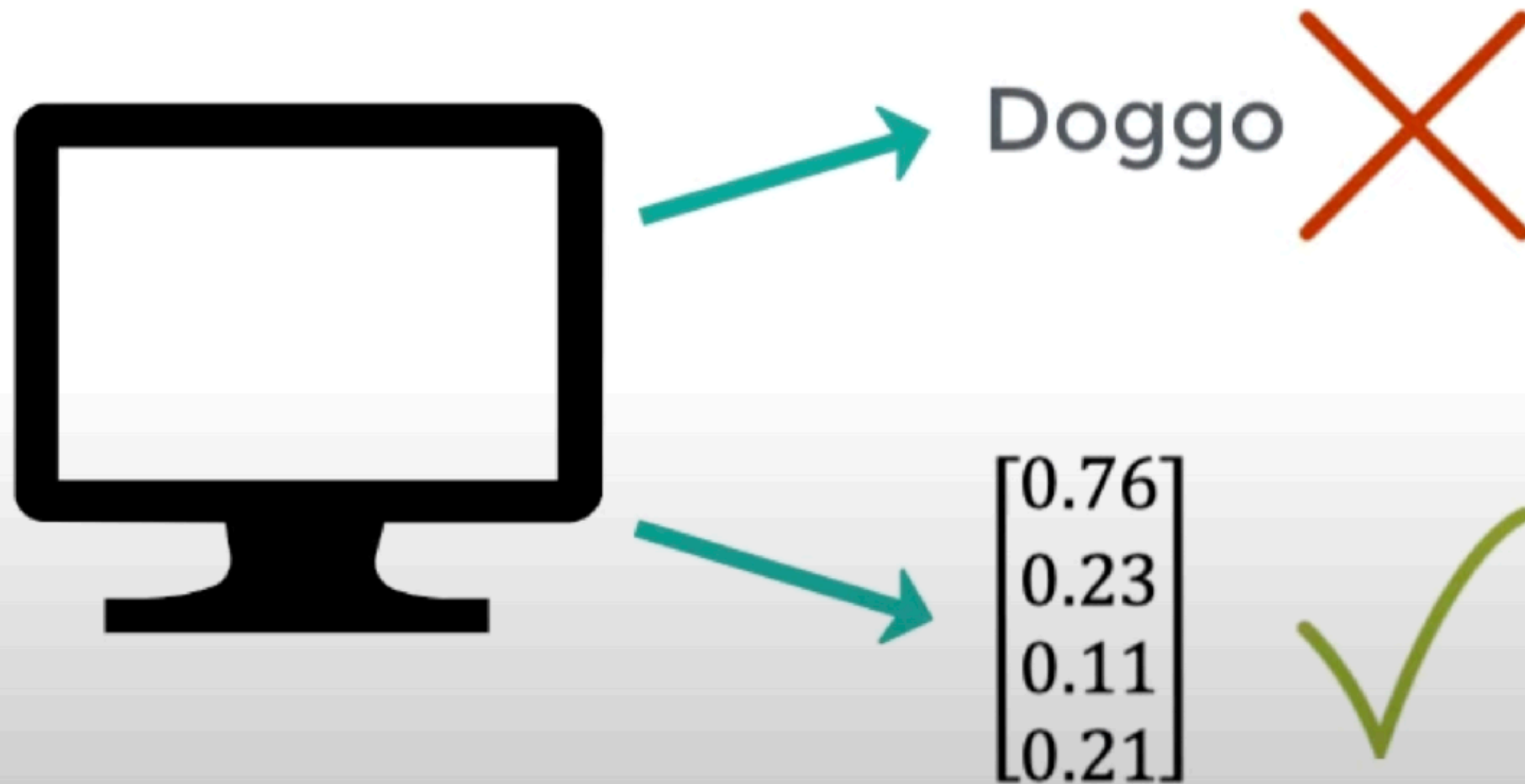


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Embedding

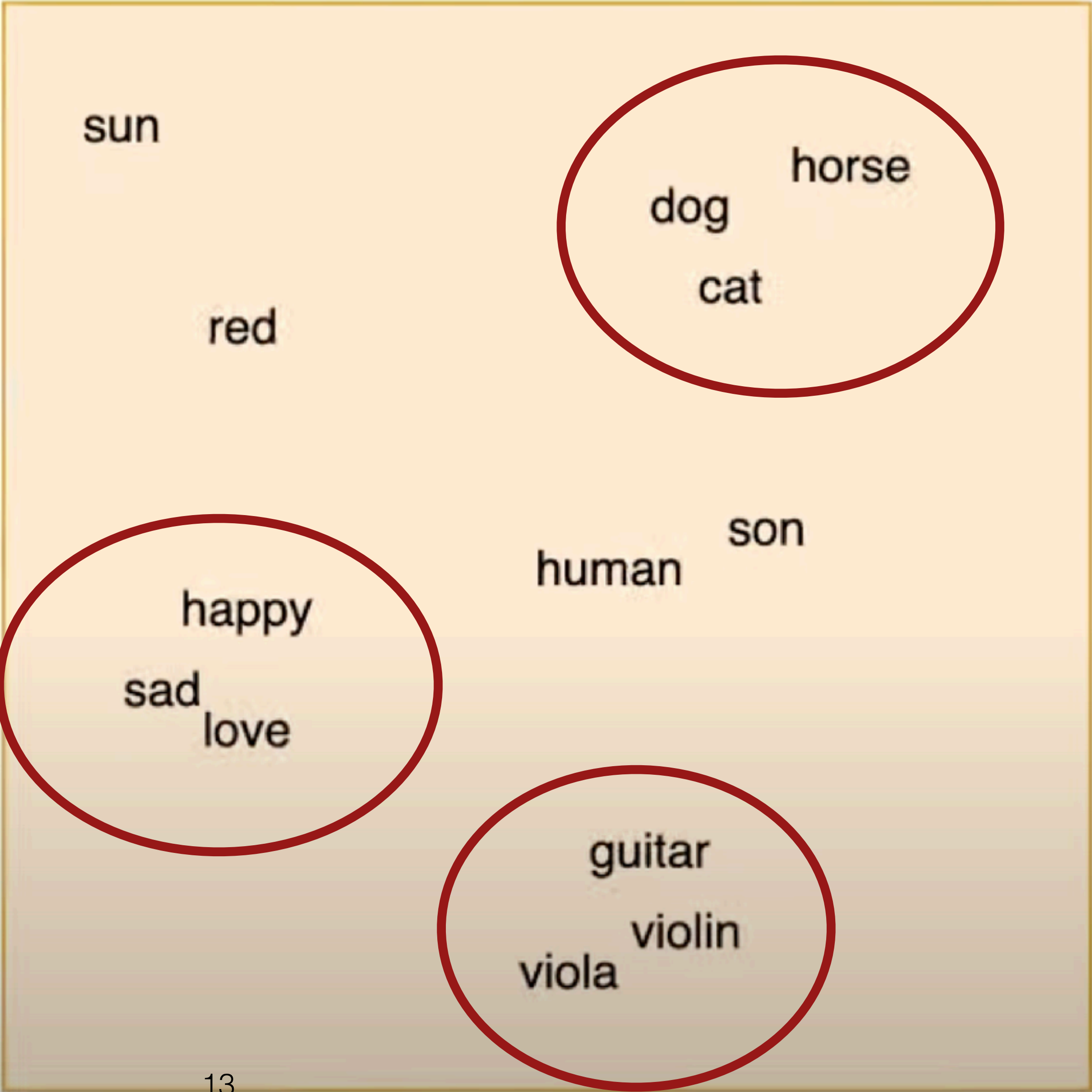


Embedding

Embedding space



learns
→



Embedding

dog



$\begin{bmatrix} 0.37 \\ 0.99 \\ 0.01 \\ 0.08 \end{bmatrix}$

Embedding

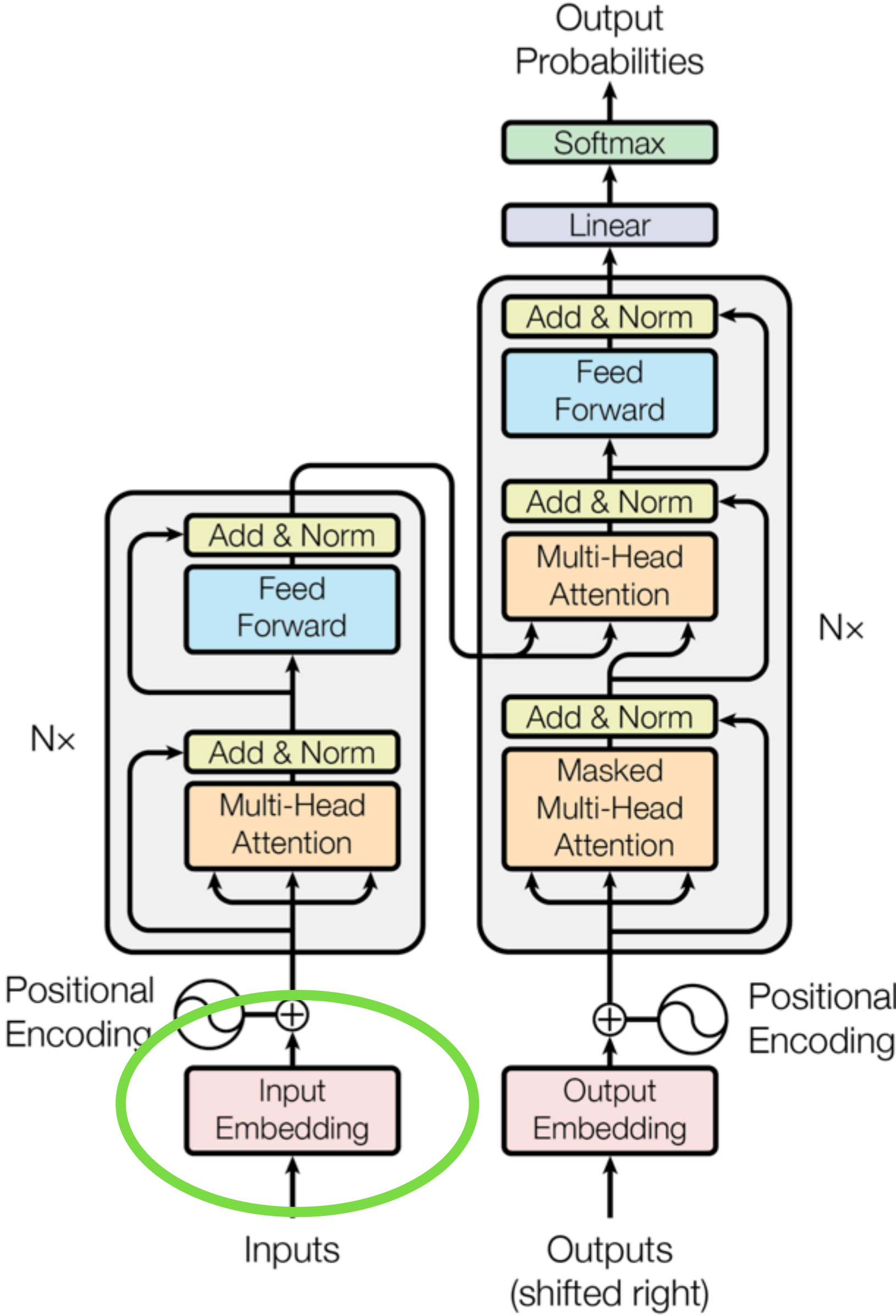


Figure 1: The Transformer - model architecture.

Positional encoding

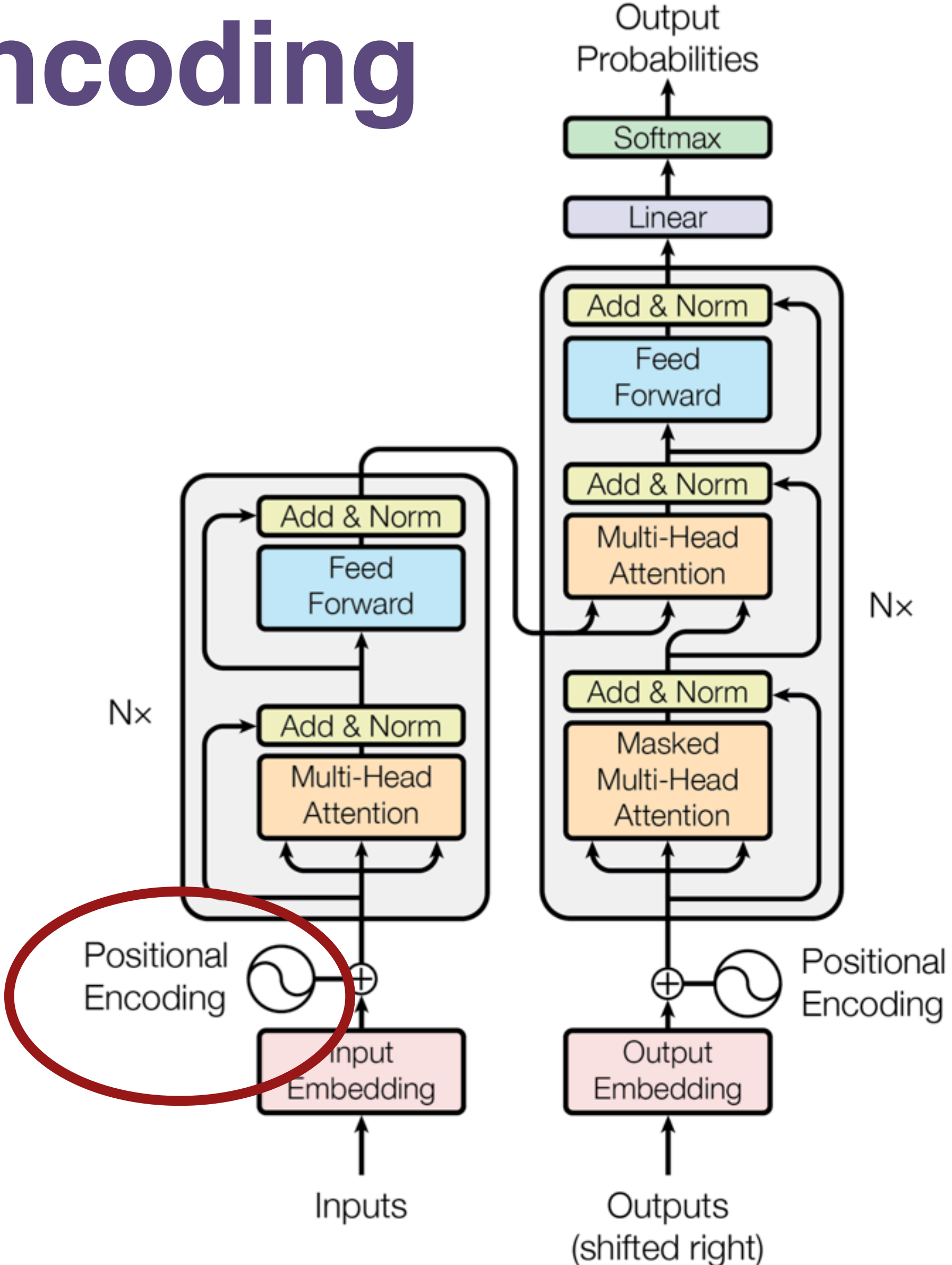


Figure 1: The Transformer - model architecture.

Positional encoding

dog



$\begin{bmatrix} 0.37 \\ 0.99 \\ 0.01 \\ 0.08 \end{bmatrix}$

AJ's **dog** is a cutie

AJ looks like a **dog**

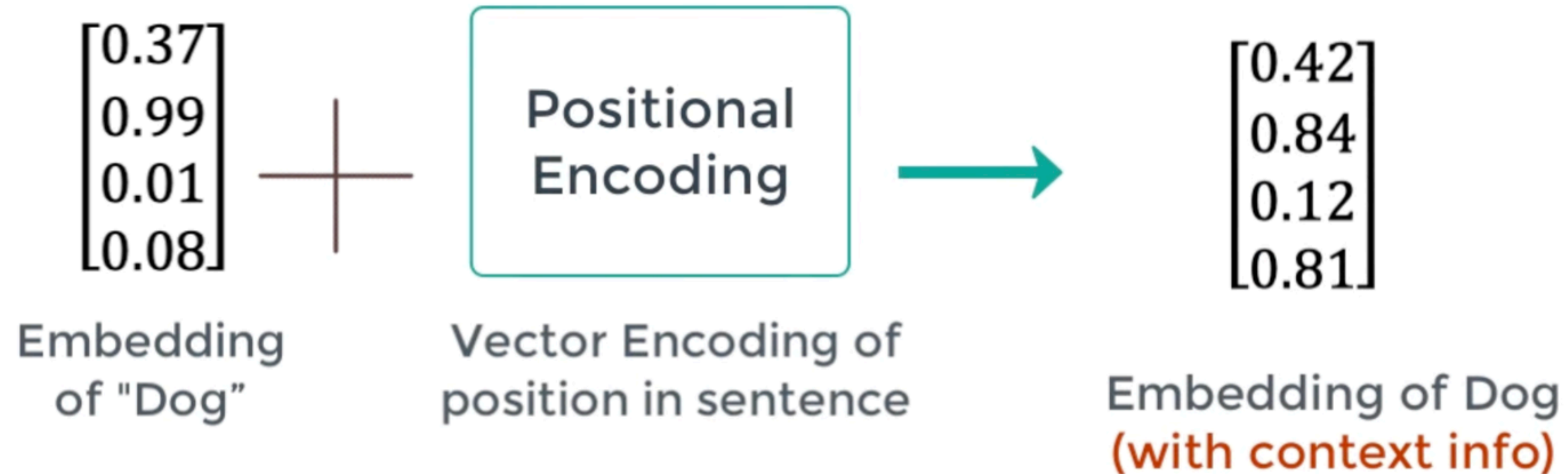
Positional Encoding

Positional encoder: Vector that gives context based on position of word in sentence

AJ's **dog** is a cutie  Position 2

AJ looks like a **dog**  Position 5

Positional Encoding



Positional encoding

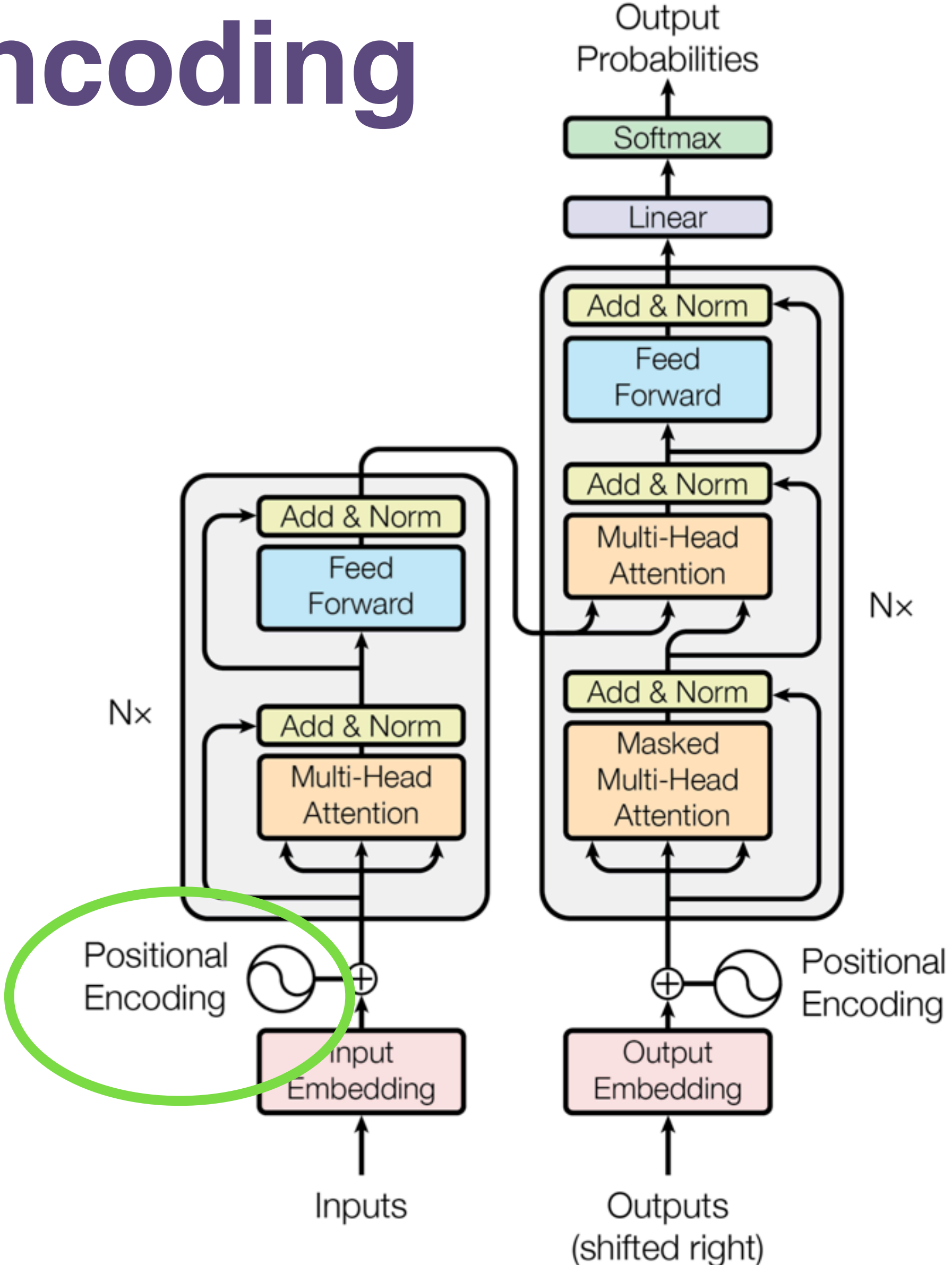


Figure 1: The Transformer - model architecture.

Attention

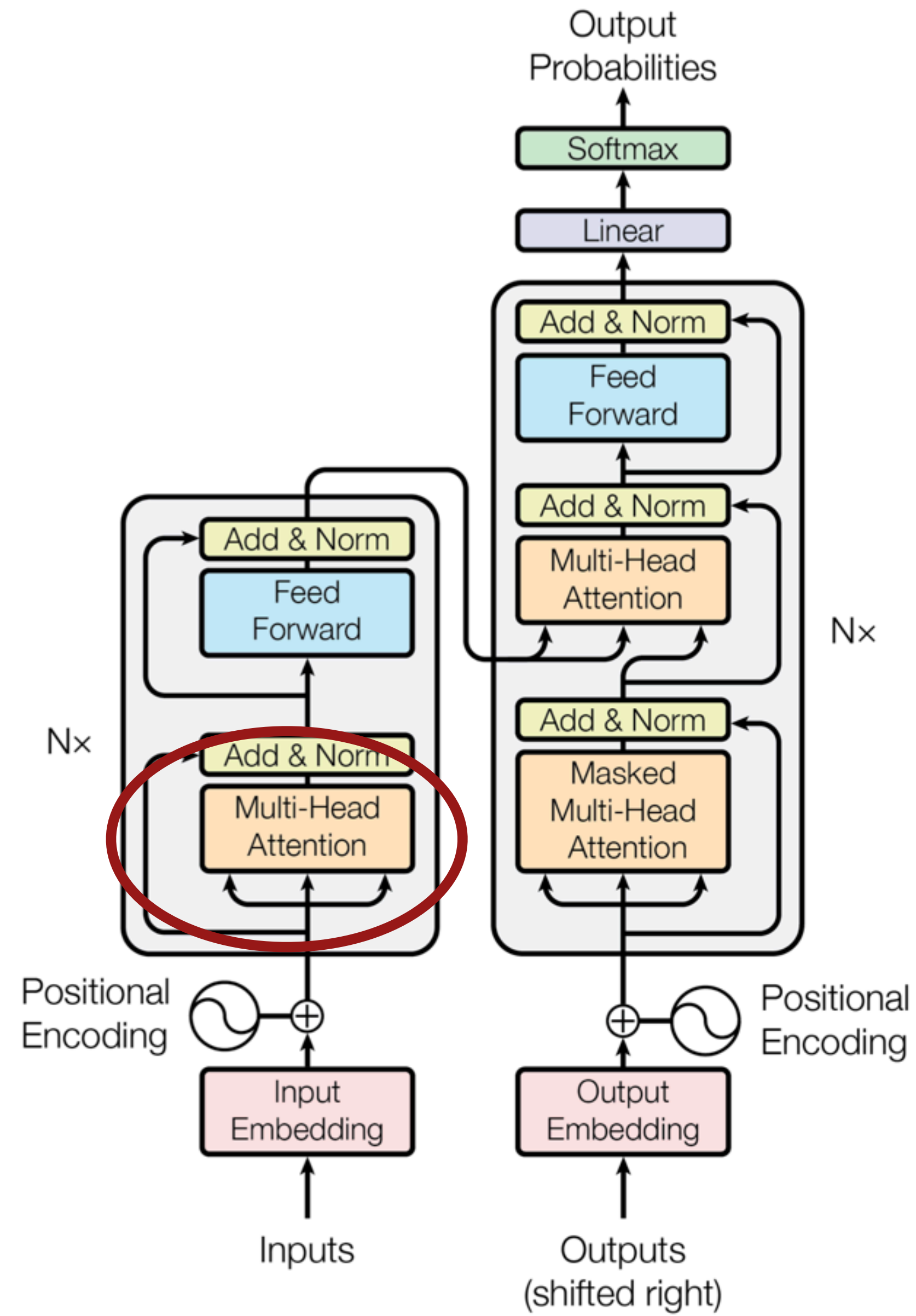
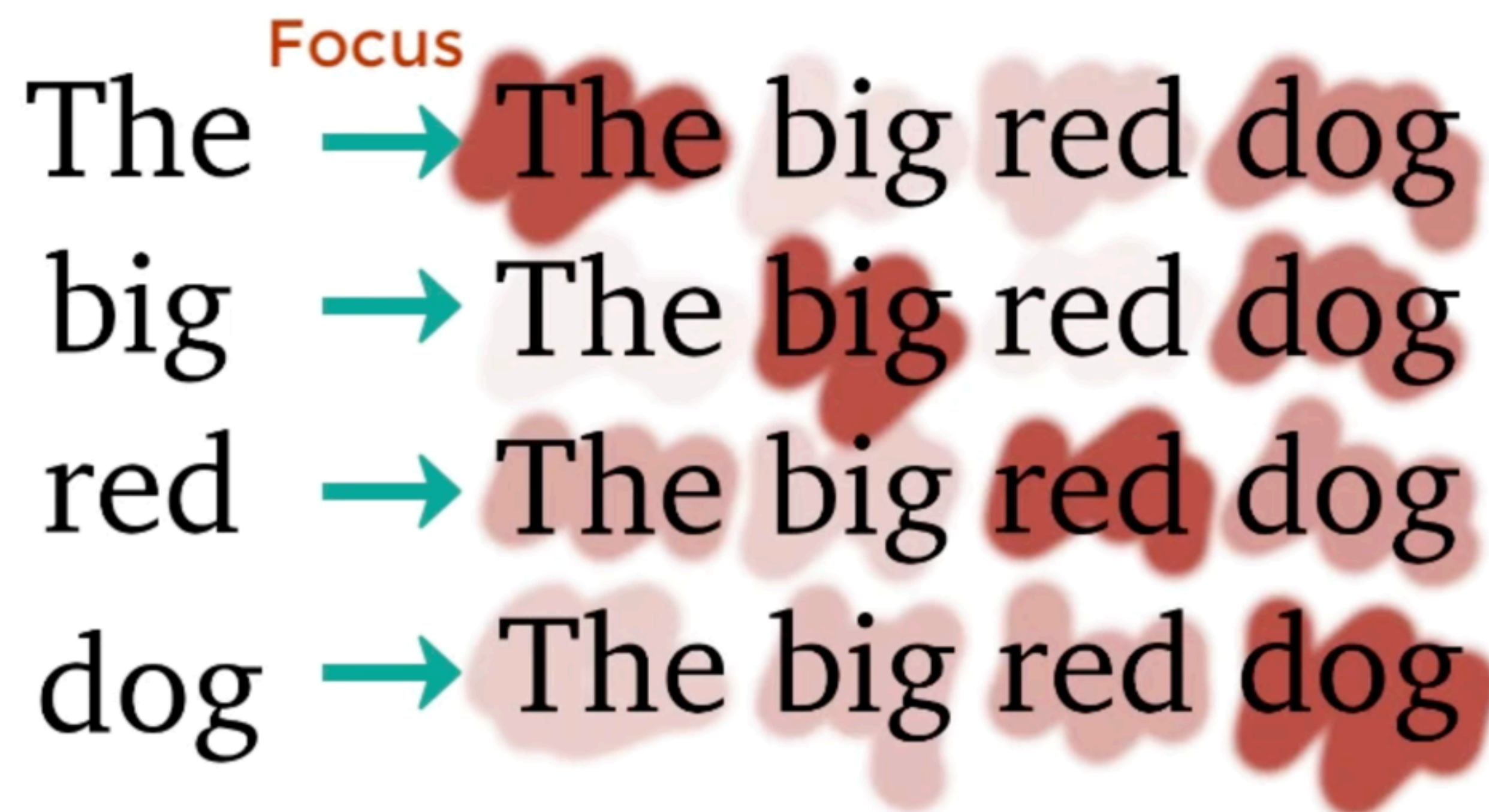


Figure 1: The Transformer - model architecture.

Attention

How relevant one word is to the others?



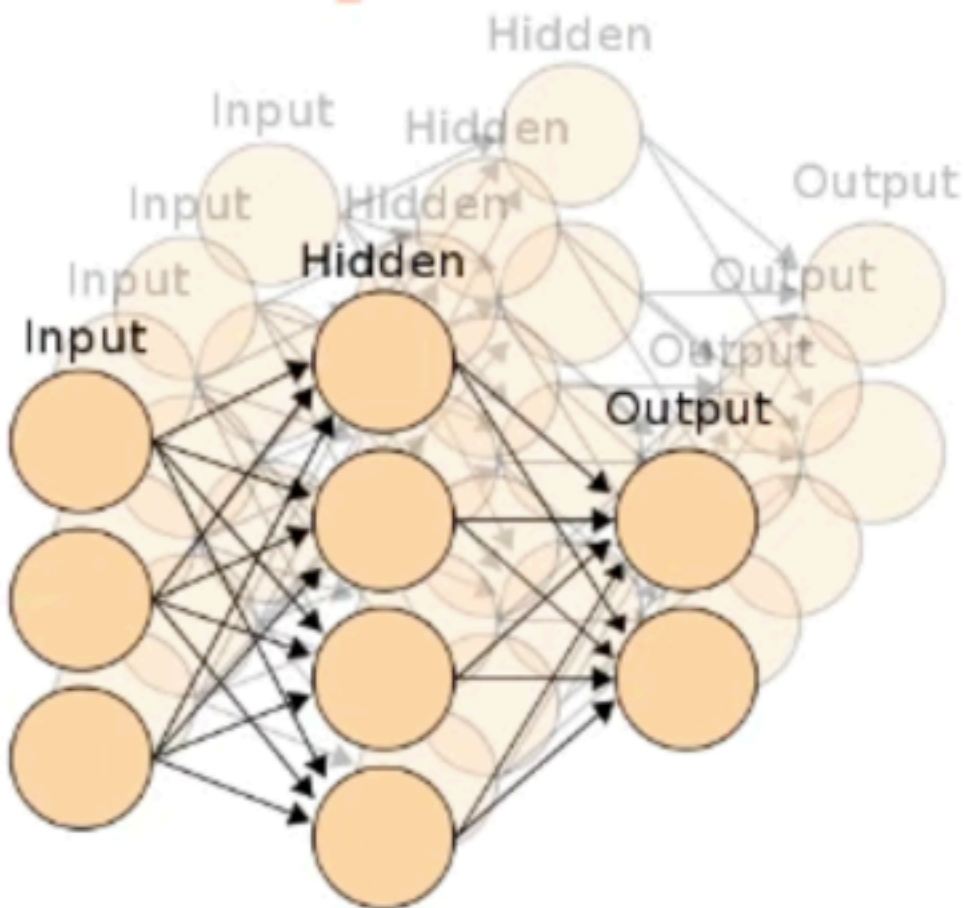
Attention matrix

$[0.71$	0.04	0.07	$0.18]^T$
$[0.01$	0.84	0.02	$0.13]^T$
$[0.09$	0.05	0.62	$0.24]^T$
$[0.03$	0.03	0.03	$0.91]^T$

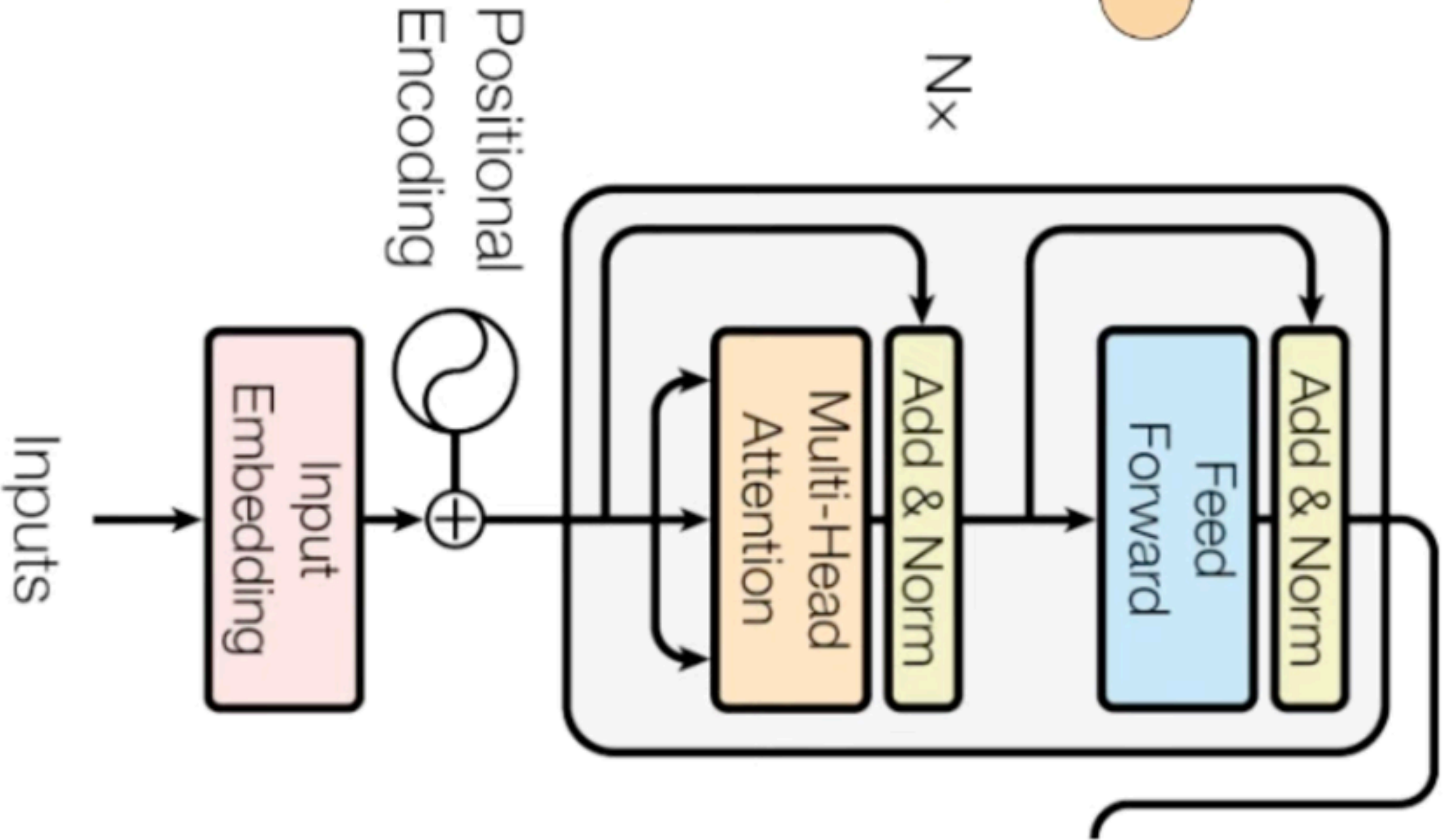
FeedForward

The big red dog

$\begin{bmatrix} 0.71 \\ 0.04 \\ 0.07 \\ 0.18 \end{bmatrix}$



$N \times$



Attention + FeedForward

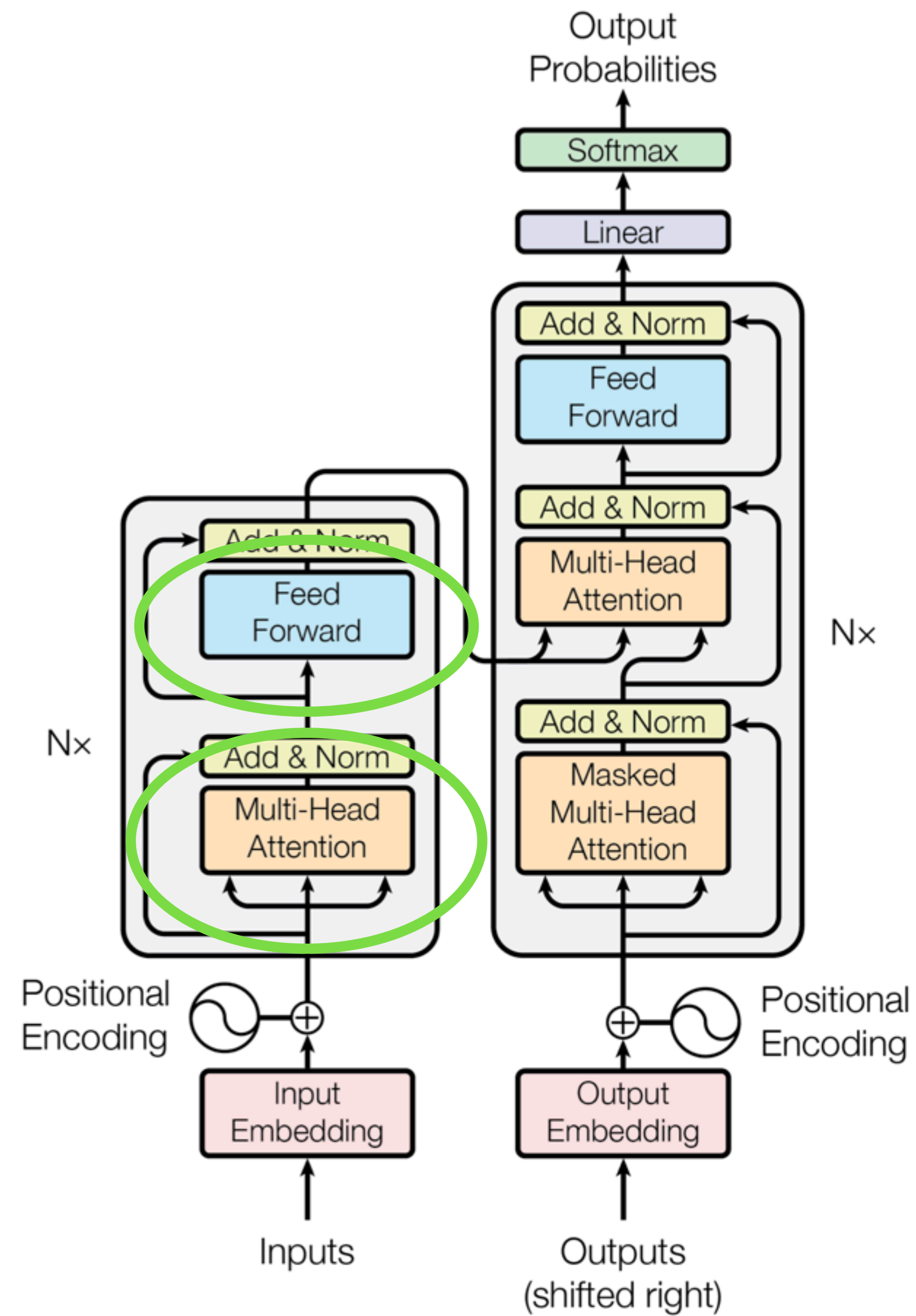


Figure 1: The Transformer - model architecture.

Decoder

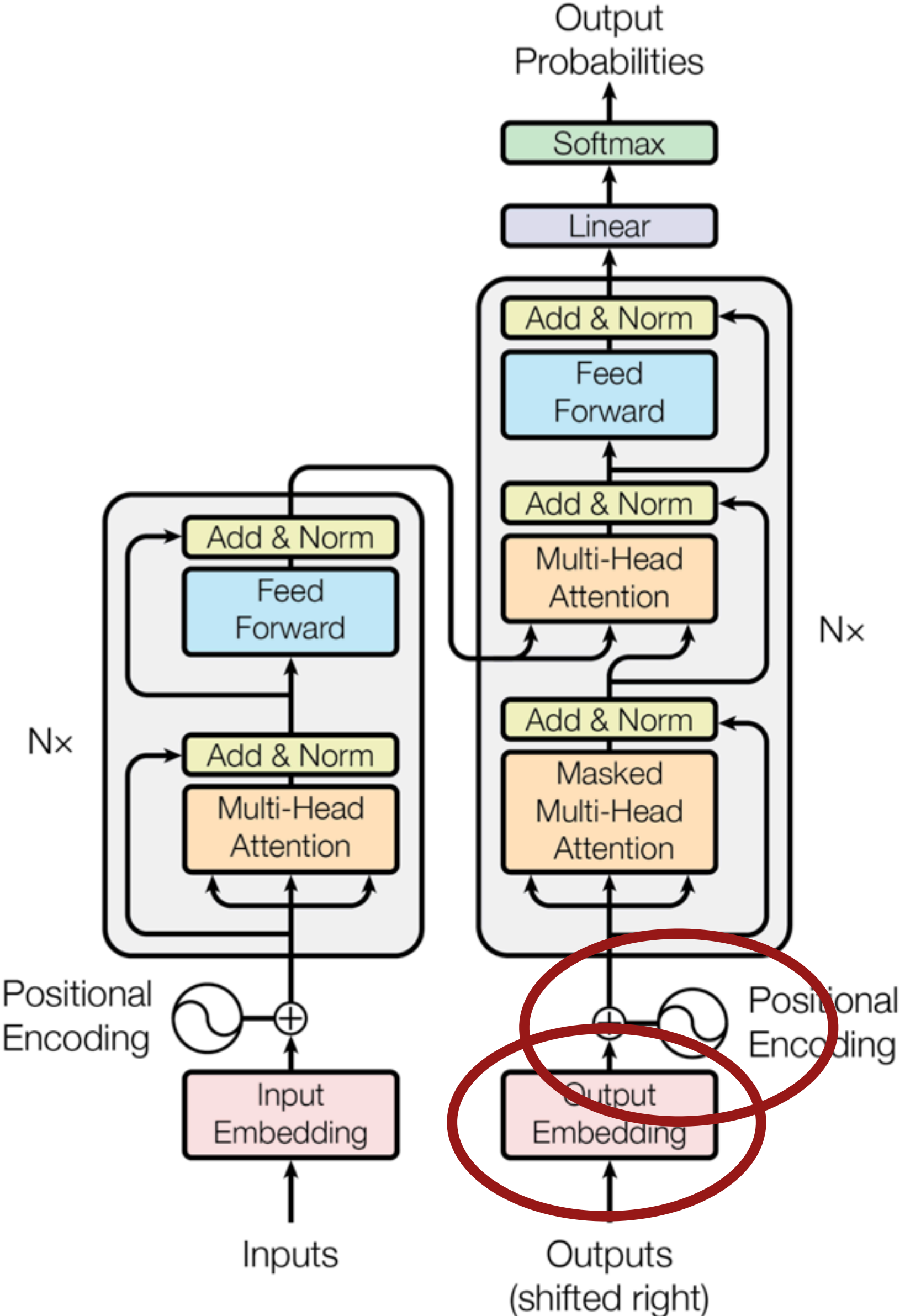


Figure 1: The Transformer - model architecture.

Decoder

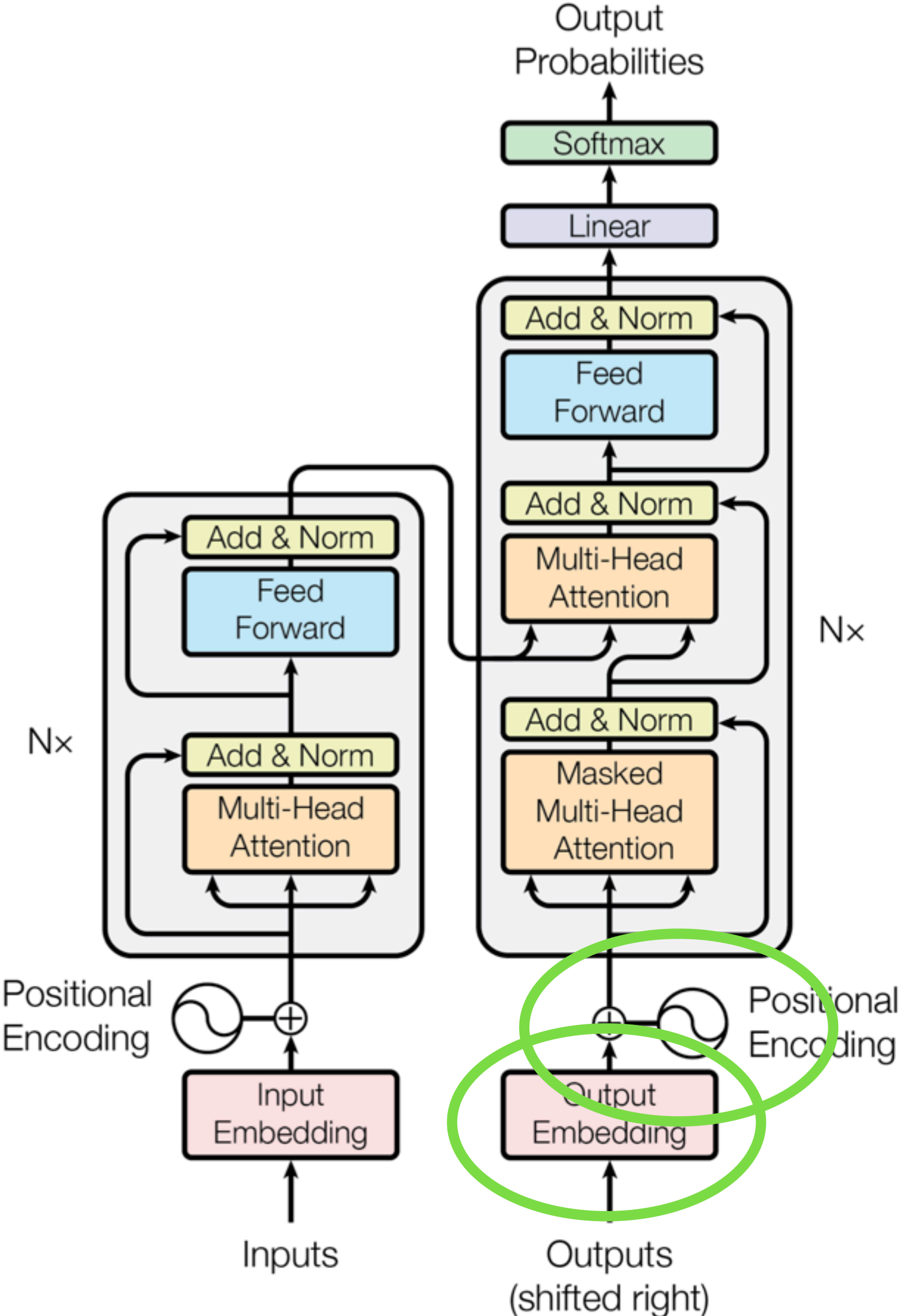


Figure 1: The Transformer - model architecture.

Masked attention

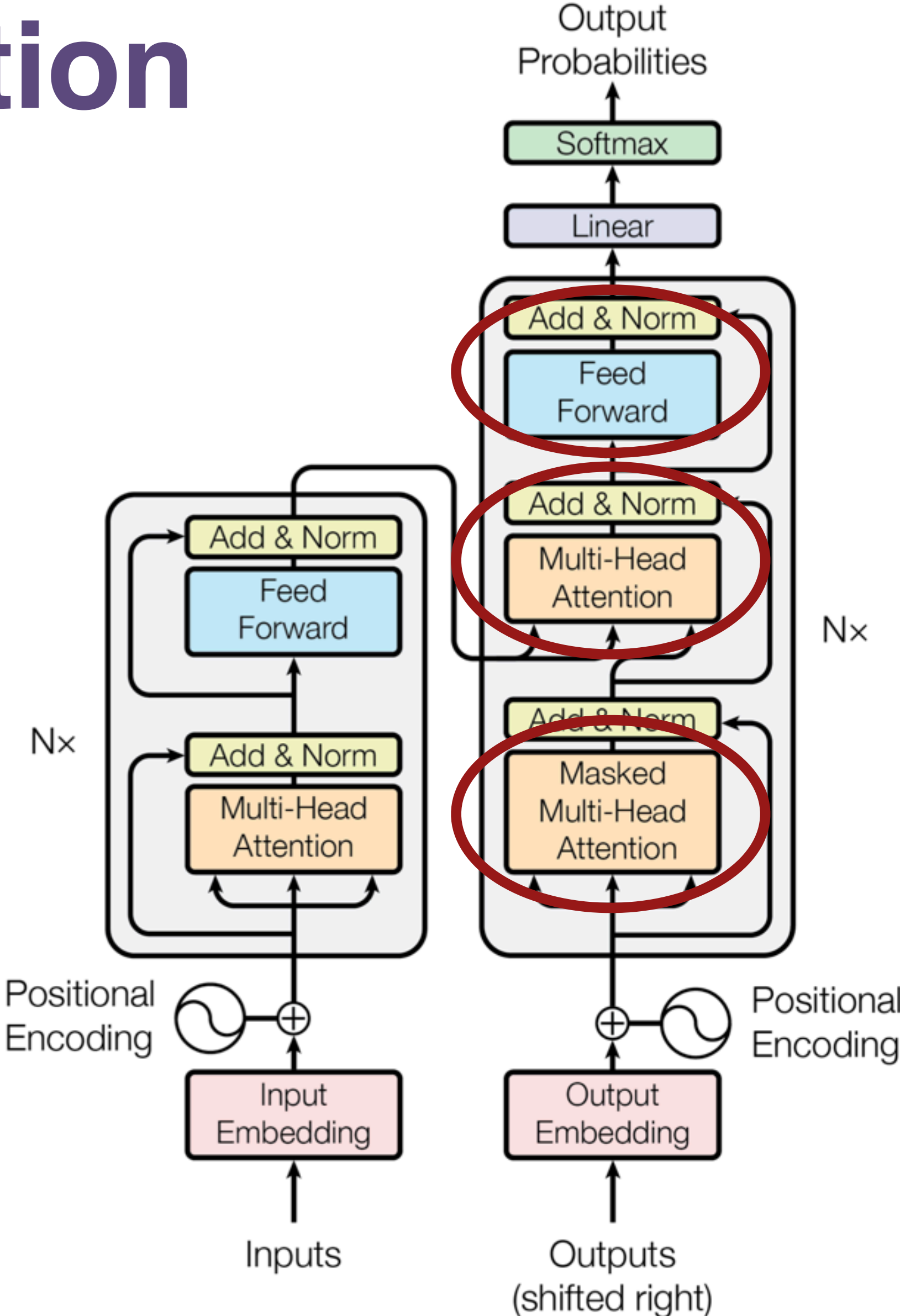


Figure 1: The Transformer - model architecture.

Self attention

Self
Attention

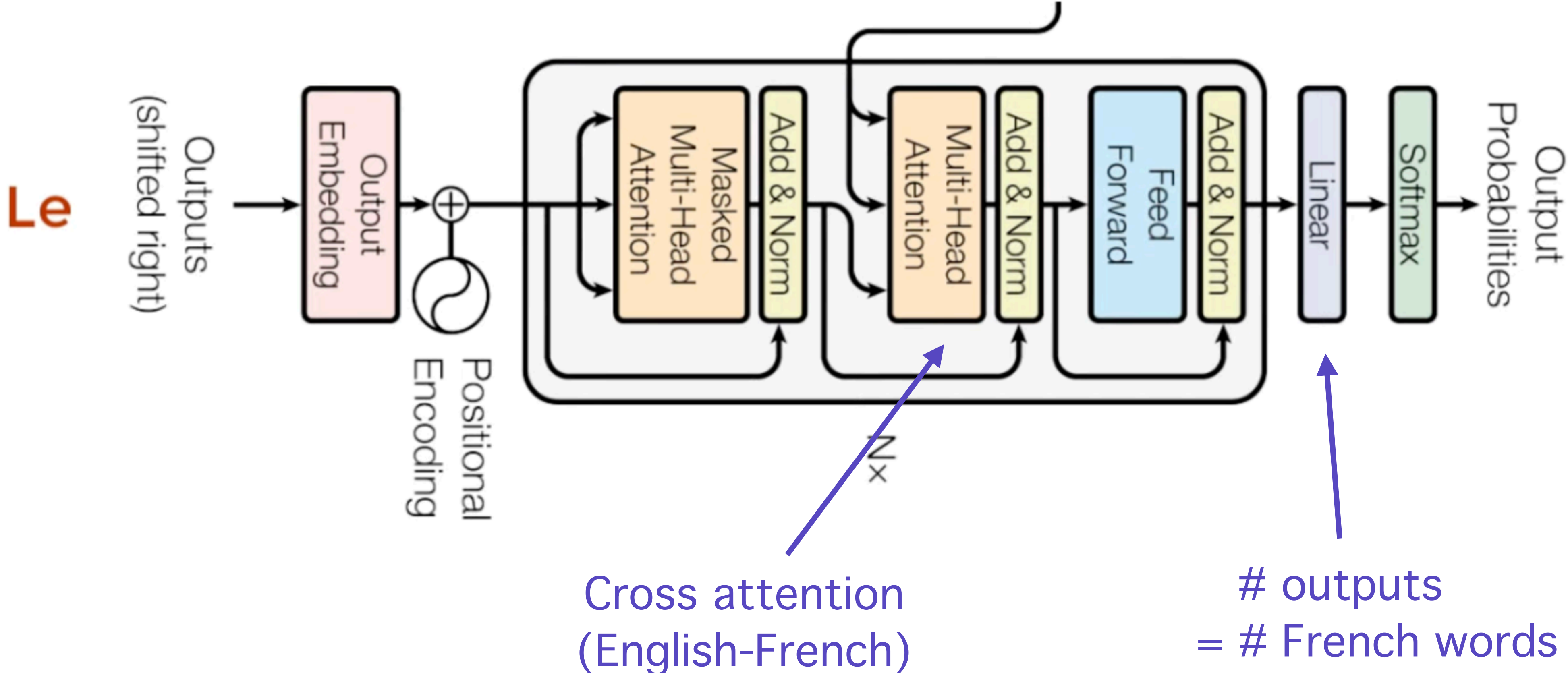
Le → Le gros chien rouge
gros → Le gros chien rouge
chien → Le gros chien rouge
rouge → Le gros chien rouge



Cross attention



Cross attention



That's pretty much it. Now let's look at some details we dropped

“Multihead” attention

- ◆ There can be **multiple relationships** to learn
 - ➔ Positional
 - ➔ “Is there” - question. “There is” - affirmative
 - ➔ Subject verb relationship
- ◆ Let’s have multiple attentions
 - ➔ **Multihead attention**
- ◆ We’ll combine all of them once they are computed

Focus
The → The big red dog
big → The big red dog
red → The big red dog
dog → The big red dog

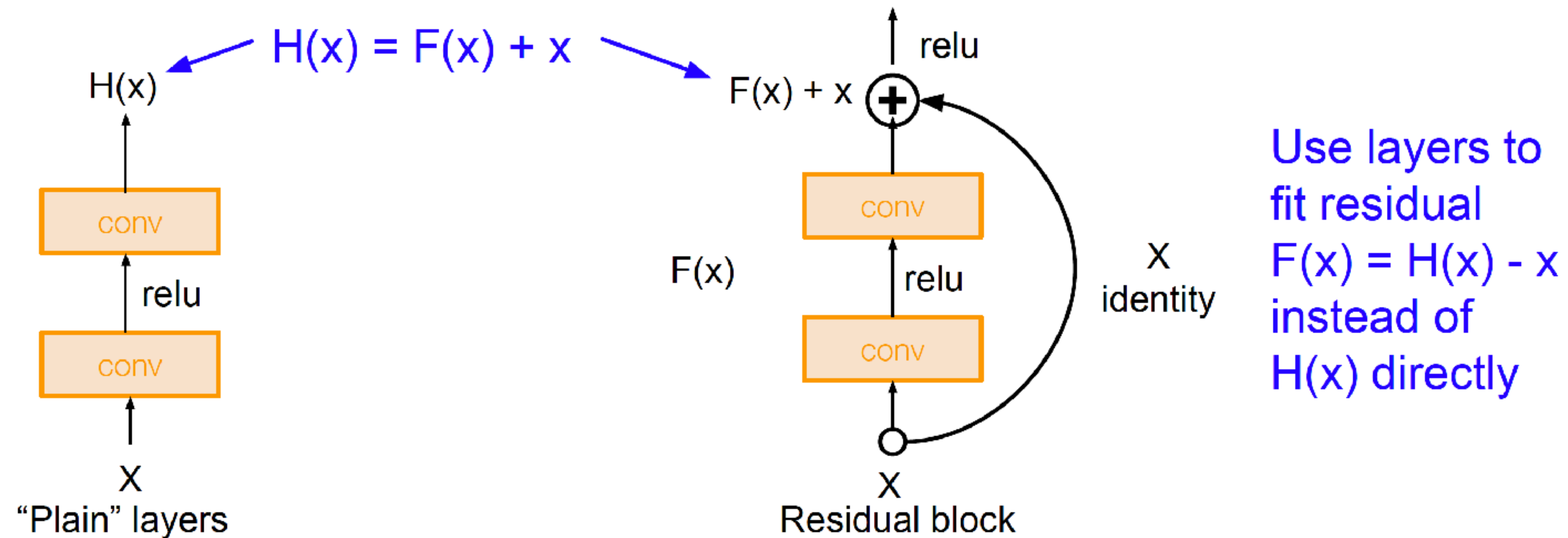
Focus
The → The big red dog
big → The big red dog
red → The big red dog
dog → The big red dog

“Masked” attention

- ◆ The initial problem we talked about
 - ➔ English: The big red dog.
 - ➔ French: Le gros chien rouge
- ◆ But, when we start we only know the first French word
 - ➔ While computing attention, during training, we only need to look at the first word
 - ➔ Mask the rest → Masked attention

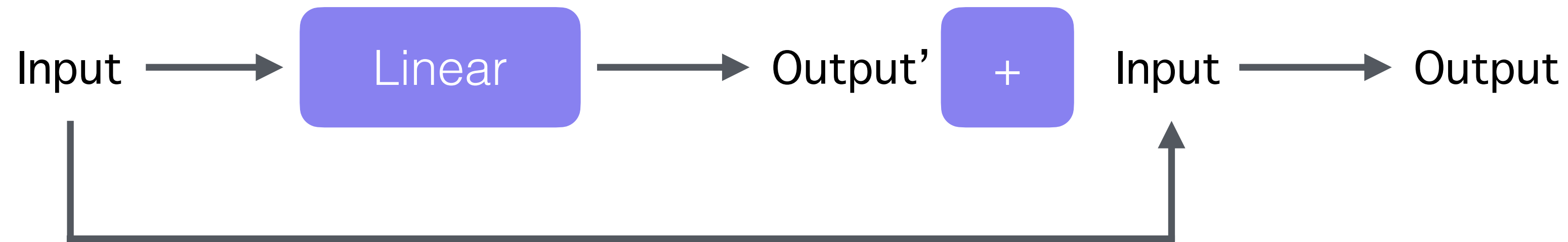


Add & Norm (RESIDUAL NETWORK)



Add & Norm

Add = skip connections



- ◆ Helps remembering where it started from
- ◆ Useful in deeper networks (in general)

Norm = normalize (layer-wise or batch-wise)

Now we understand the principle

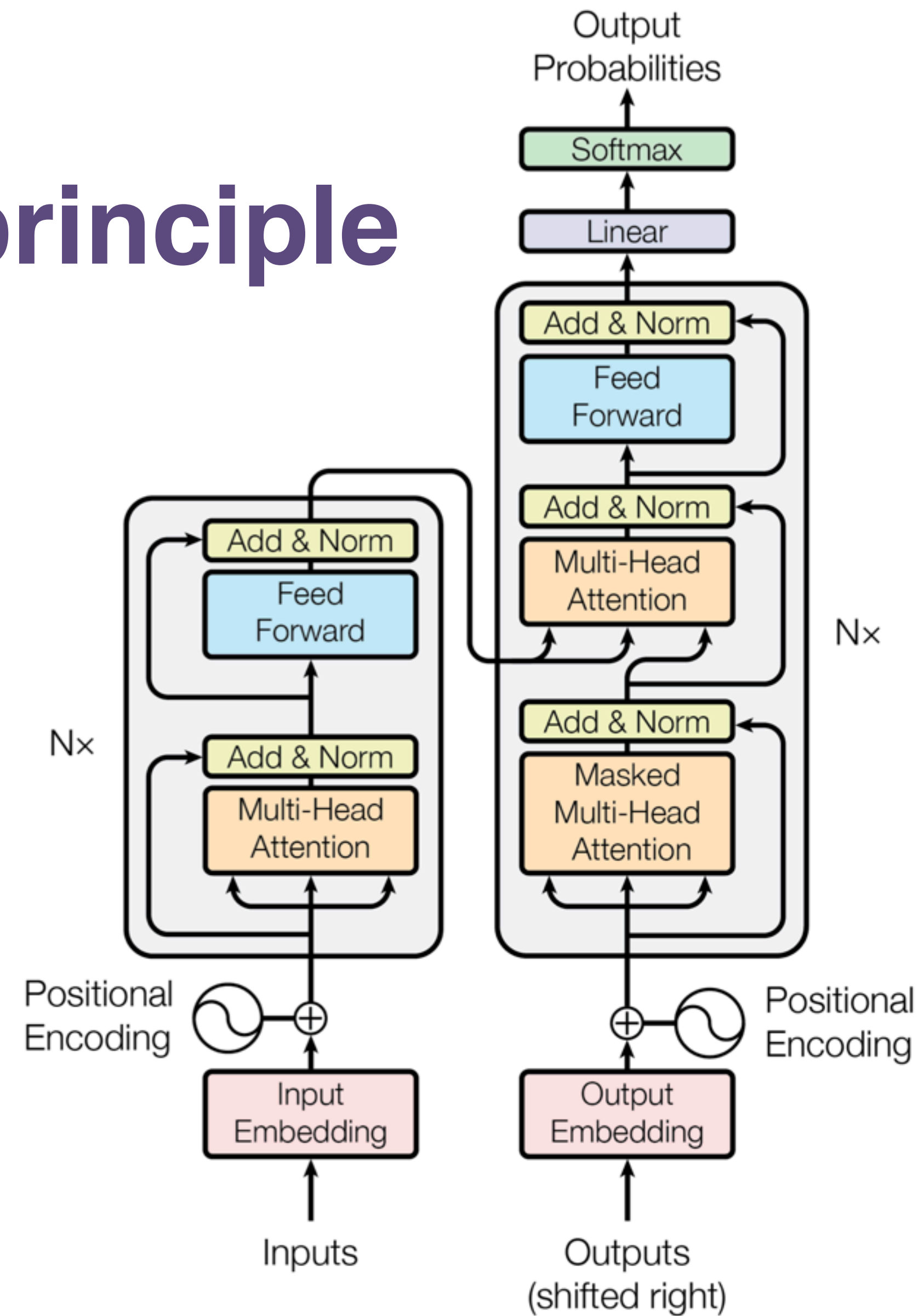


Figure 1: The Transformer - model architecture.

Attention is All You Need

Level 3 E. Gross

[Jay Alammar: The Illustrated Transformer](#)

[Mehreen Saeed: Positional Encoding](#)

<https://arxiv.org/abs/1706.03762>

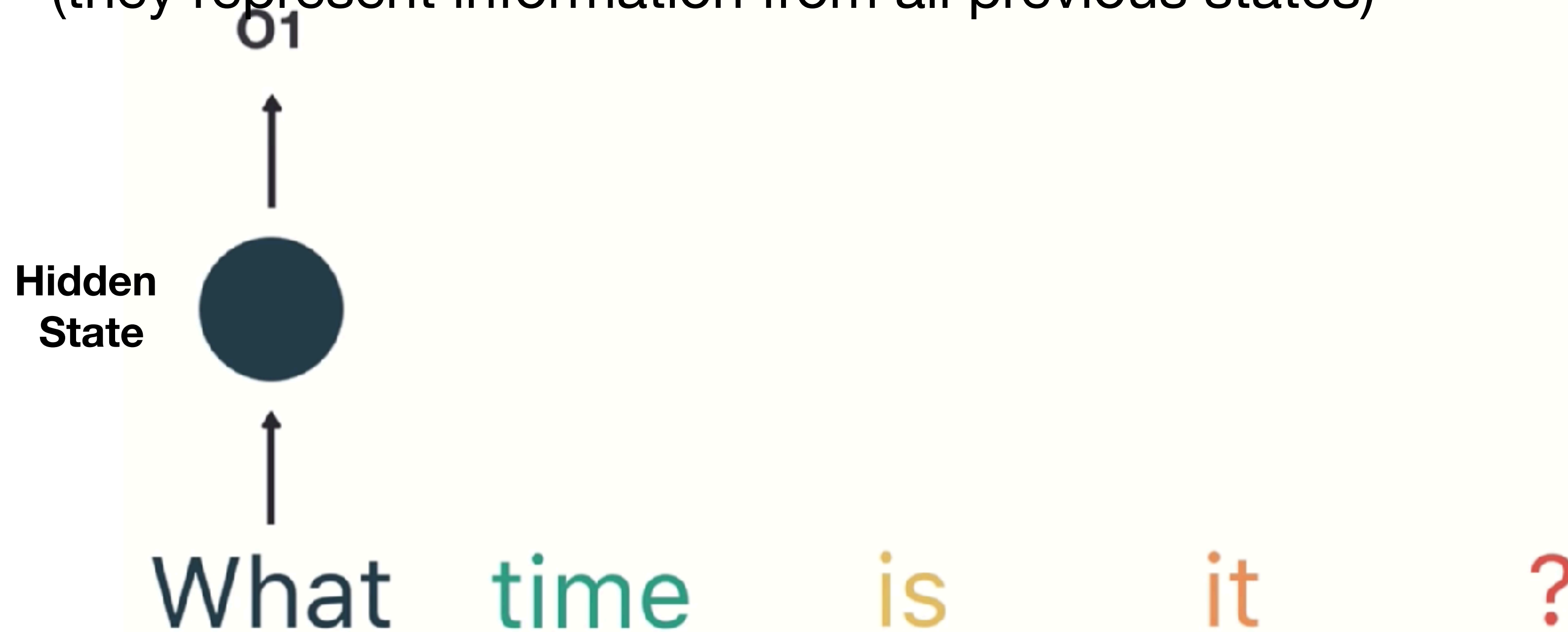
Recurrent Neural Net in a NutShell

RNN's are good at processing sequence data for predictions

<https://www.youtube.com/watch?v=LHXXI4-IEns>

Recurrent Neural Net in a NutShell

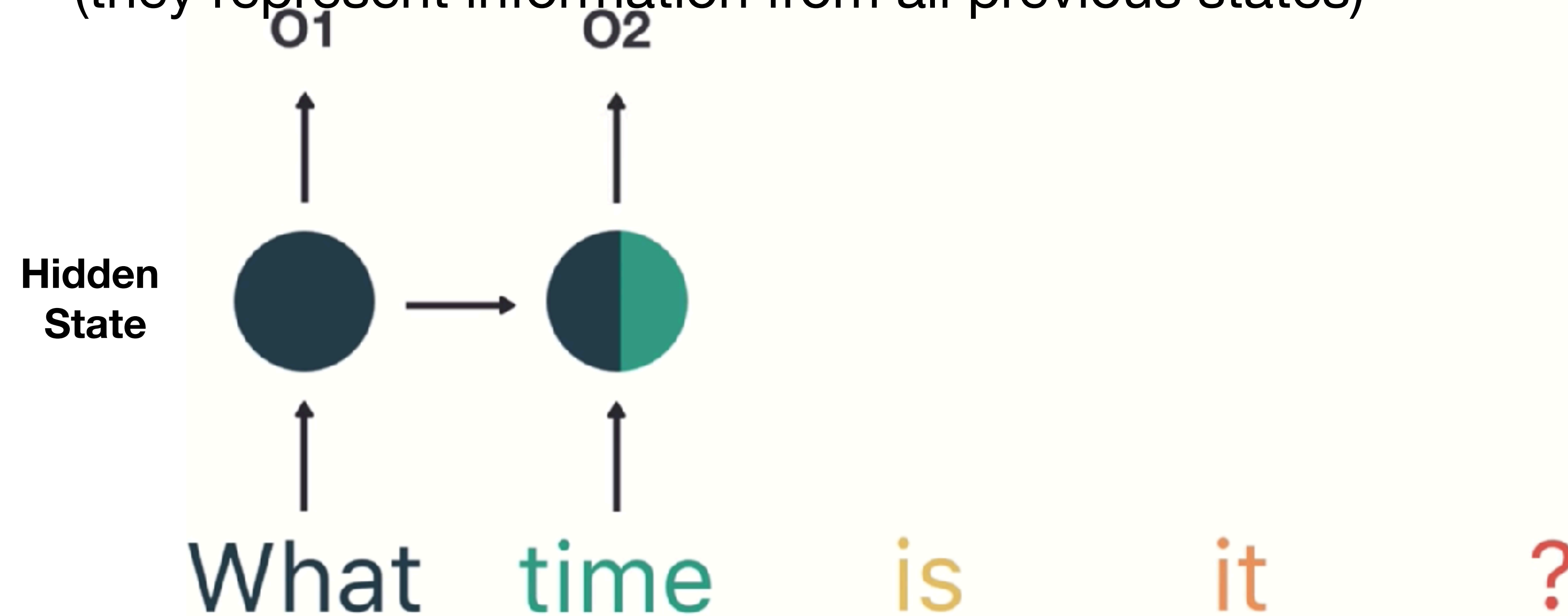
- How do we do it?
- We use hidden states as memory
(they represent information from all previous states)



<https://www.youtube.com/watch?v=LHXXI4-IEs>

Recurrent Neural Net in a NutShell

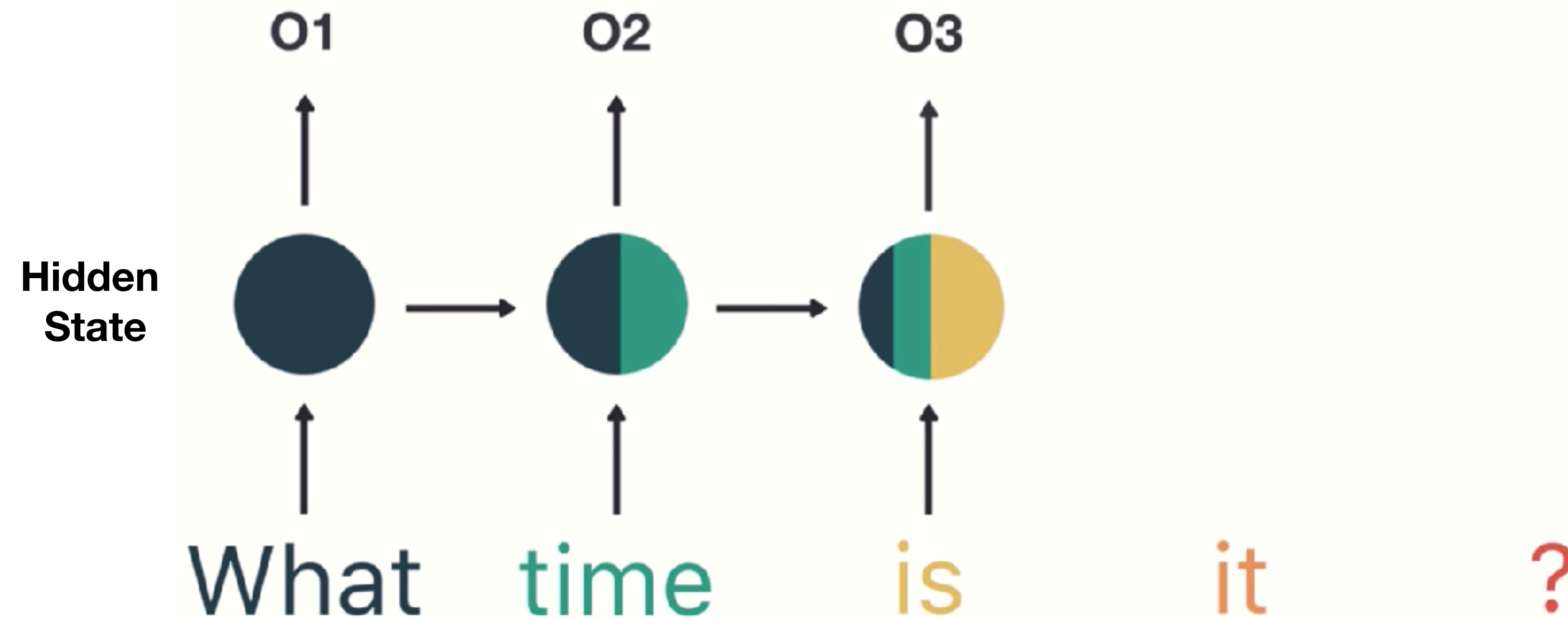
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Recurrent Neural Net in a NutShell

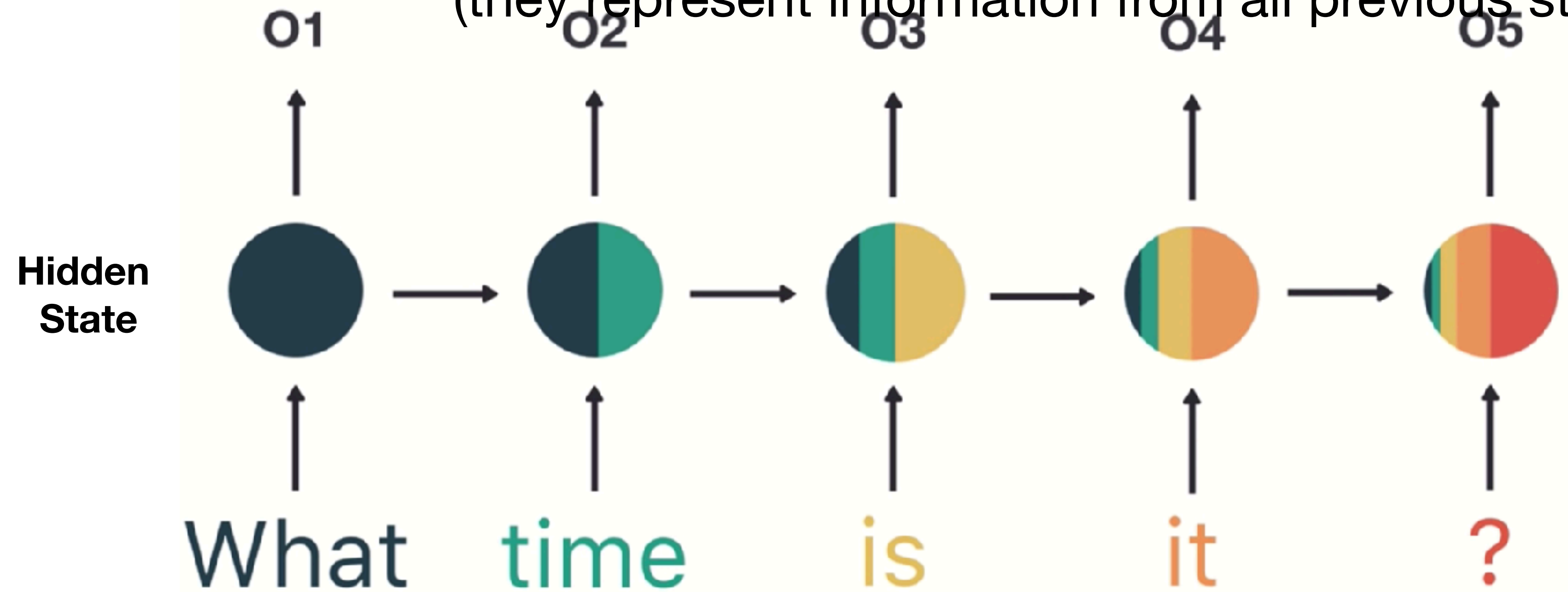
- How do we do it?
- We use hidden states as memory



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Recurrent Neural Net in a NutShell

- How do we do it?
- We use hidden states as memory (they represent information from all previous states)



<https://www.youtube.com/watch?v=LHXXI4-IEns>

Recurrent Neural Net in a NutShell

- Issue of RNN with Short Time Memory



<https://www.youtube.com/watch?v=LHXXI4-IEns>

Recurrent Neural Net in a NutShell

- Issue of RNN with Short Time Memory
- Back propagation with time \rightarrow Vanishing Gradient
We do not learn very early layers....



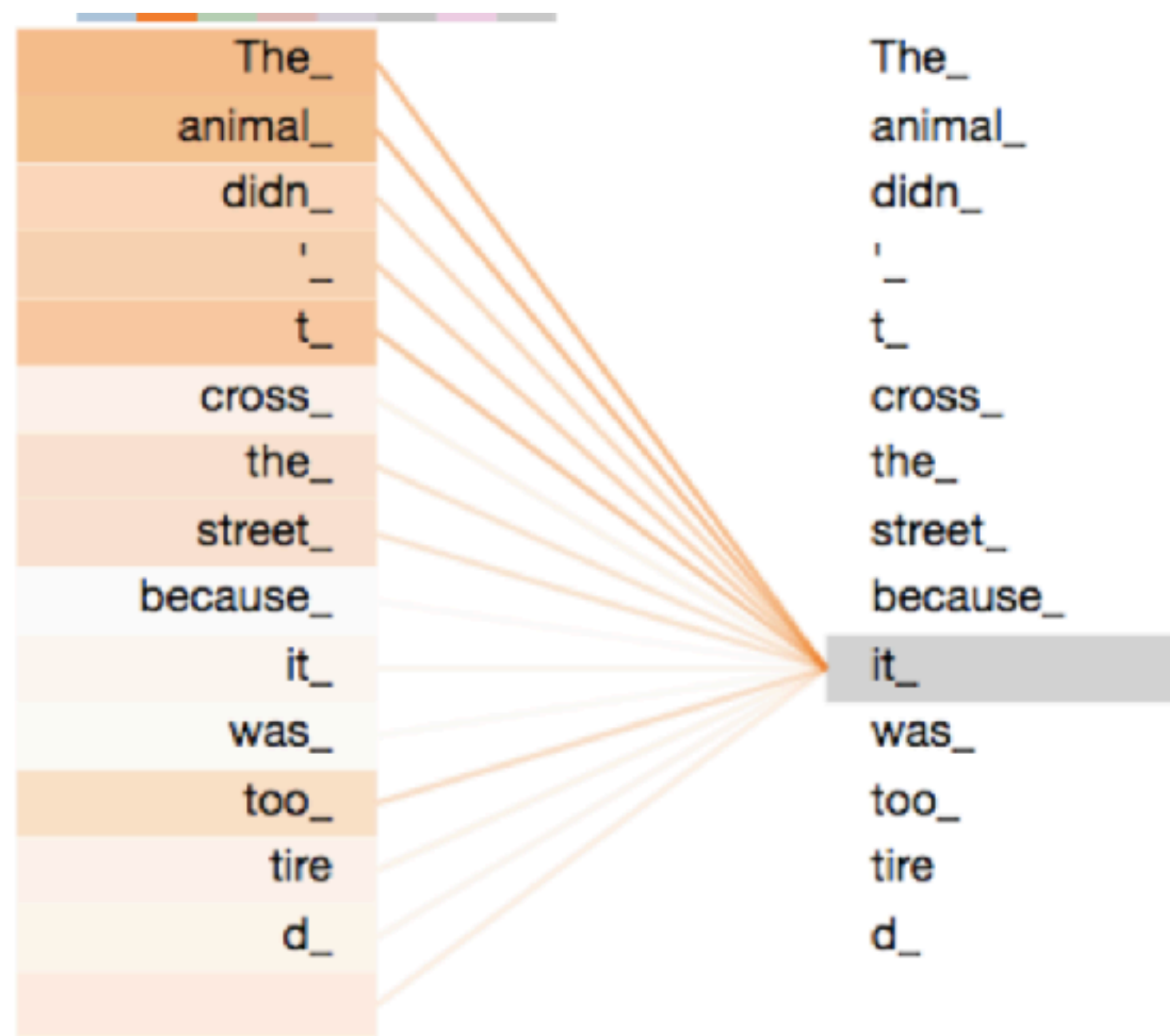
<https://www.youtube.com/watch?v=LHXXI4-IEns>

Transformer Keypoints

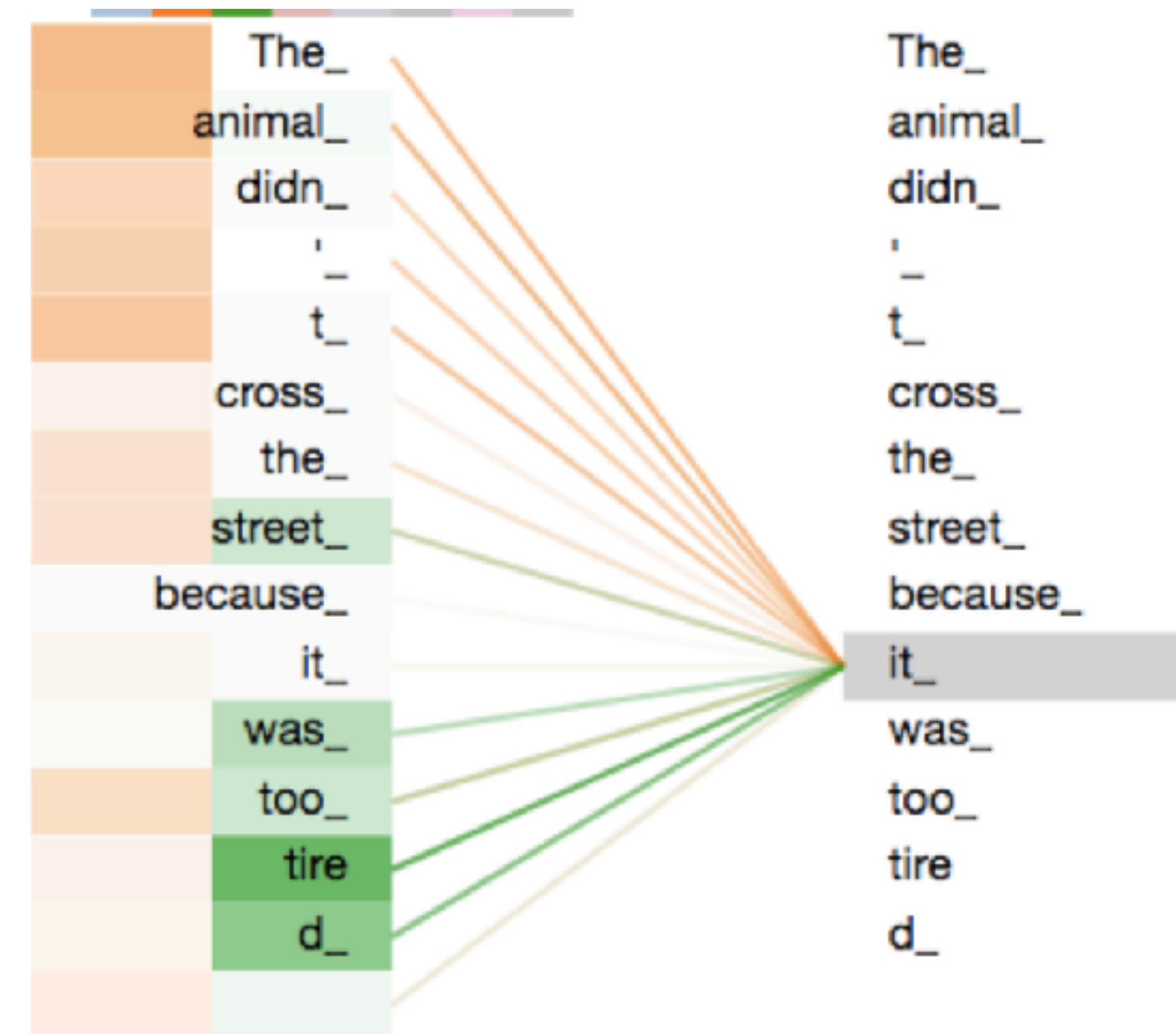
- RNN: Seq to Seq
Suffers from long term memory
Transformer not sequential like RNN
All input fed once through the model and calculation is performed once
- Introduce the concept of Self Attention
- Multi Head Attention

God commanded Abraham to sacrifice his son in order to test his faith

One Attention



two Heads



<http://jalammar.github.io/illustrated-transformer/>

paper :

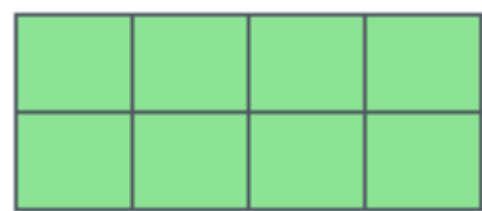
$$d_{model} = 512$$

$$d_K = d_V = \frac{d_{model}}{h}$$

$$d_K = d_V = \frac{512}{8} = 64$$

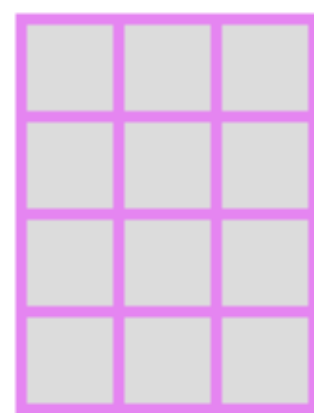
$$d_K = d_V = \frac{d_{model}}{h}$$

X



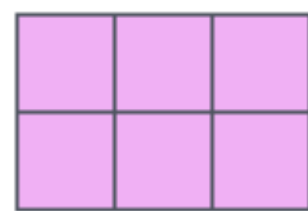
×

W^Q



=

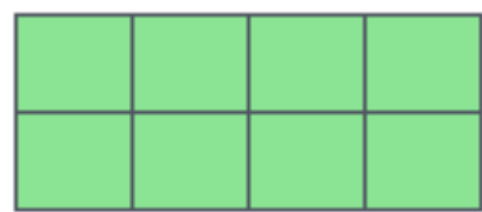
Q



$$X \in R^{N \times d_{model}}$$

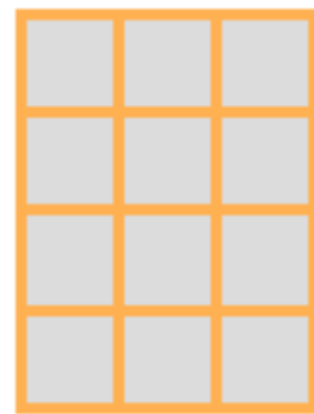
$$W^K, W^Q \in R^{d_{model} \times d_k} \quad Q, K \in R^{N \times d_k}$$

X



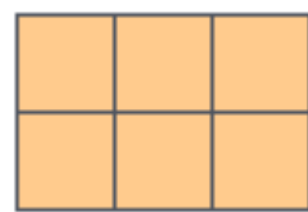
×

W^K



=

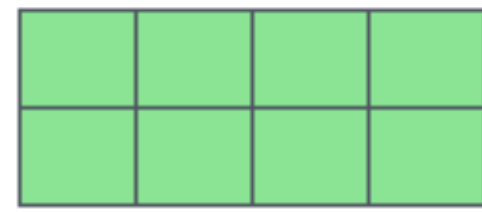
K



$$X \in R^{N \times d_{model}}$$

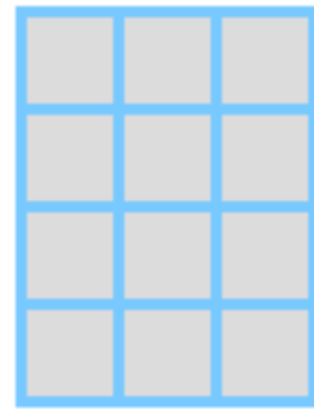
$$W^V \in R^{d_{model} \times d_v} \quad V \in R^{N \times d_v}$$

X



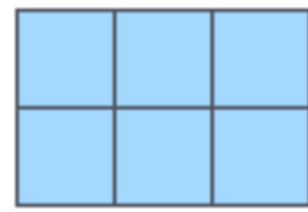
×

W^V



=

V



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

$$Z_i = \sum_{\ell} \text{softmax}\left(\frac{1}{\sqrt{d_k}} Q_i \cdot K_{\ell}^T\right) V_{\ell}$$

$$X \in R^{N \times d_{\text{model}}}$$

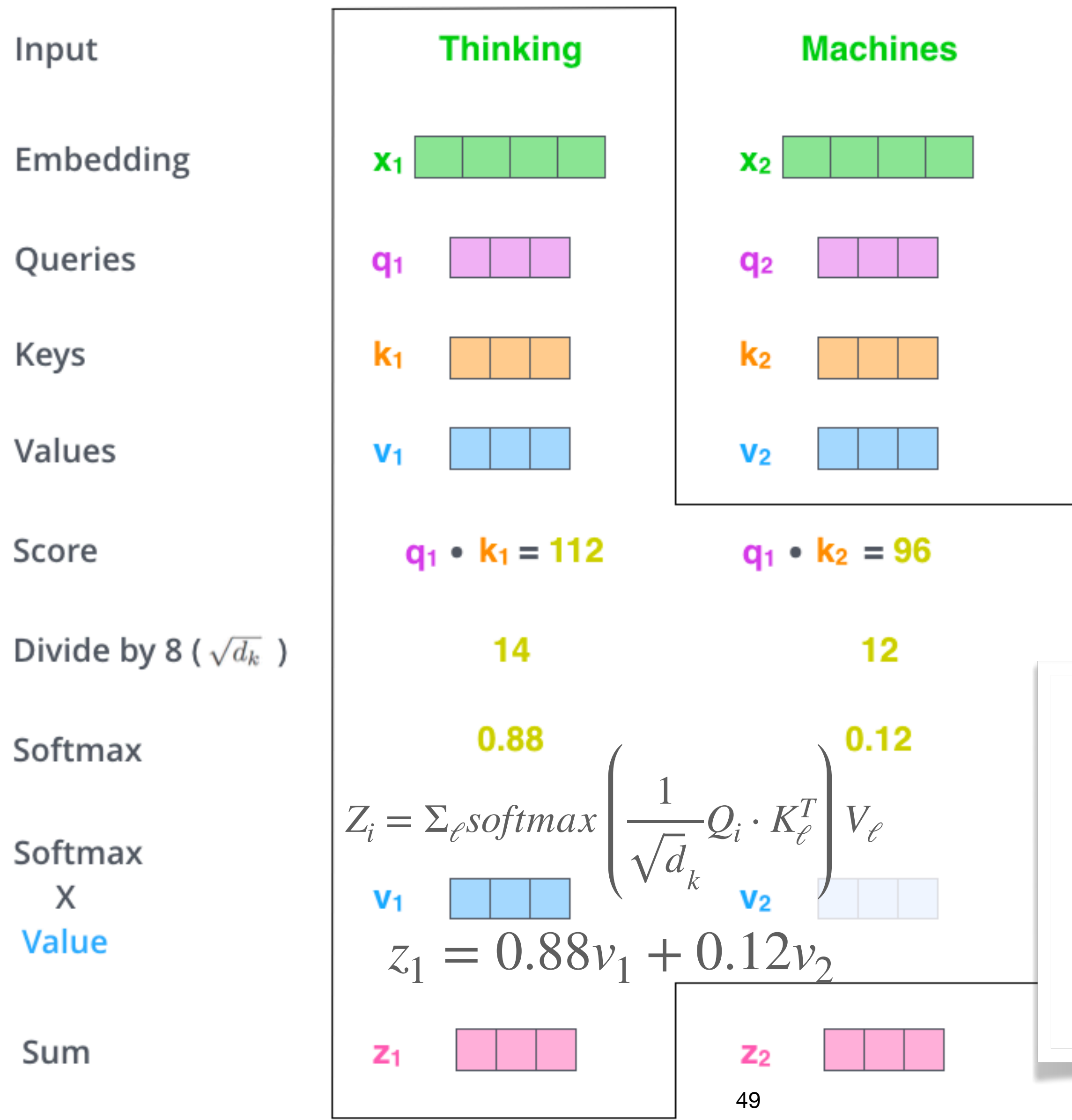
$$Q, K \in R^{N \times d_k}$$

$$Q \times K^T \in R^{N \times N}$$

$$V \in R^{N \times d_v}$$

$$\text{softmax}\left(\frac{\begin{matrix} \text{Q} & & \text{K}^T \\ \begin{matrix} \text{2x3 grid} & \times & \begin{matrix} \text{3x2 grid} \end{matrix} \end{matrix}}{\sqrt{d_k}}\right) \begin{matrix} \text{V} \\ \begin{matrix} \text{2x3 grid} \end{matrix} \end{matrix}$$

$$= \begin{matrix} \text{Z} \\ \begin{matrix} \text{2x3 grid} \end{matrix} \end{matrix} \quad Z \in R^{N \times d_v}$$



$$z_i = \sum_{\ell} \text{softmax} \left(\frac{1}{\sqrt{d_k}} Q_i \cdot K_{\ell}^T \right) v_{\ell}$$

$$\text{softmax} \left(\frac{Q \times K^T}{\sqrt{d_k}} \right) \cdot V = Z$$

$$head_i = Attention(Q_i, K_i, V_i)$$

$X \in R^{N \times d_{model}}$ Thinking Machines 

$$d_K = d_V = \frac{d_{model}}{h}$$

Calculating attention separately in eight different attention heads

ATTENTION HEAD #0

ATTENTION HEAD #1

...

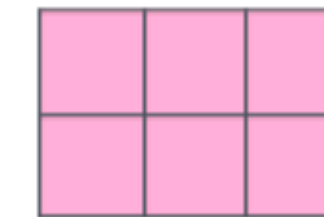
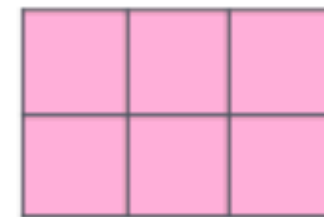
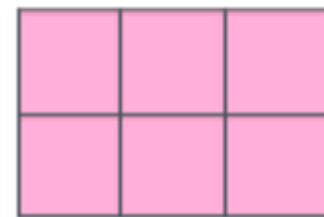
ATTENTION HEAD #7

Z_0

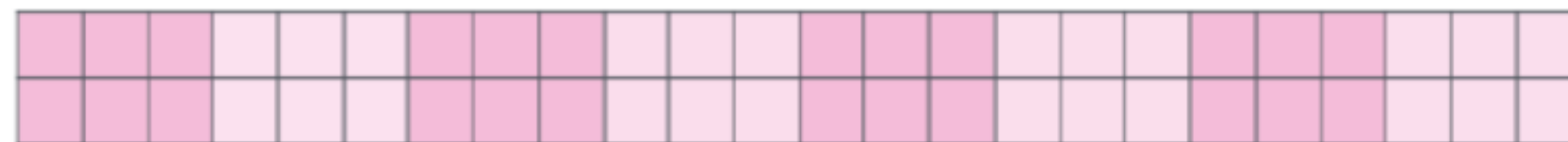
Z_1

Z_7

$Z \in R^{N \times d_V}$



Z_0 Z_1 Z_2 Z_3 Z_4 Z_5 Z_6 Z_7

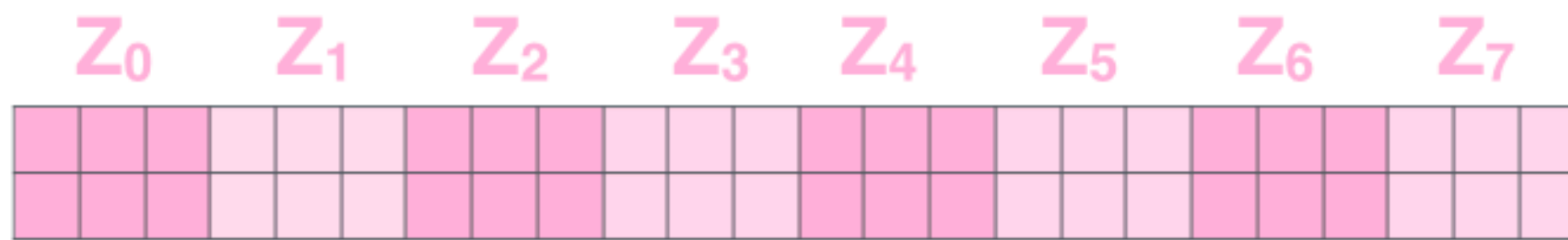


$$\in R^{N \times (hd_V)} = R^{N \times d_{model}}$$

Concat(head₁, ..., head_h)

$$\text{MultiHead}(Q, K, V) = \text{Concat}(\text{head}_1, \dots, \text{head}_h)W^O$$

1) Concatenate all the attention heads



$$\in \mathbb{R}^{N \times hd_V}$$

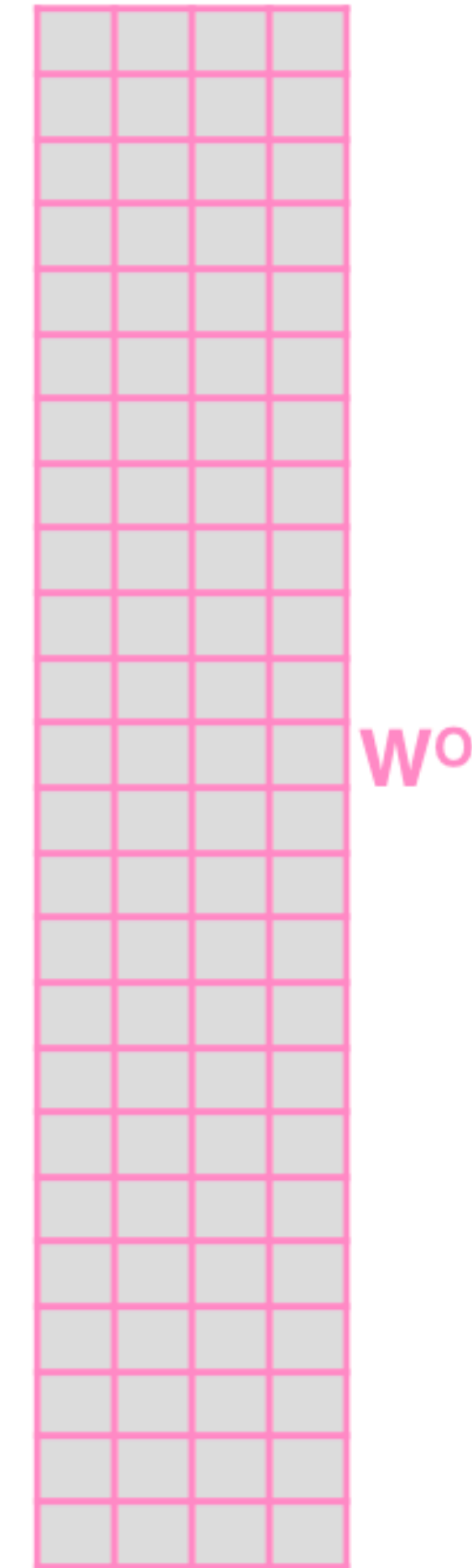
2) Multiply with a weight matrix W^O that was trained jointly with the model

x

$$W^O \in \mathbb{R}^{hd_V \times d_{model}}$$

3) The result would be the Z matrix that captures information from all the attention heads. We can send this forward to the FFNN

=  $Z \in \mathbb{R}^{N \times d_{model}}$



1) This is our input sentence*

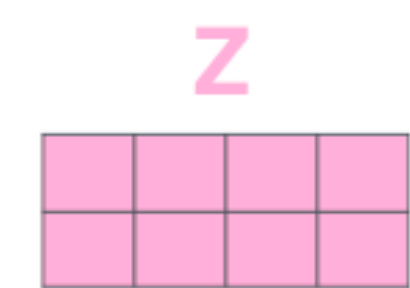
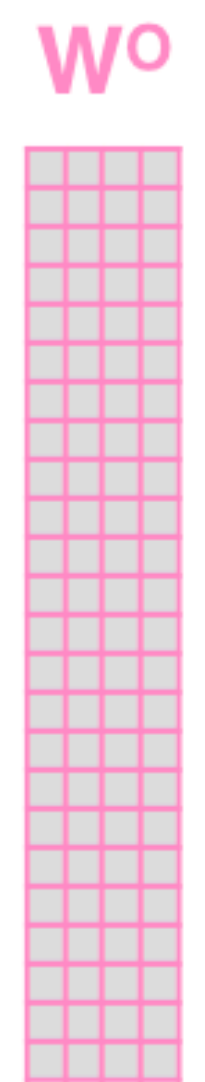
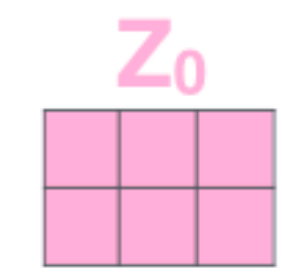
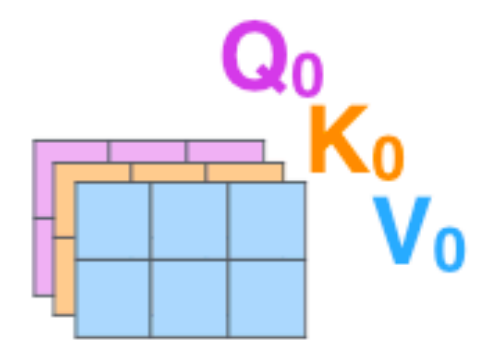
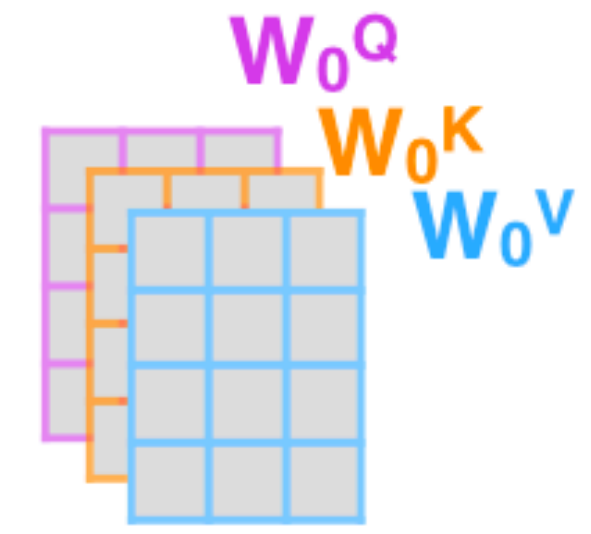
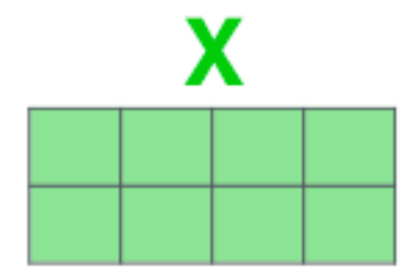
2) We embed each word*

3) Split into 8 heads. We multiply X or R with weight matrices

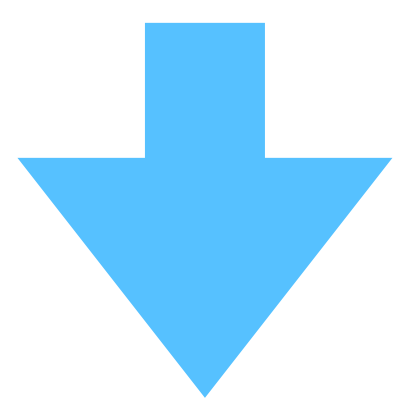
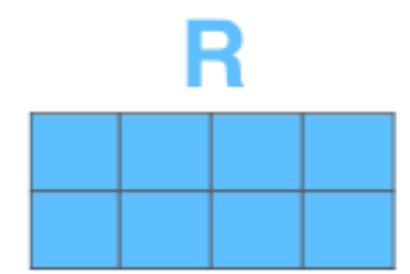
4) Calculate attention using the resulting $Q/K/V$ matrices

5) Concatenate the resulting Z matrices, then multiply with weight matrix W^O to produce the output of the layer

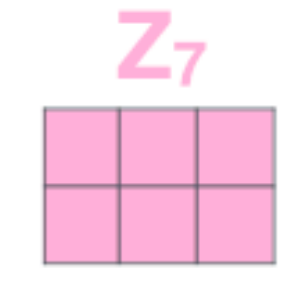
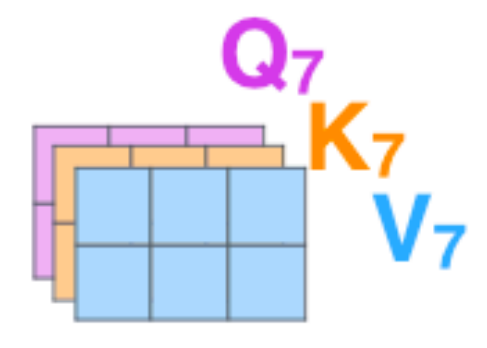
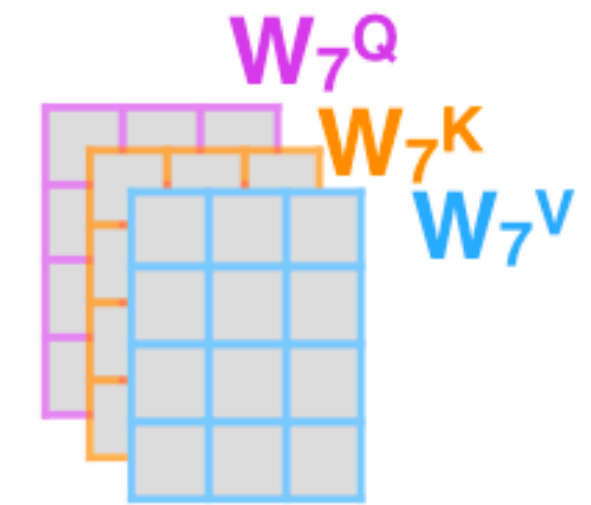
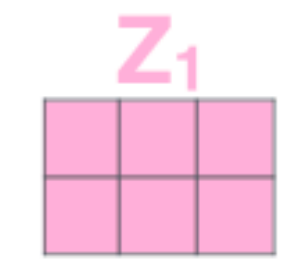
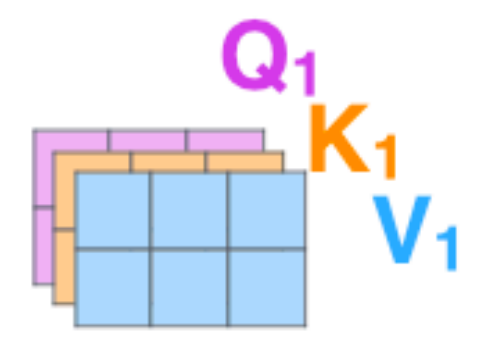
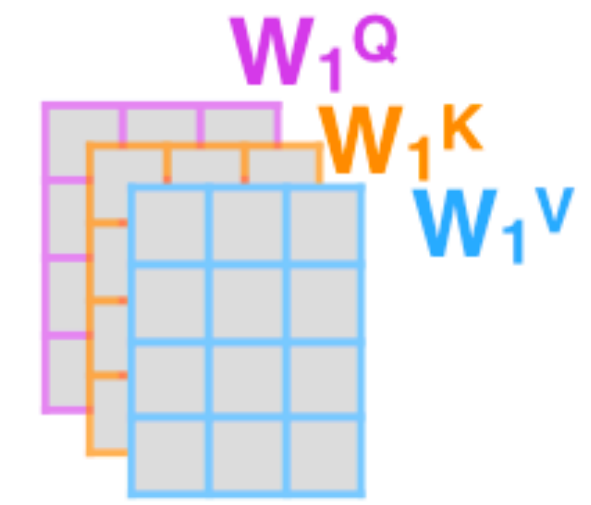
Thinking Machines

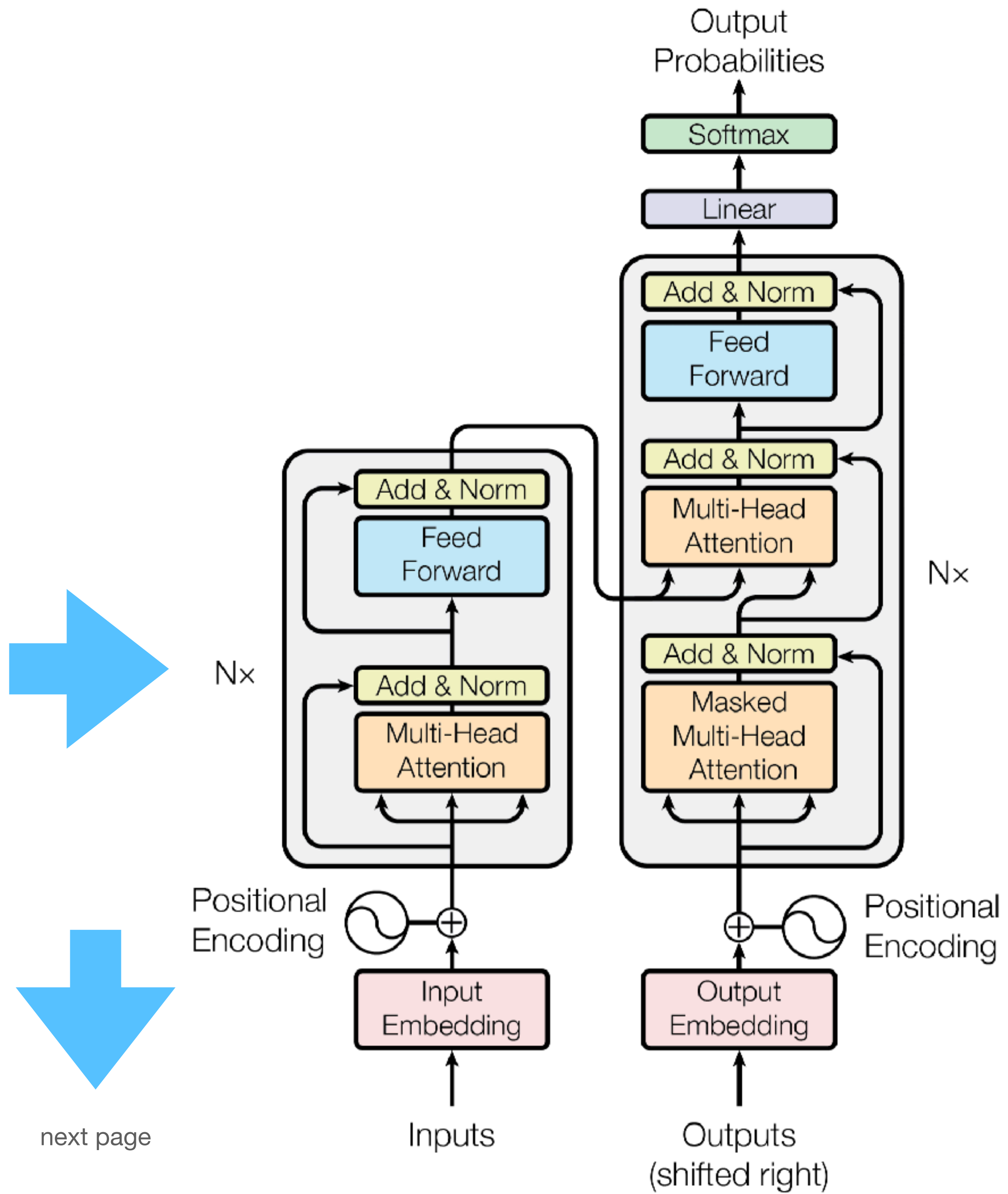


* In all encoders other than #0, we don't need embedding. We start directly with the output of the encoder right below this one



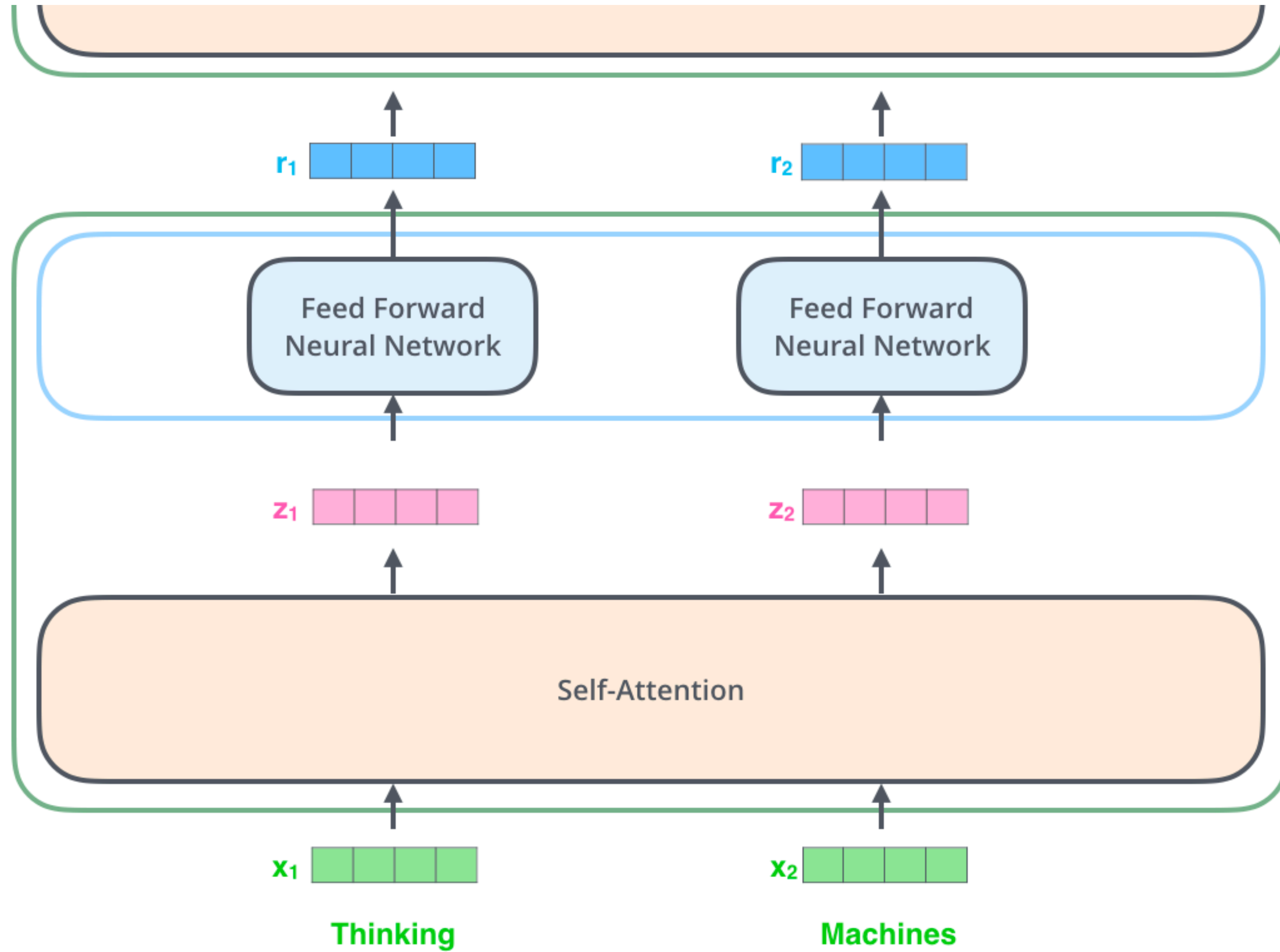
next page





ENCODER #2

ENCODER #1

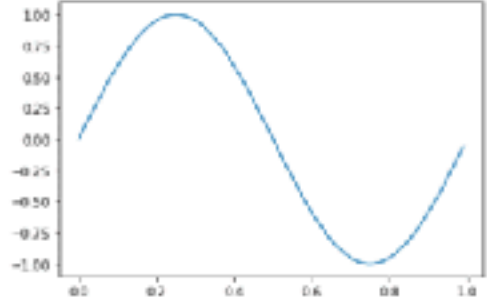
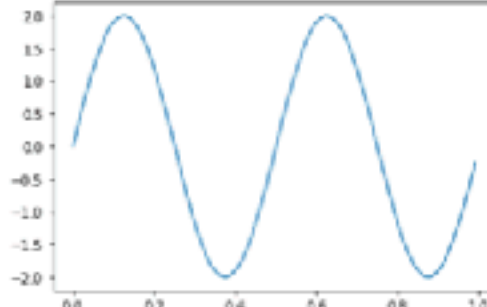
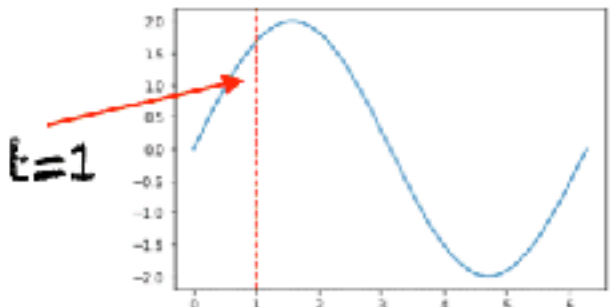


Position ENCODING

Sequence Length = L Varies
 $2i=0, \dots, L$

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

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

Equation	Graph	Frequency	Wavelength
$\sin(2\pi t)$		1	1
$\sin(2 * 2\pi t)$		2	1/2
$\sin(t)$		$1/2\pi$	2π
$\sin(ct)$	Depends on c	$c/2\pi$	$2\pi/c$

Position ENCODING

Sequence Length = L Varies
 $2i=0, \dots, d_model$

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

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

Positional Encoding
Matrix with $d=4, n=100$

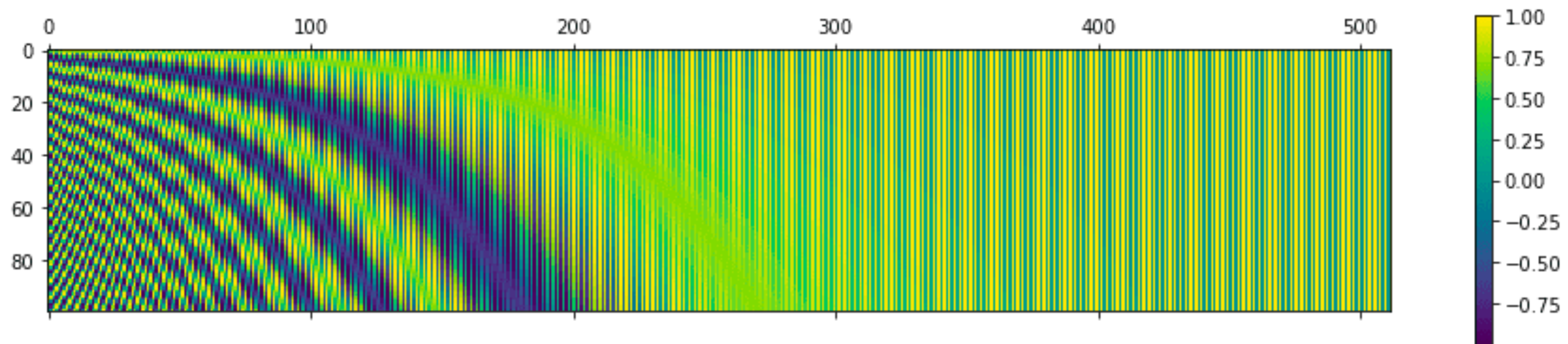
Sequence	Index of token, k	$i=0$	$i=0$	$i=1$	$i=1$
I	0	$P_{00} = \sin(0) = 0$	$P_{01} = \cos(0) = 1$	$P_{02} = \sin(0) = 0$	$P_{03} = \cos(0) = 1$
am	1	$P_{10} = \sin(1/1) = 0.84$	$P_{11} = \cos(1/1) = 0.54$	$P_{12} = \sin(1/10) = 0.10$	$P_{13} = \cos(1/10) = 1.0$
a	2	$P_{20} = \sin(2/1) = 0.91$	$P_{21} = \cos(2/1) = -0.42$	$P_{22} = \sin(2/10) = 0.20$	$P_{23} = \cos(2/10) = 0.98$
Robot	3	$P_{30} = \sin(3/1) = 0.14$	$P_{31} = \cos(3/1) = -0.99$	$P_{32} = \sin(3/10) = 0.30$	$P_{33} = \cos(3/10) = 0.96$

Positional Encoding Matrix for the sequence 'I am a robot'

Position ENCODING

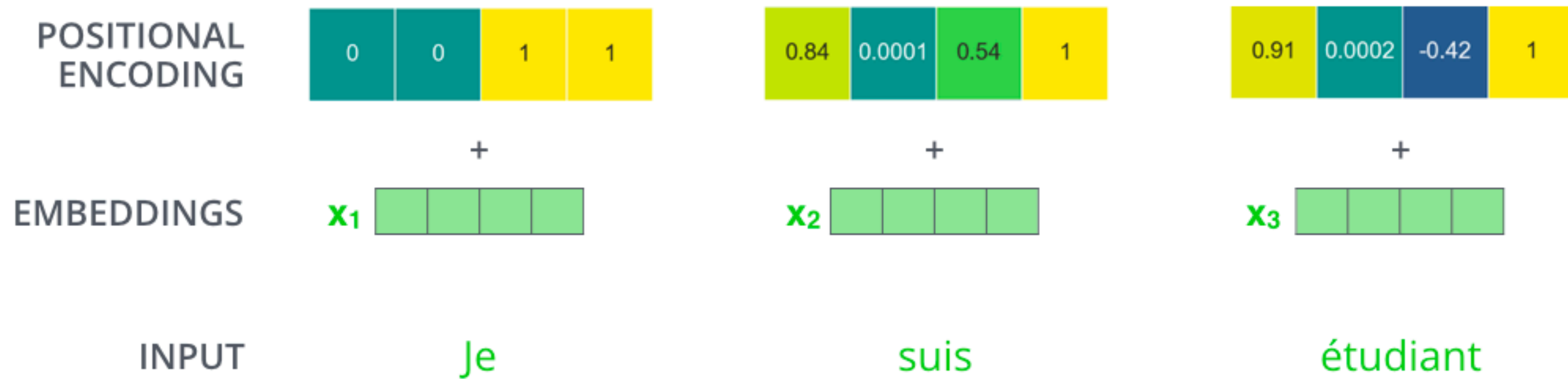
Sequence Length = L Varies
 $2i=0, \dots, d_{\text{model}}$

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

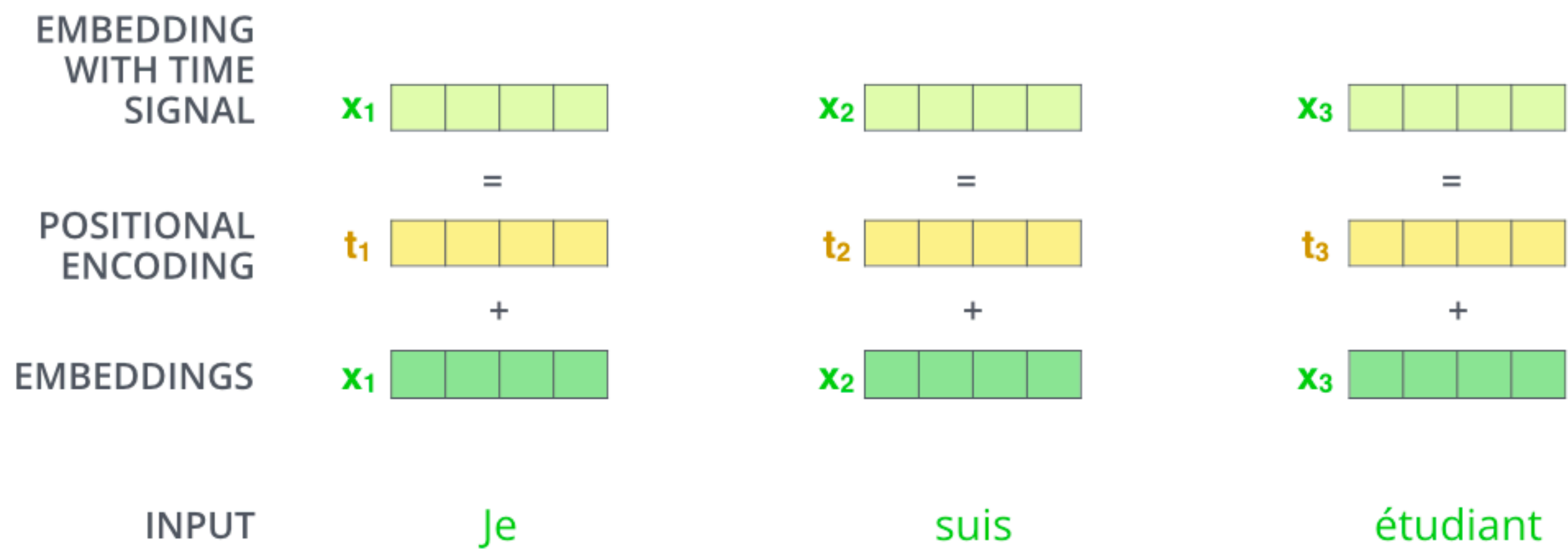
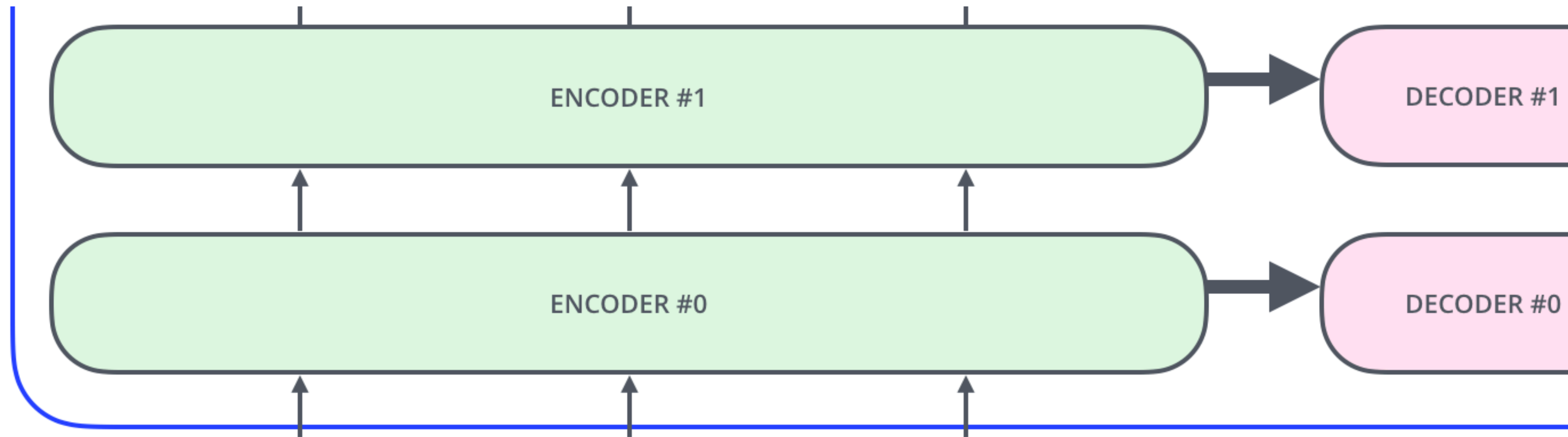


The positional encoding matrix for $n=10,000$, $d=512$, sequence length=100

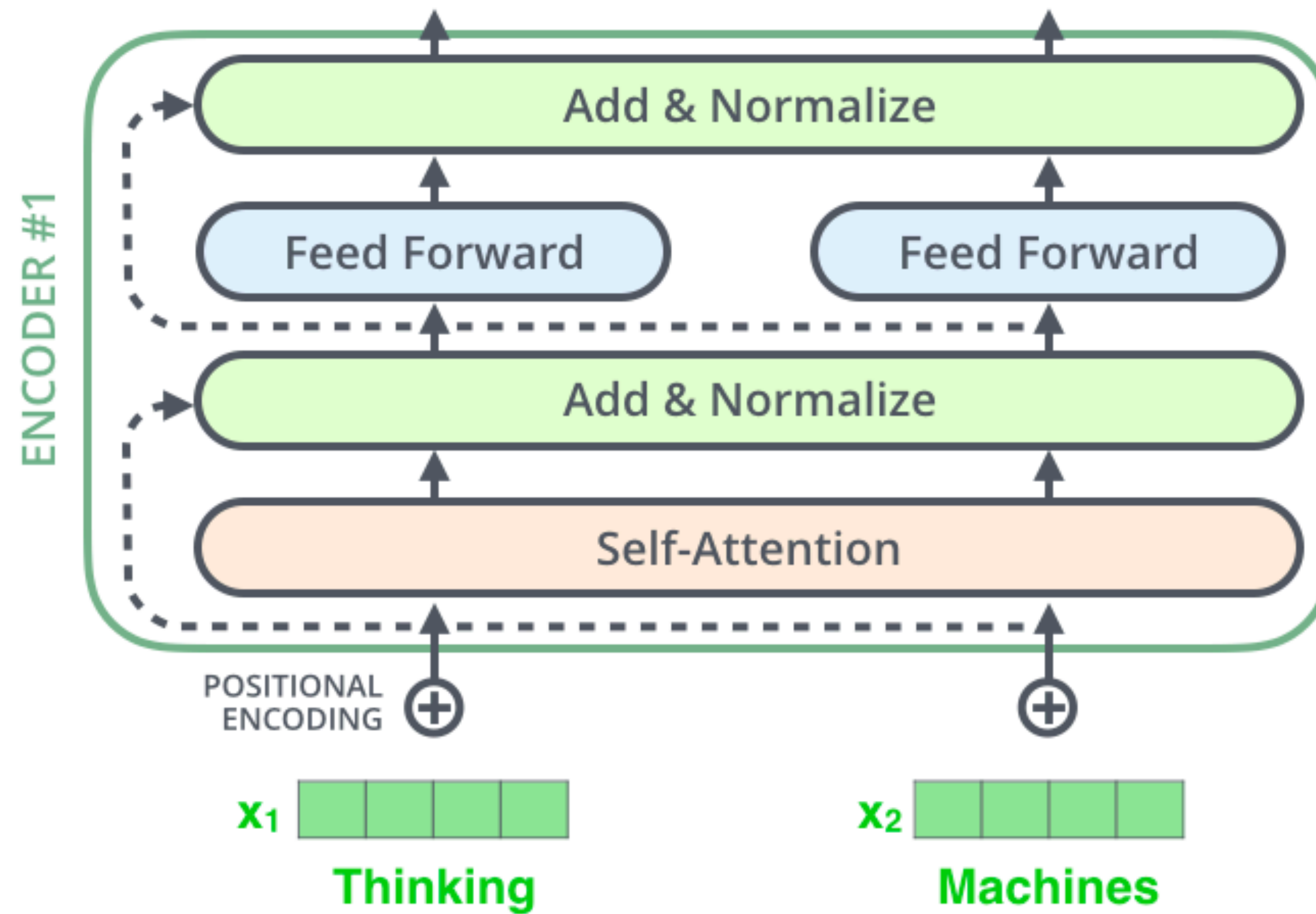
Position ENCODING



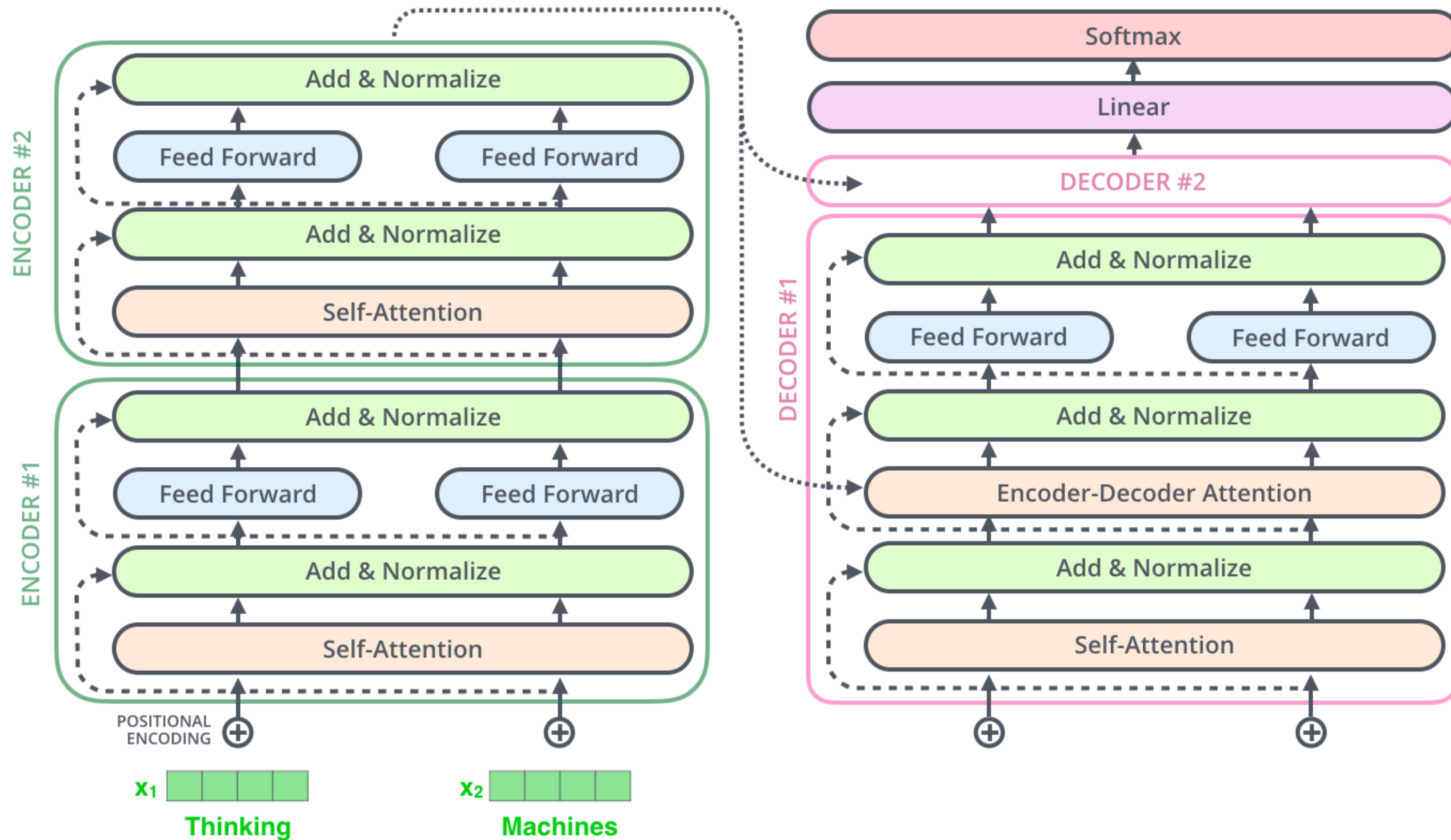
Position ENCODING



Residual Net



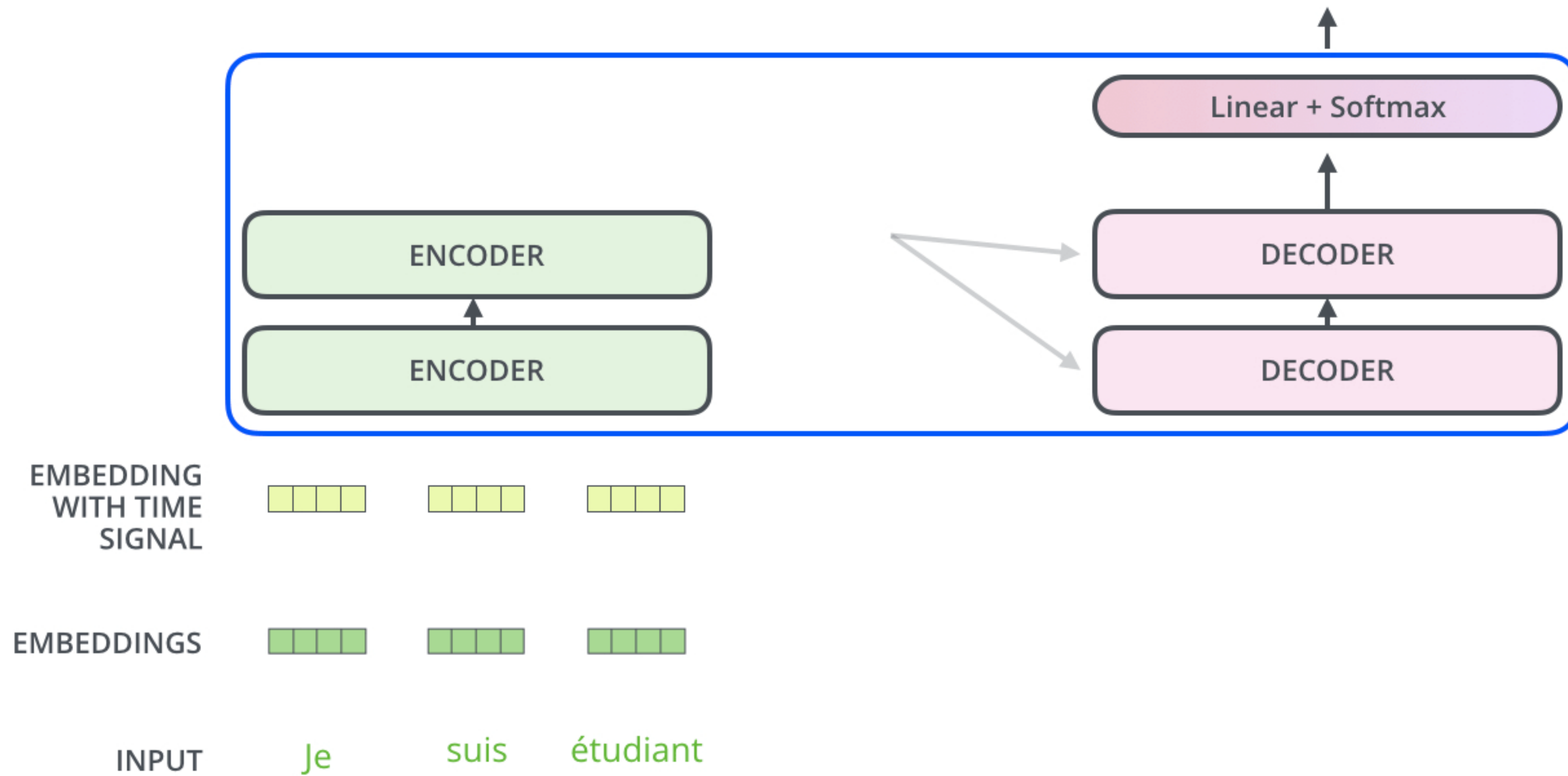
Stack 6 Encoders & Decoders



Cross Attention

Decoding time step: 1 2 3 4 5 6

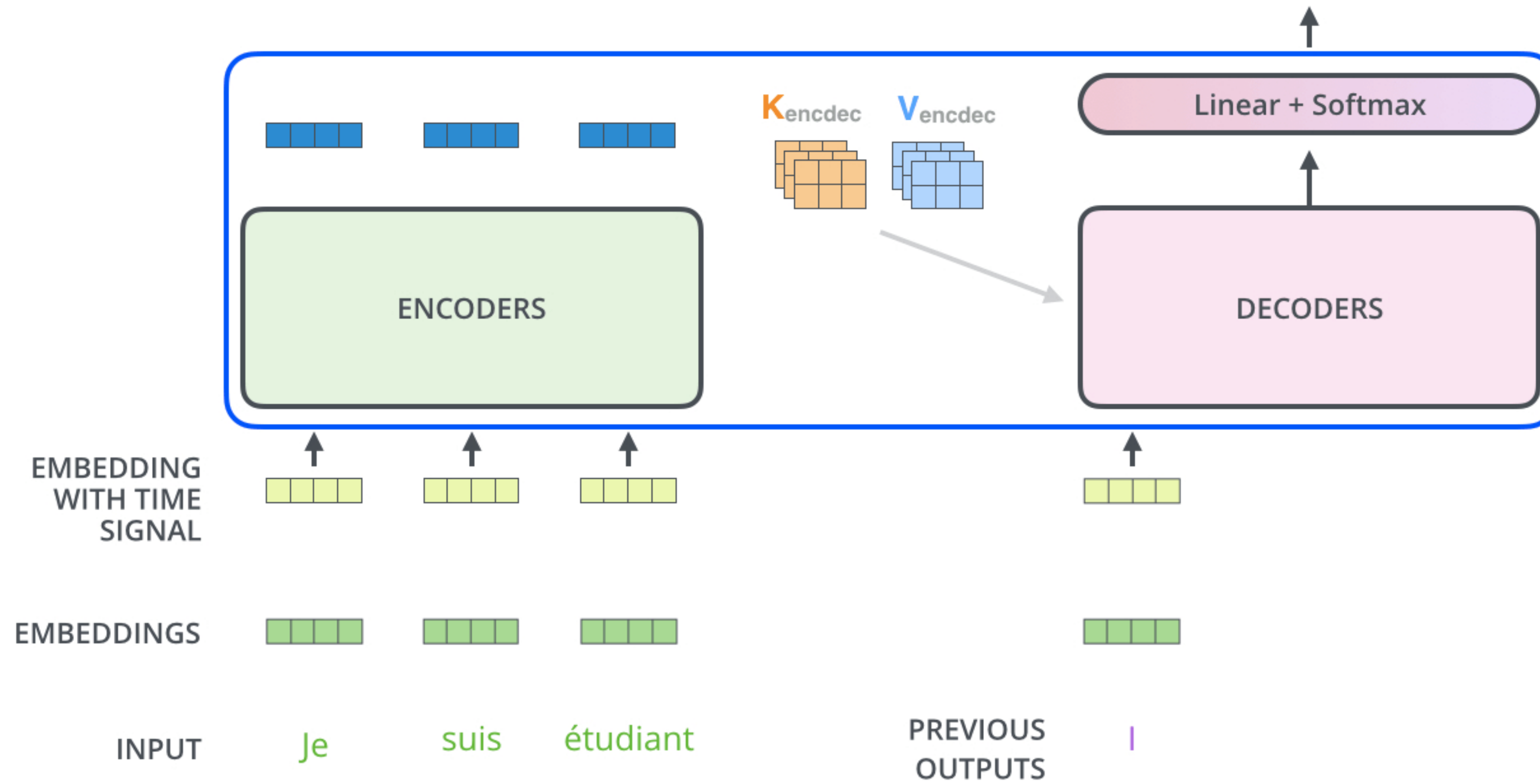
OUTPUT



Decoder

Decoding time step: 1 2 3 4 5 6

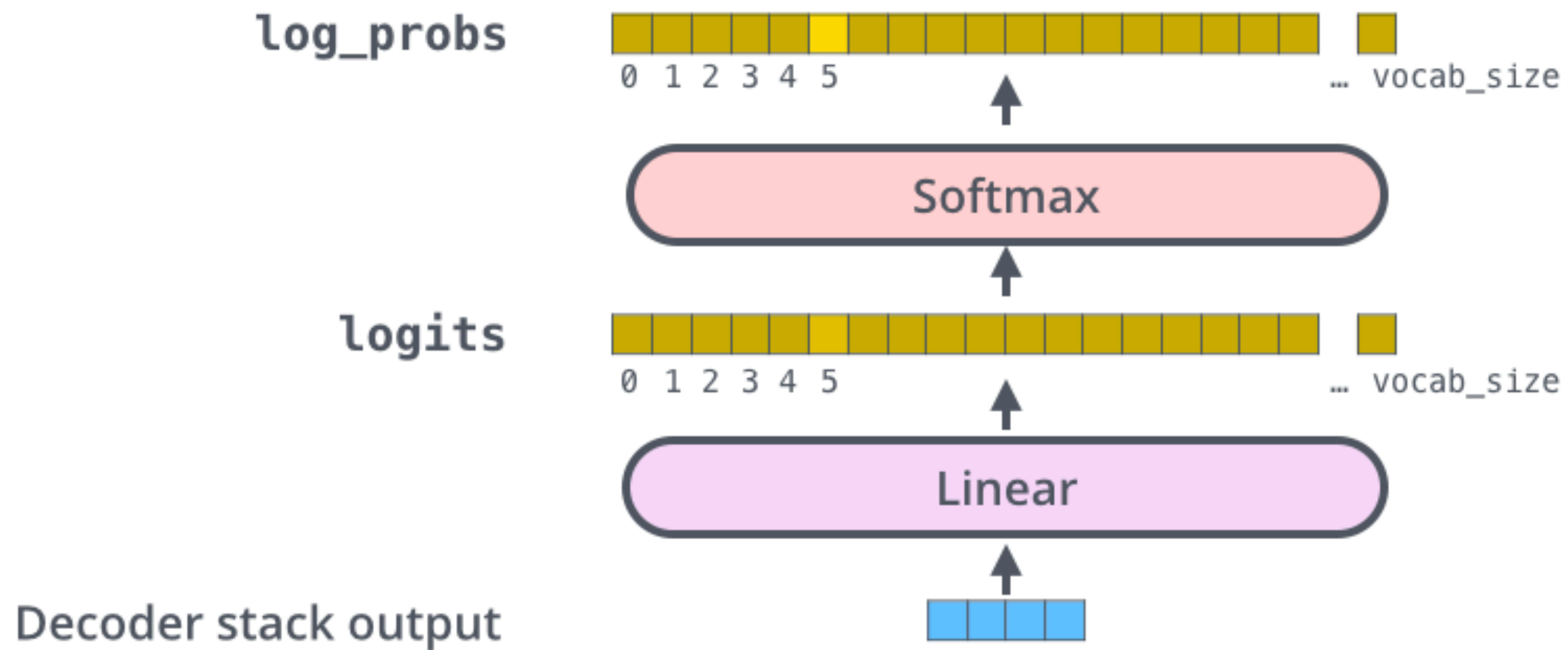
OUTPUT |



Softmax

Which word in our vocabulary
is associated with this index?

Get the index of the cell
with the highest value
(**argmax**)



End of Lecture 2

✓ Seriously? Where is the Physics?

Fast Simulation for Particle Reconstruction with GNN and Slot Attention

Conditional Generative Modelling of Reconstructed Particles at Collider Experiments

**Francesco Armando Di Bello¹, Etienne Dreyer², Sanmay Ganguly³,
Eilam Gross², Lukas Heinrich⁴, Marumi Kado^{4,5}, Nilotpal Kakati²,
Jonathan Shlomi², Nathalie Soybelman²**

¹ University of Genova

² Weizmann Institute of Science

³ ICEPP, University of Tokyo

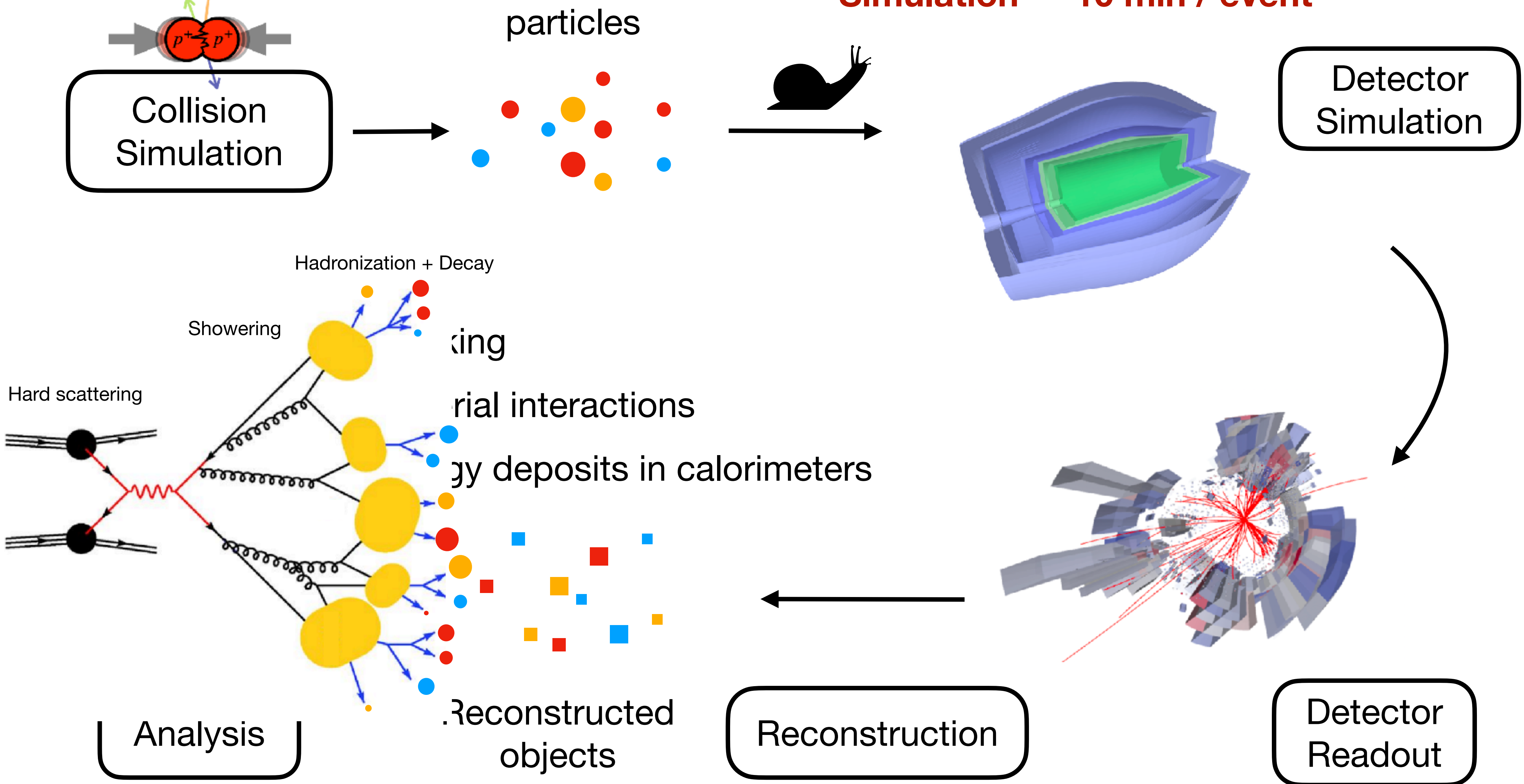
⁴ Technical University of Munich

⁵ Sapienza University of Rome

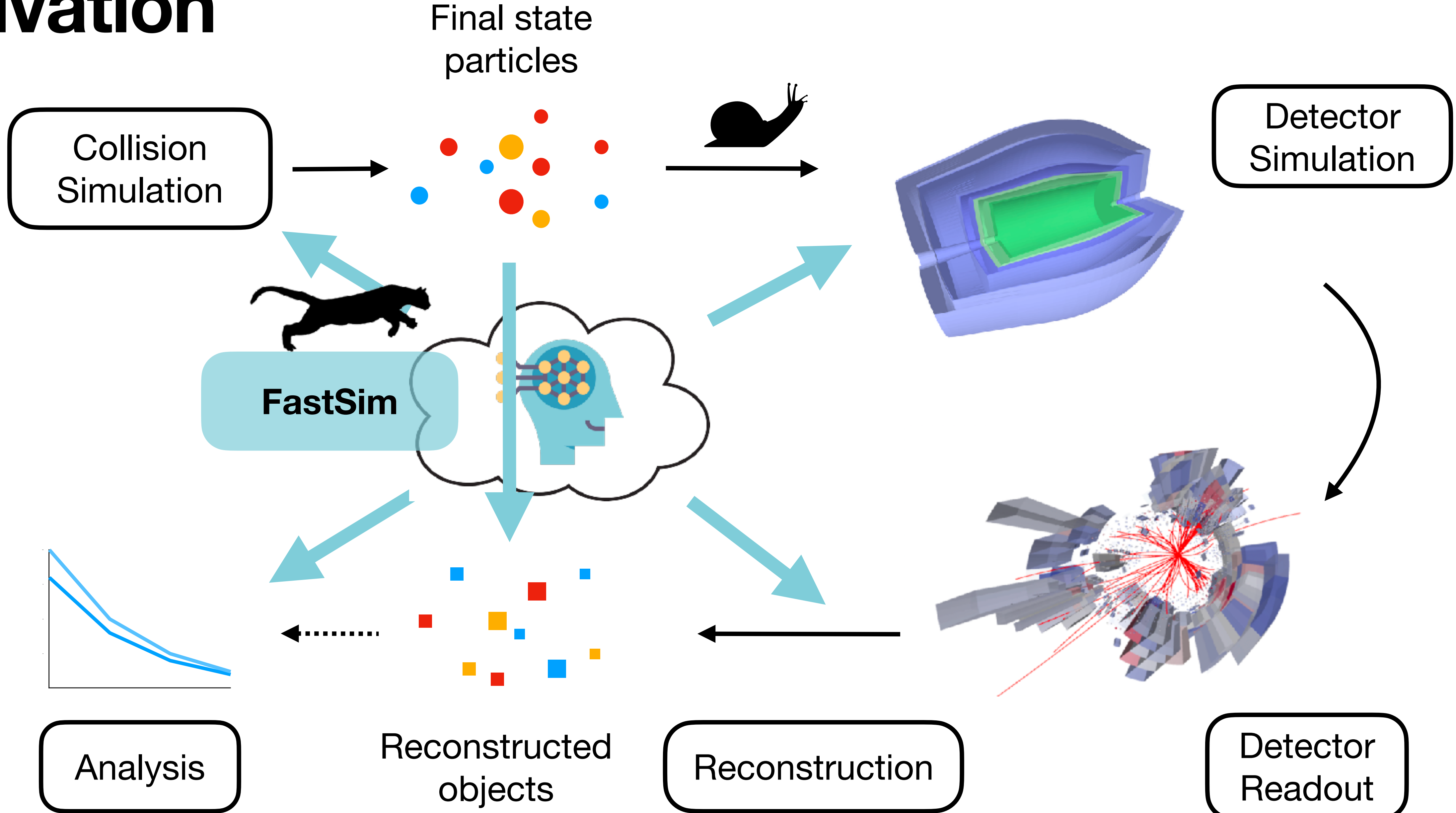
Motivation

Data taking – 1000 events / sec

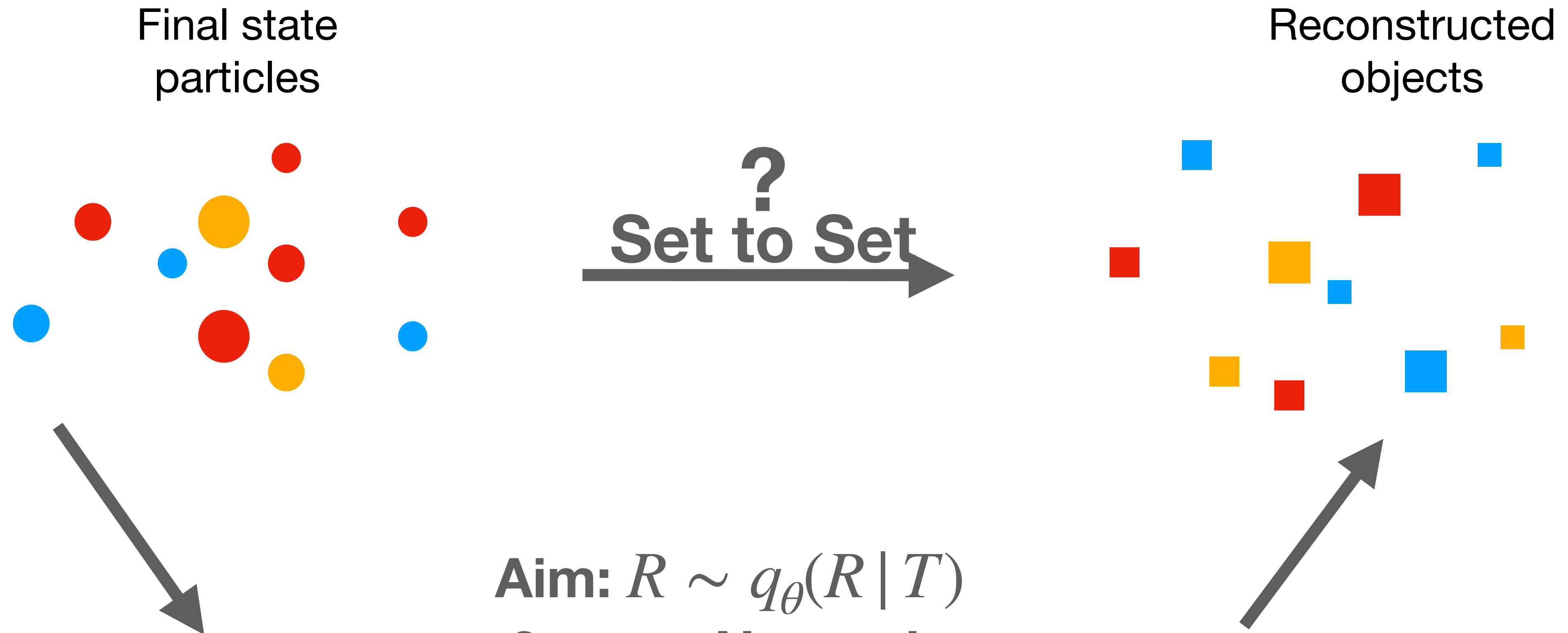
Simulation – 10 min / event



Motivation



Problem to solve



Aim: $R \sim q_{\theta}(R | T)$

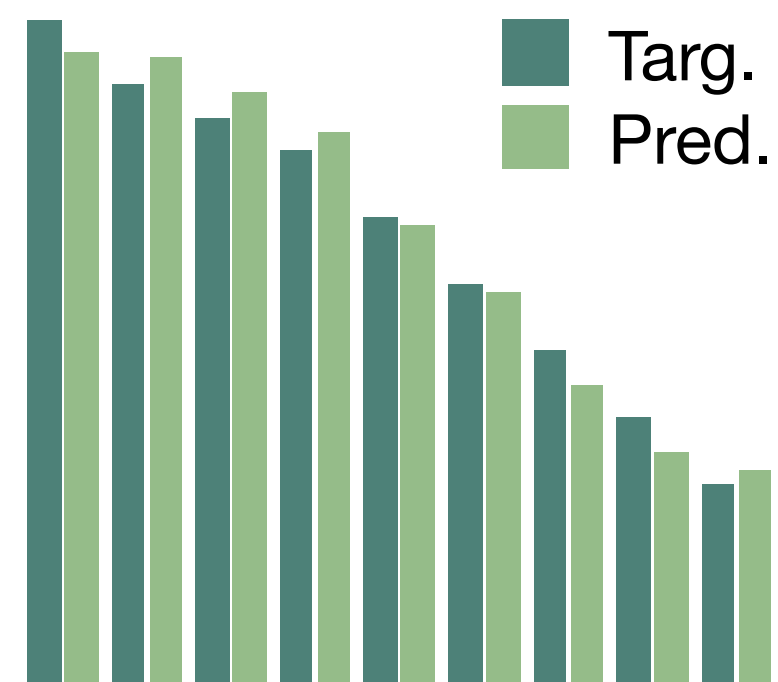
2 stage Network:

$$R \sim q_{\theta_2}(R | N_R, T) q_{\theta_1}(N_R | T)$$

Goals

$$p(R) = \int dT p(R|T)p(T)$$

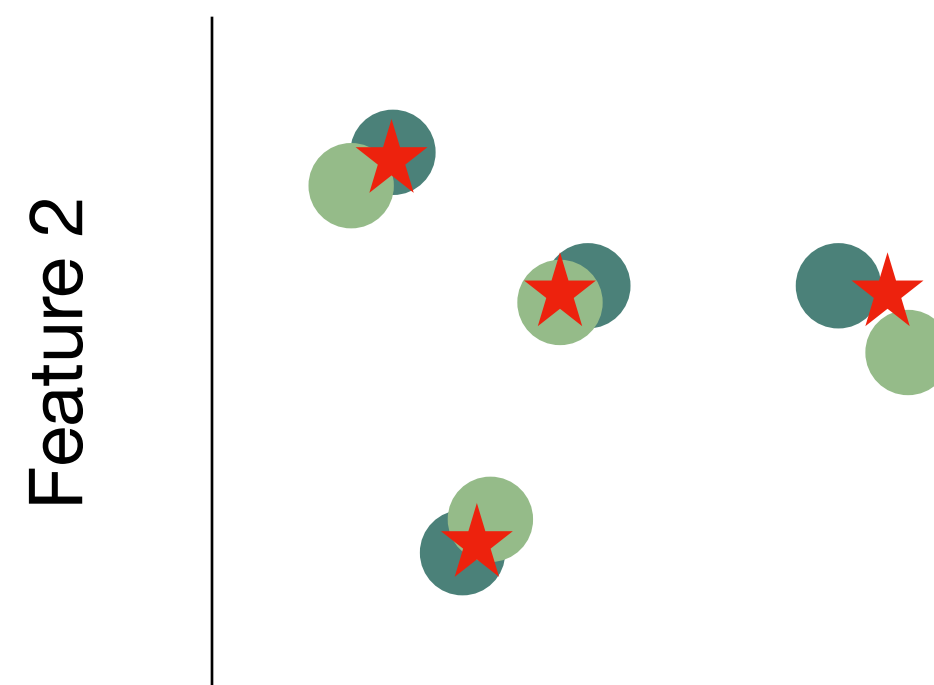
Marginal
distributions



Feature

$$(d_0, z_0, q/p_T, \theta, \phi)$$

Reconstruct
constituents

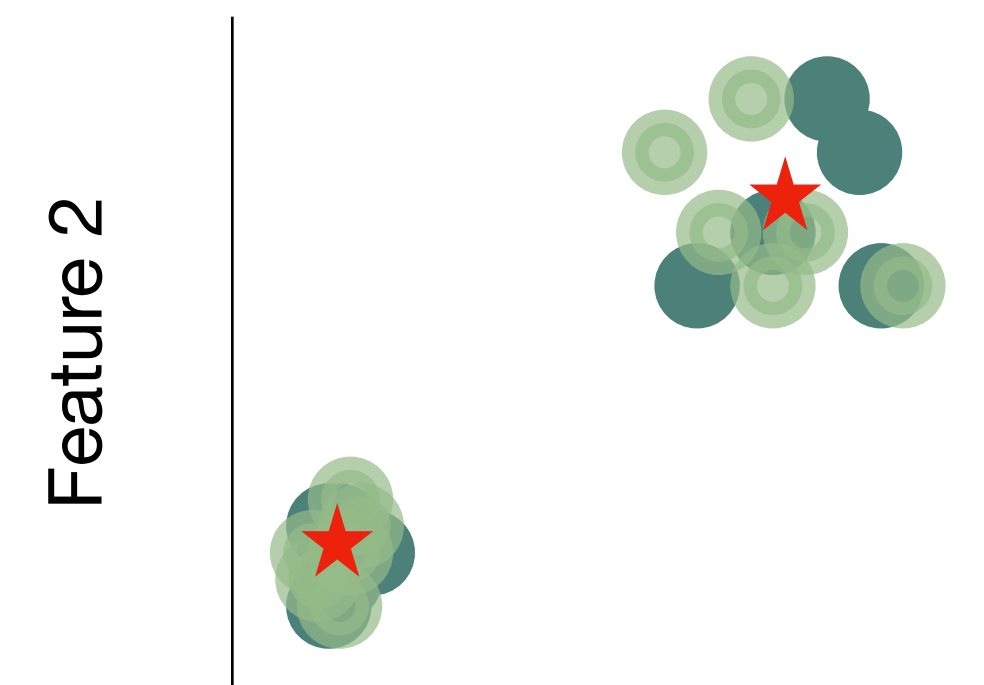


Feature 1

70

$$P(f_R|f_T)$$

Resolution



Feature 1

Goals: RESOLUTION

How to obtain the correct resolution?

Resolution depends on features

→ difficult to learn smearing from one reconstructed sample per truth event

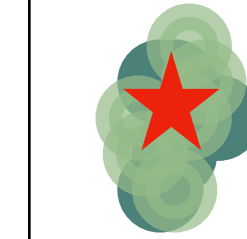
→ need in principle very large dataset

Solution

Introduce *replicas*:

Generate many reconstructions per truth event,
i.e. replicas for the SAME truth event

Feature 2

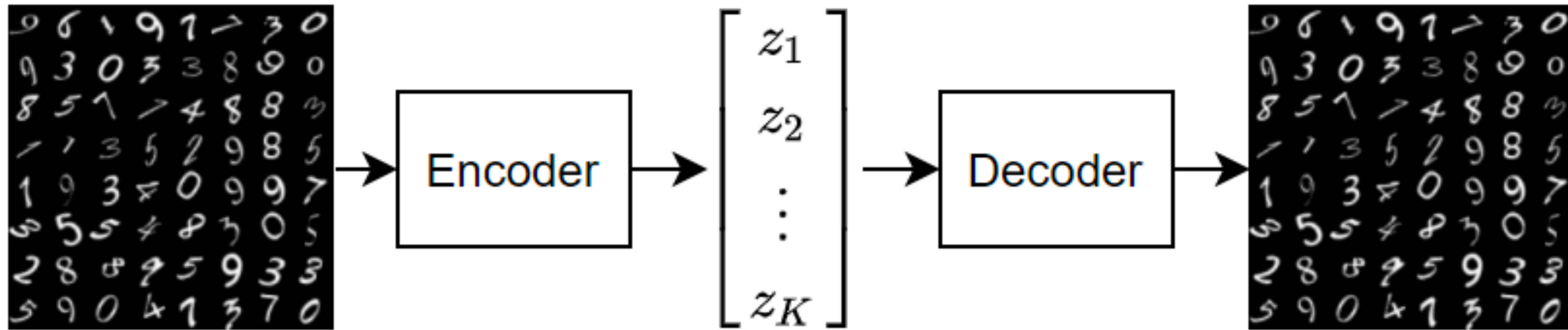


Feature 1

Dataset

- SET of CHARGED particles within a single jet
- Detector Simulation GEANT based COCOA (tomorrow)
- 1-12 charged particles/jet
- Toy example: Smearred tracks as targets
- Reconstruction efficiency, no fakes $\longrightarrow n_{reco} \leq n_{truth}$
- 100 replicas per event (train on 25 for speed)

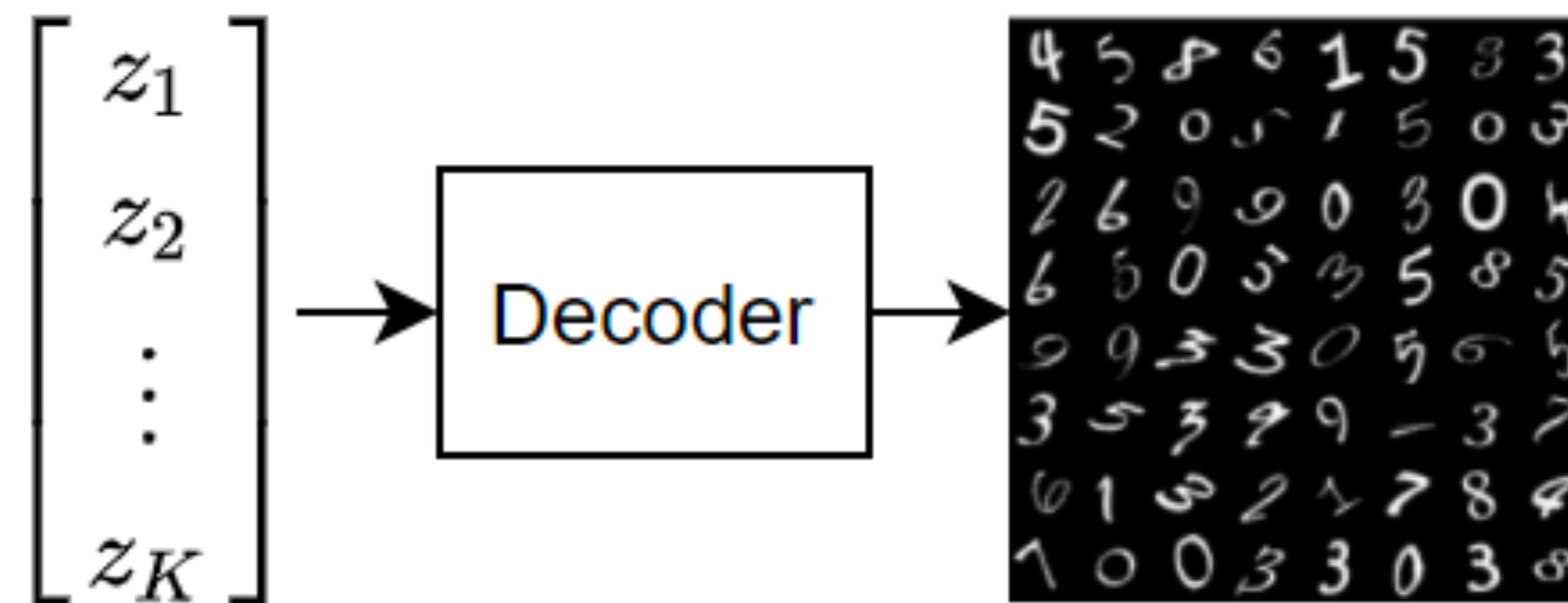
Variational Auto Encoder



Input Images

Image Encodings

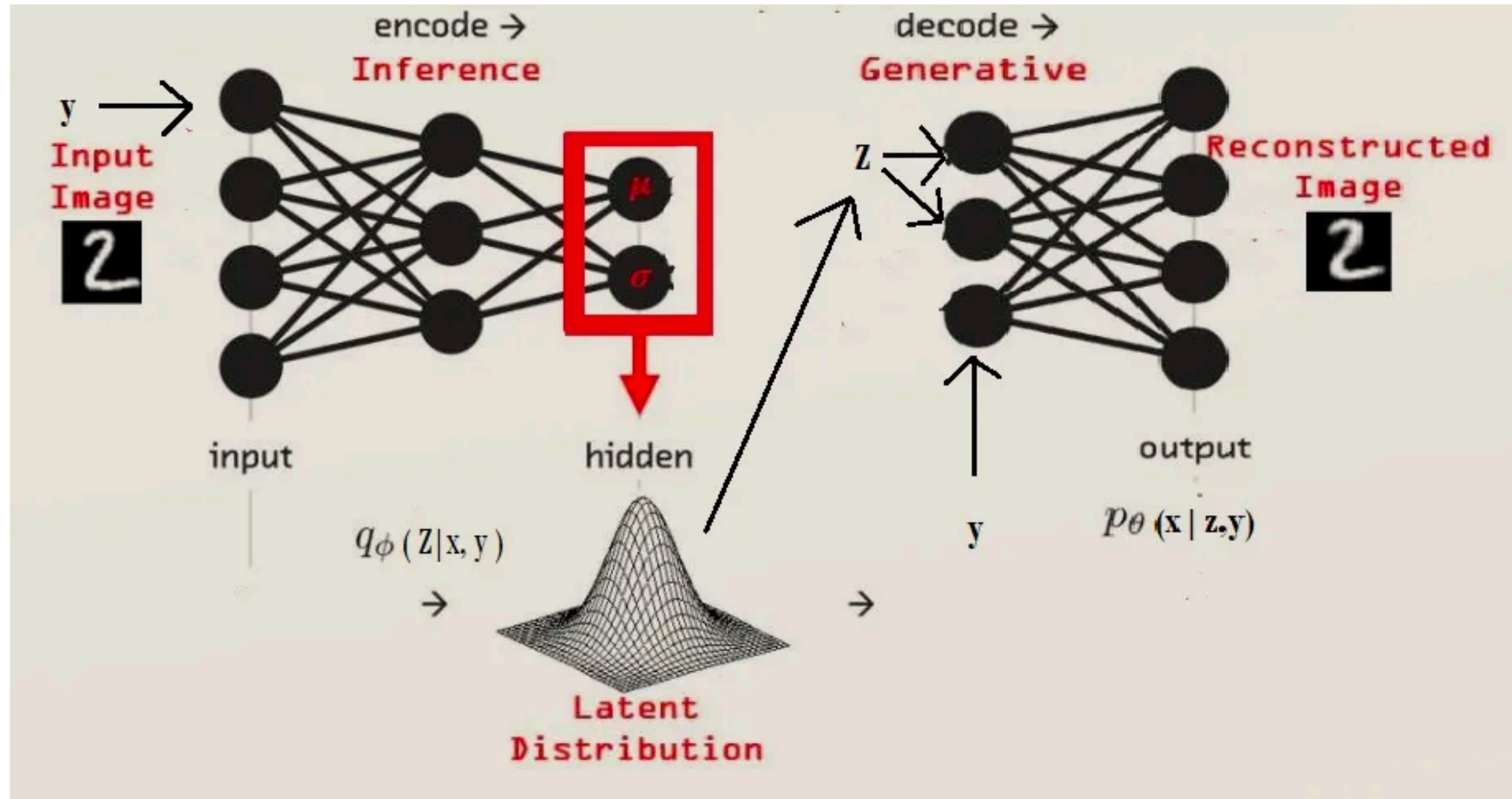
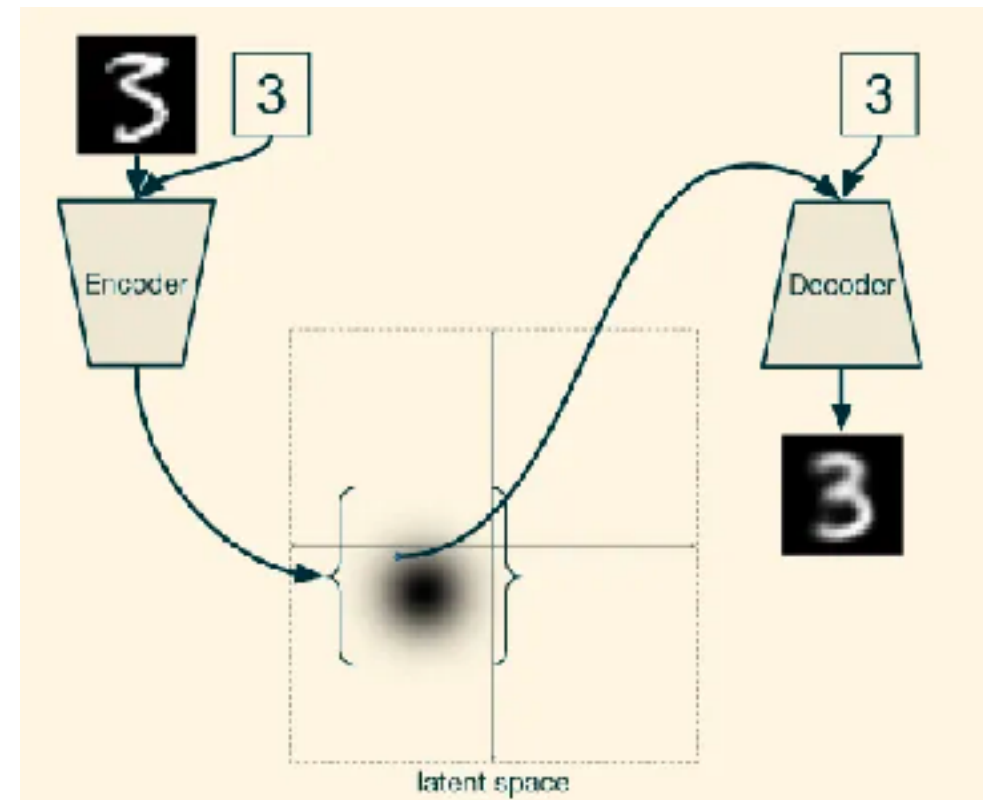
Reconstructed Images



Random Vectors

Generated Images

cVAE



Variational Auto Encoder as Baseline

VAE in a NUTSHELL

- Start by picking a prior to Z , $p(Z) \sim \mathcal{N}(0,1)$
The details are in the conditional $P(X|Z)$

- The decoder learns the distribution of $x|z$, it learns two functions

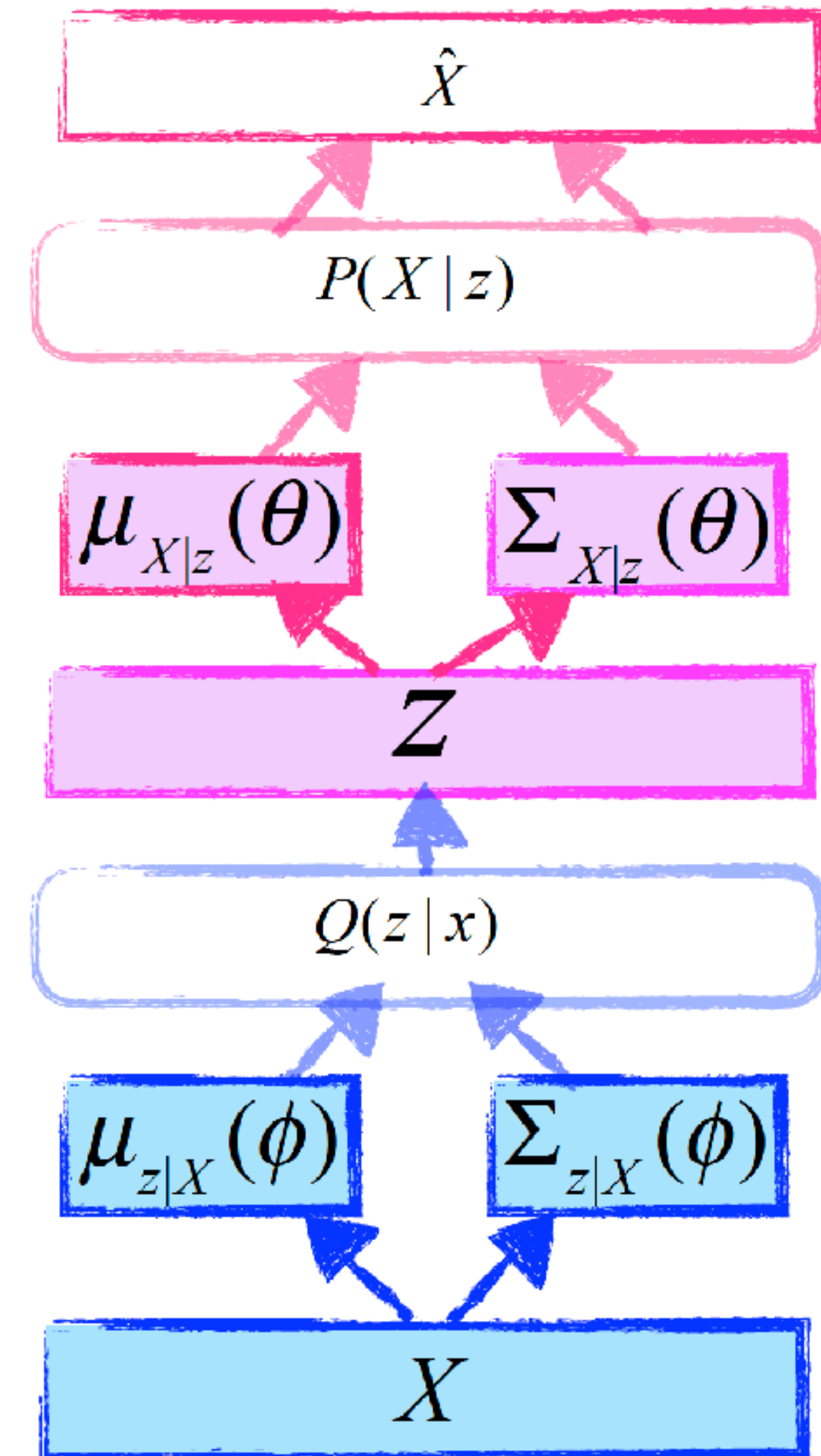
$$\mu_{X|z}(\theta) \quad \Sigma_{X|z}(\theta)$$

Sample $x|z$ from $x|z \sim \mathcal{N}(\mu_{x|z}, \Sigma_{x|z})$

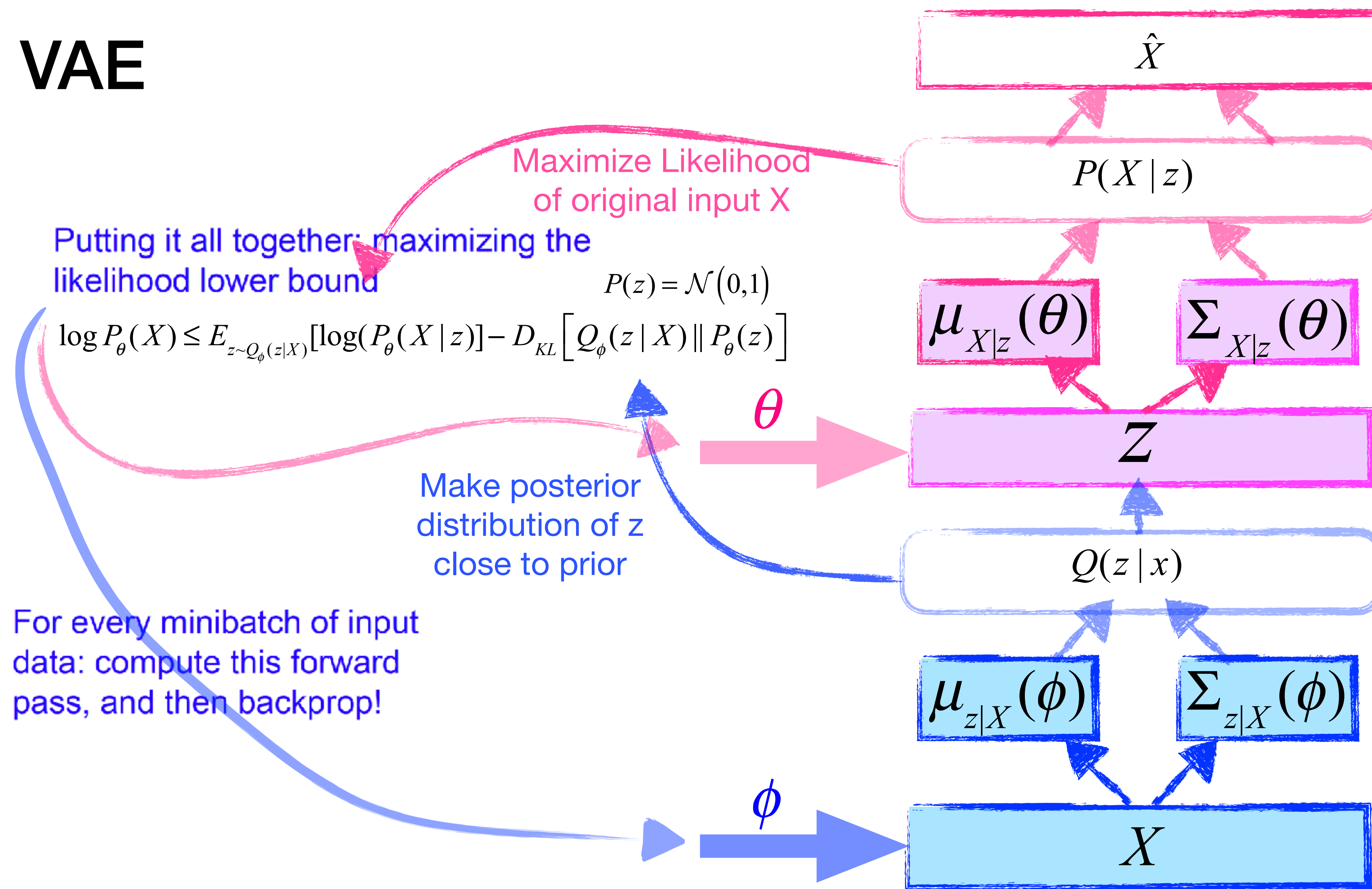
- To ensure that the latent space contains z that lead to a DATA-like X the encoder learns an **approximate** distribution of $\mathbf{P(Z|X)}$; $\mathbf{Q(Z|X)}$ by learning two functions

$$\mu_{z|X}(\phi) \quad \Sigma_{z|X}(\phi)$$

from which $Z|x$ is sampled

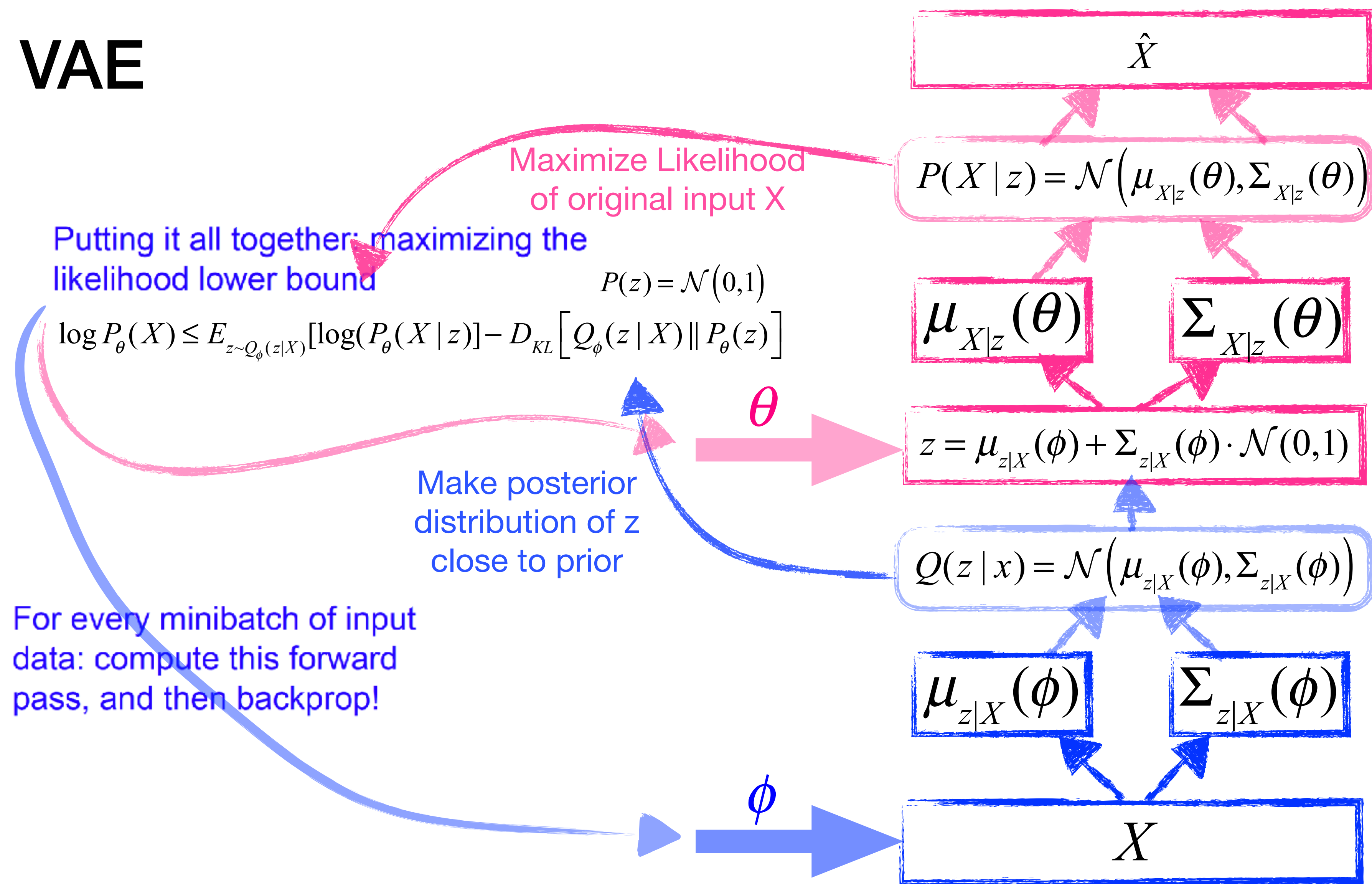


VAE



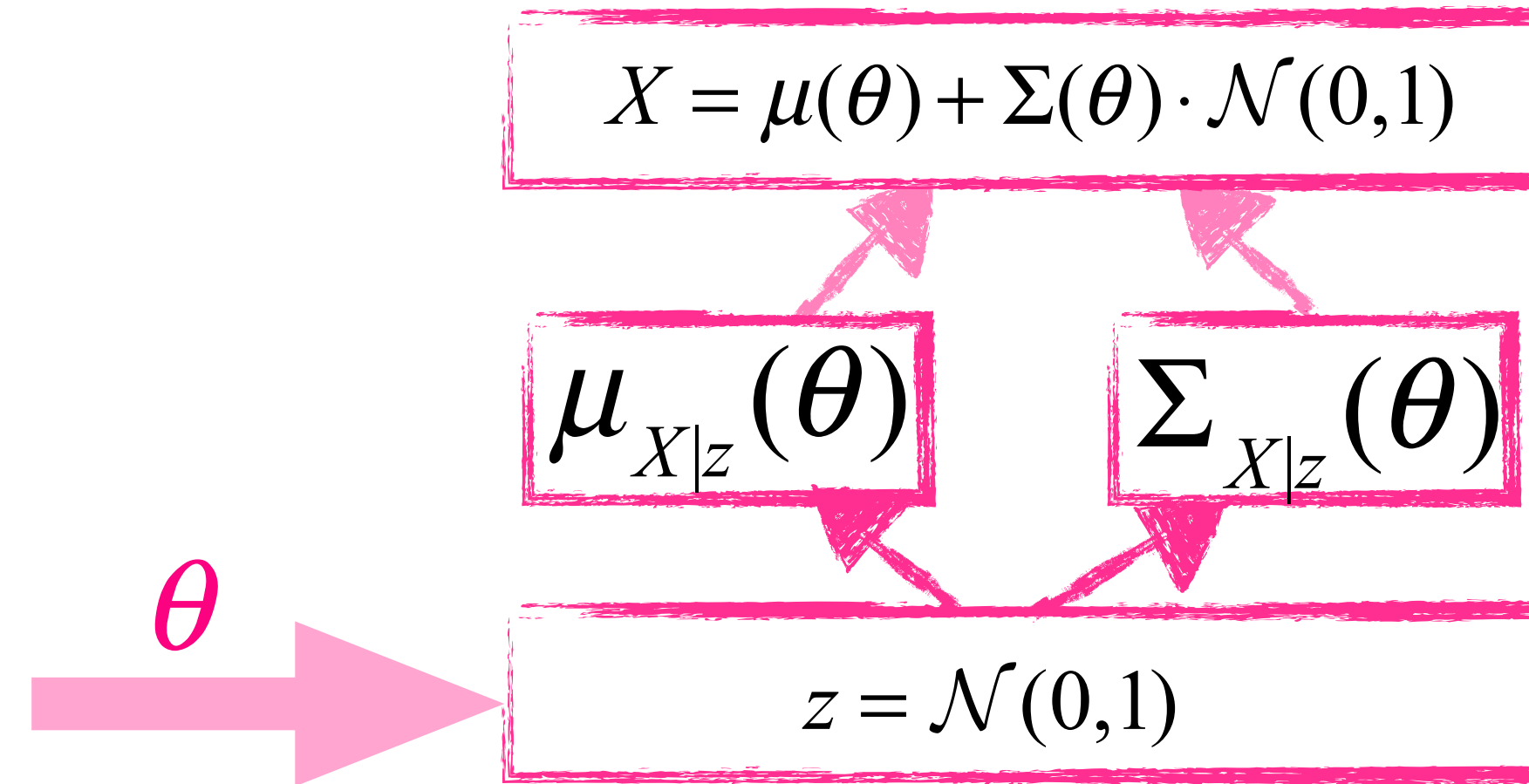
We update our model by continuously update the decoder and encoder parameters, Φ and Θ

VAE

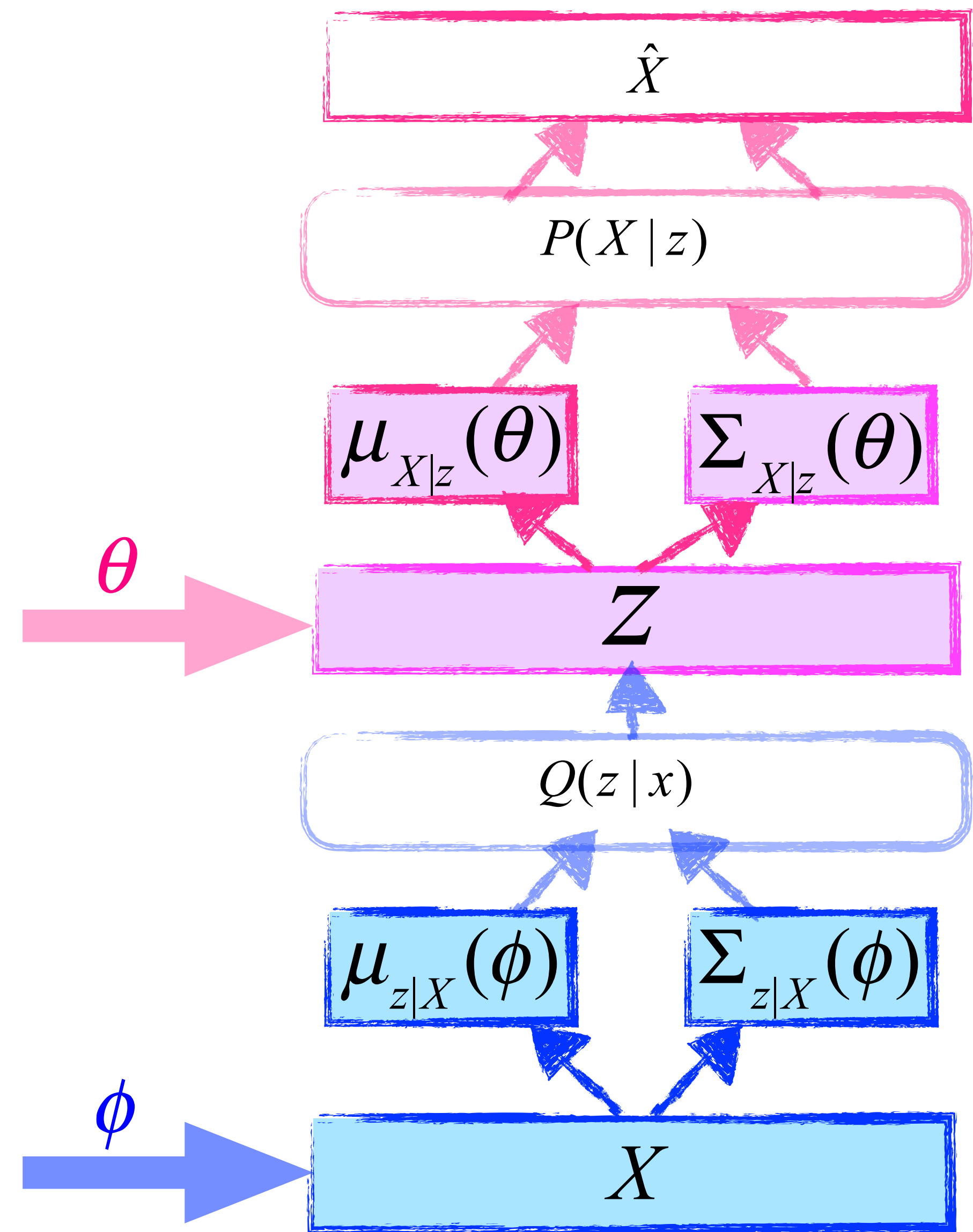
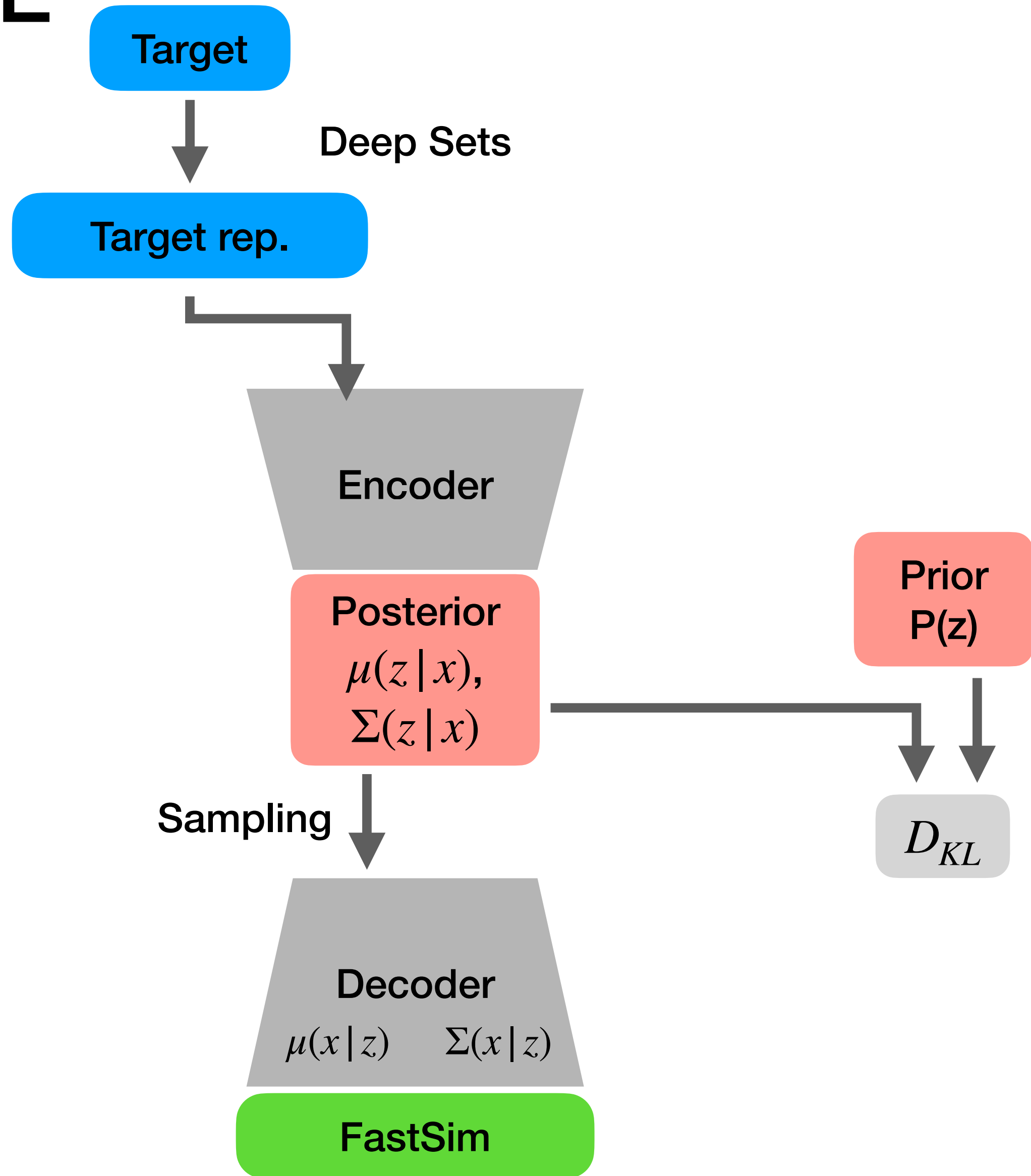


We update our model by continuously update the decoder and encoder parameters, Φ and Θ

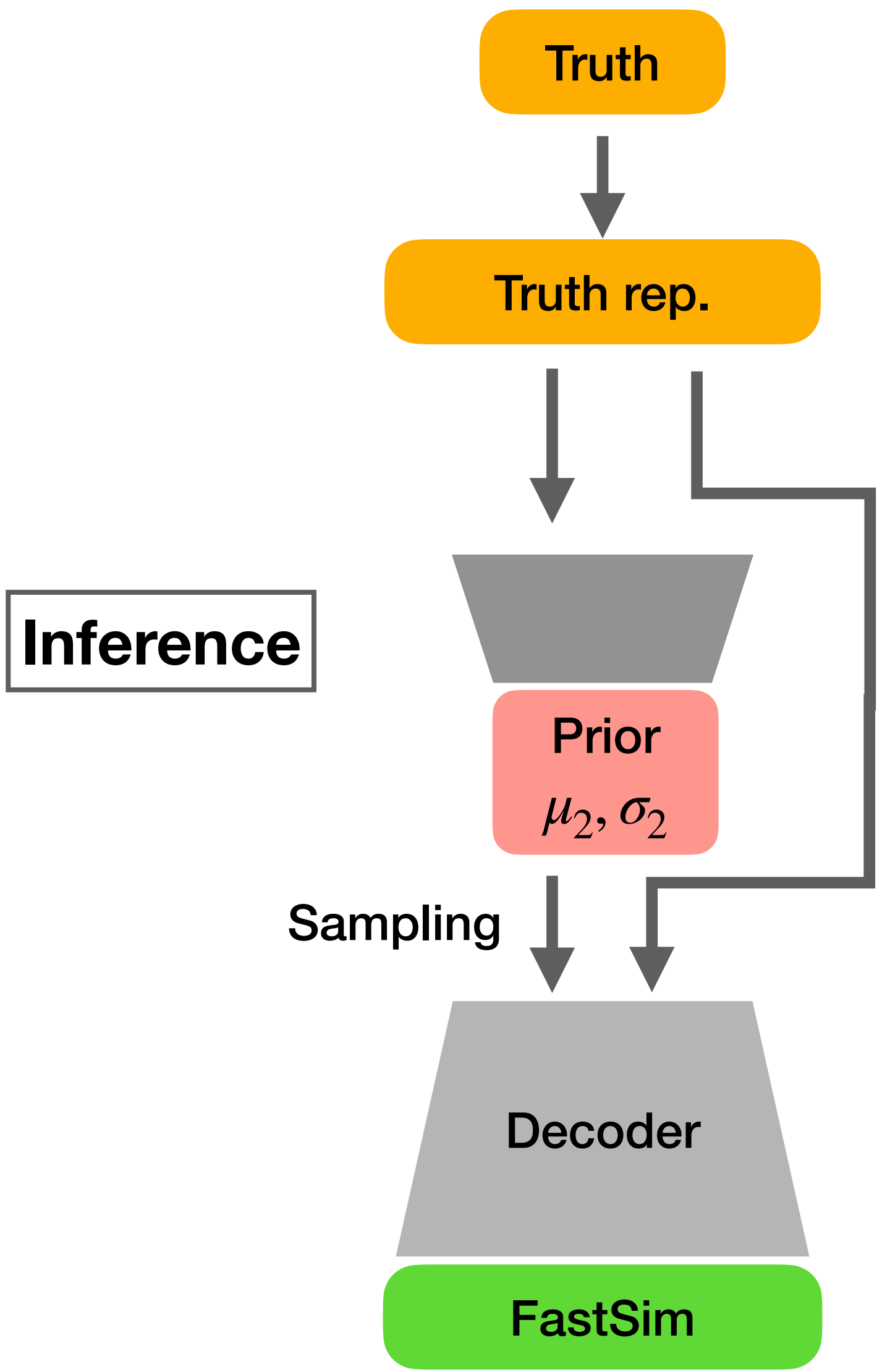
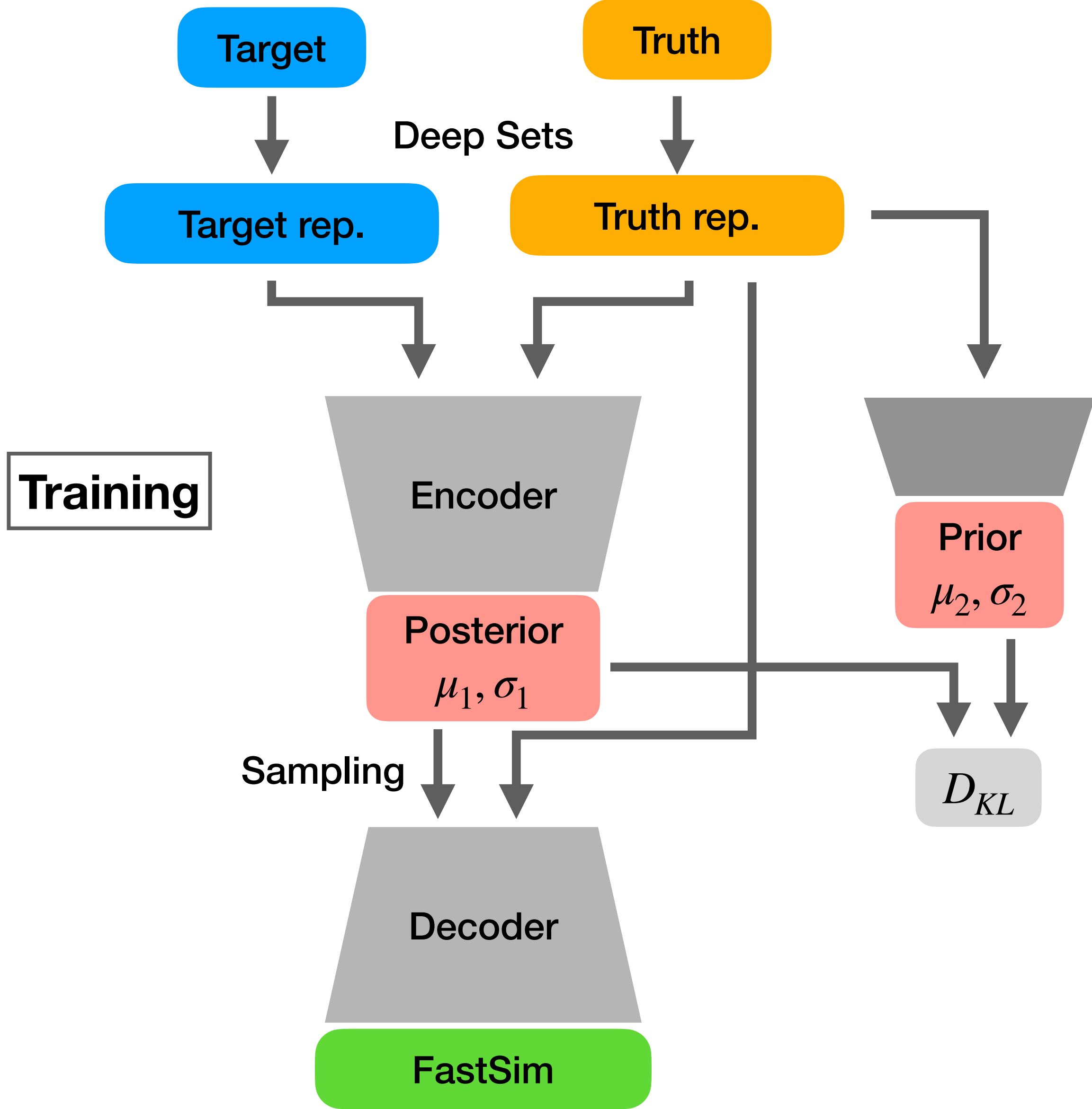
VAE



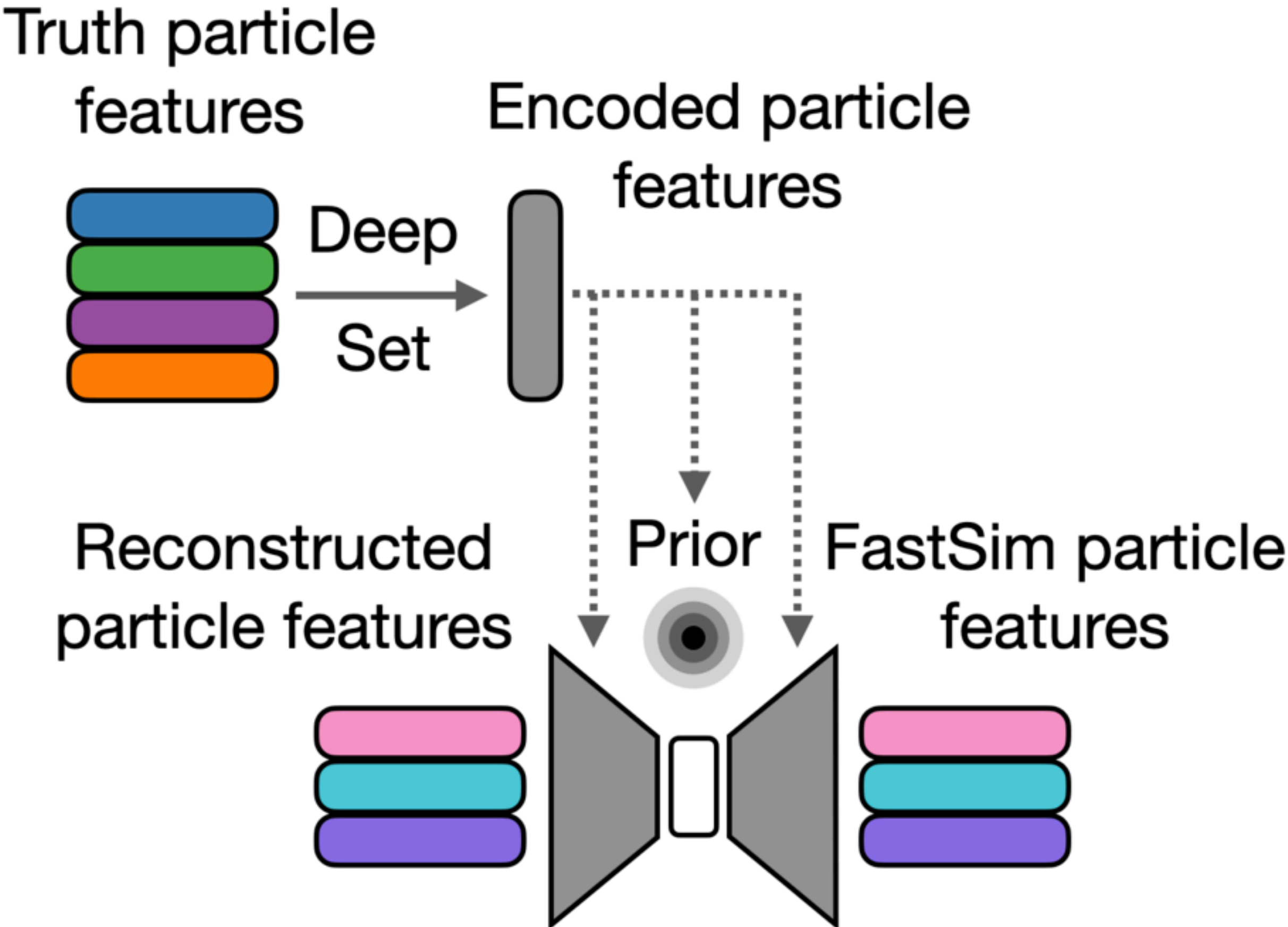
VAE



cVAE Architecture

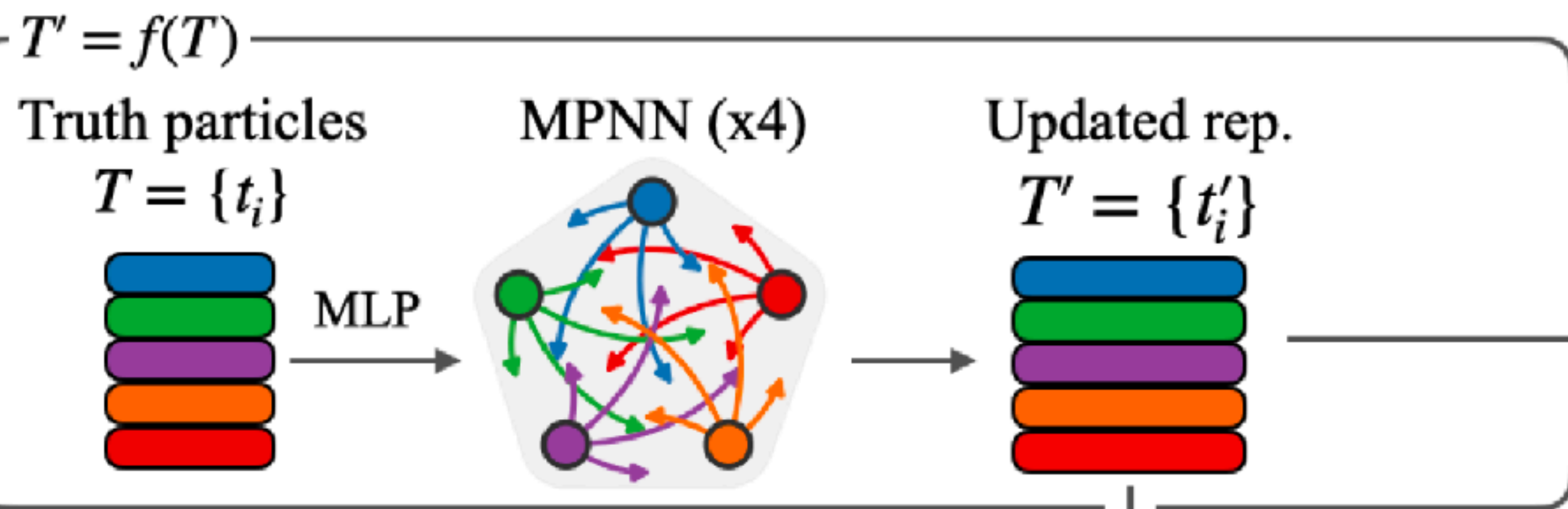


cVAE Architecture

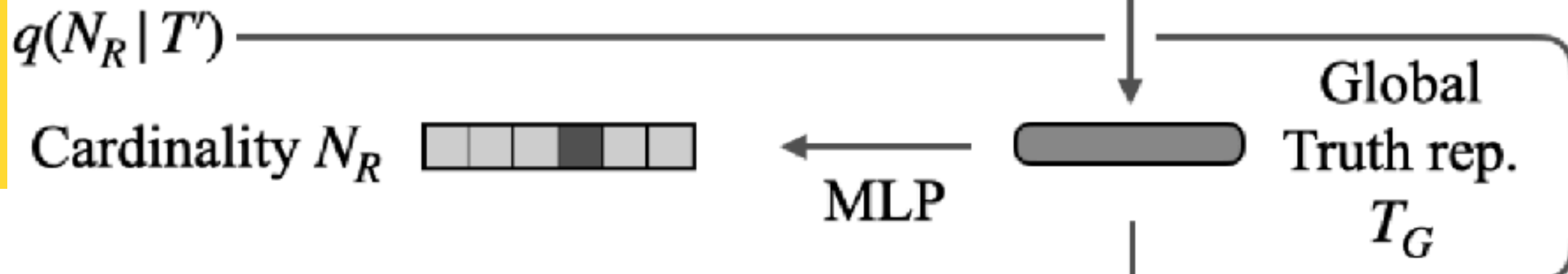


GNN Architecture

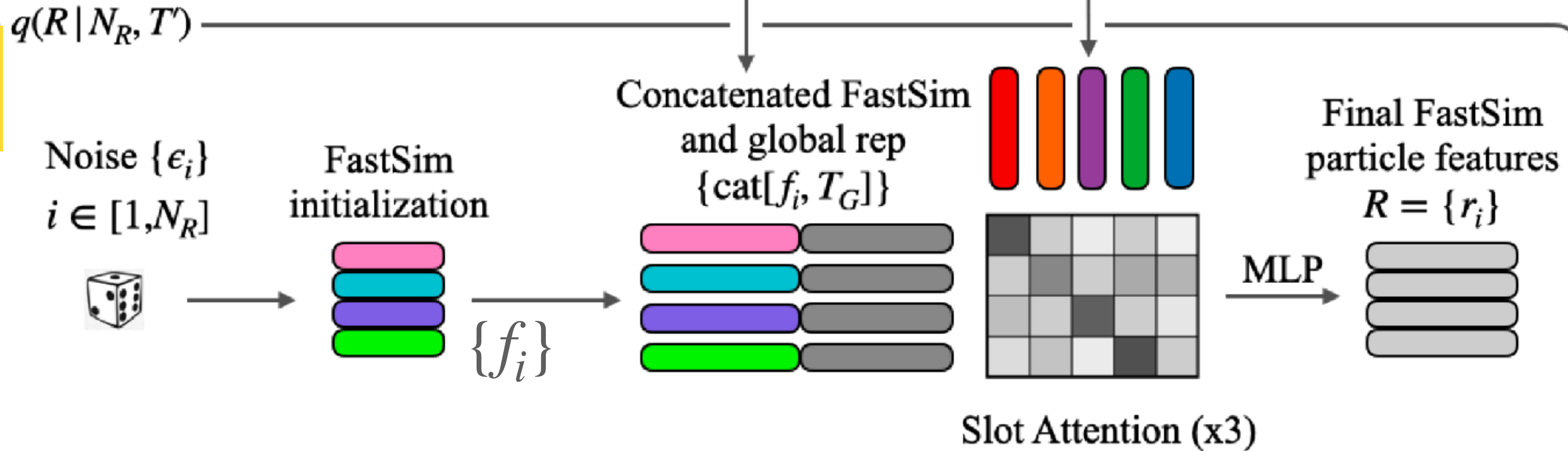
Input Set Encoding



Cardinality Prediction



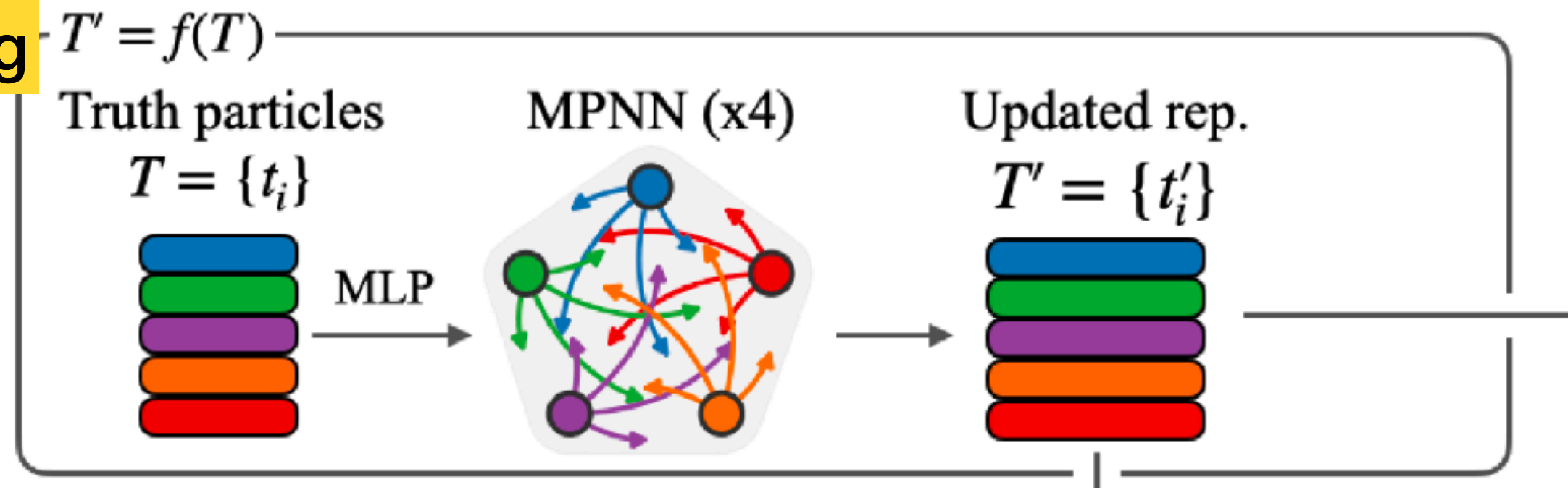
Conditional Set Generation



$$R = \{r_i\} = f_{\theta_2}(\{\epsilon_i\}, \{t'_i\})$$

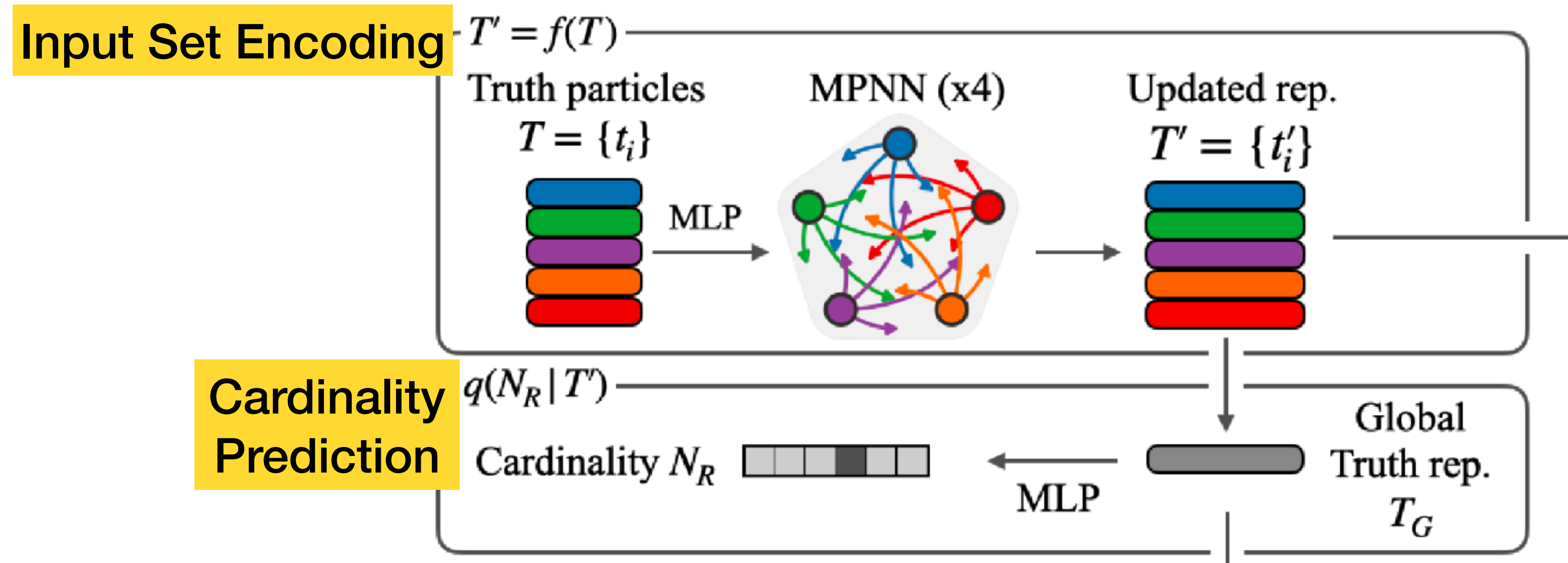
GNN Architecture

Input Set Encoding



$$\{f_i\} = \{p_{T,i}, n_i, \phi_i\}$$

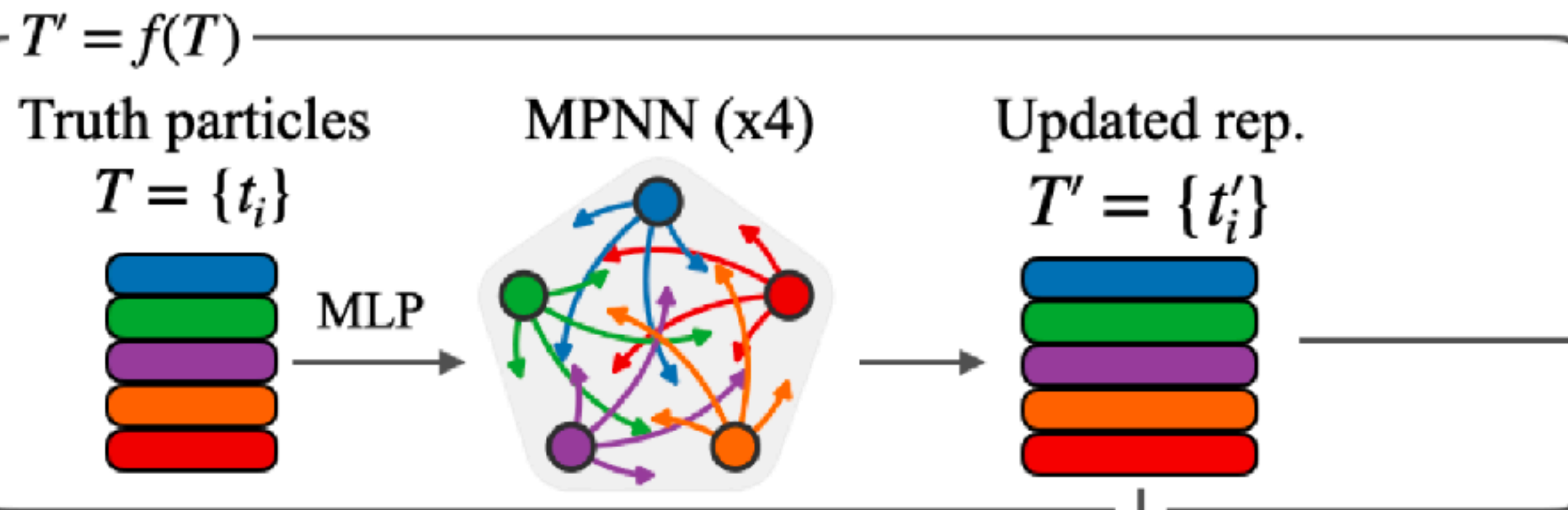
GNN Architecture



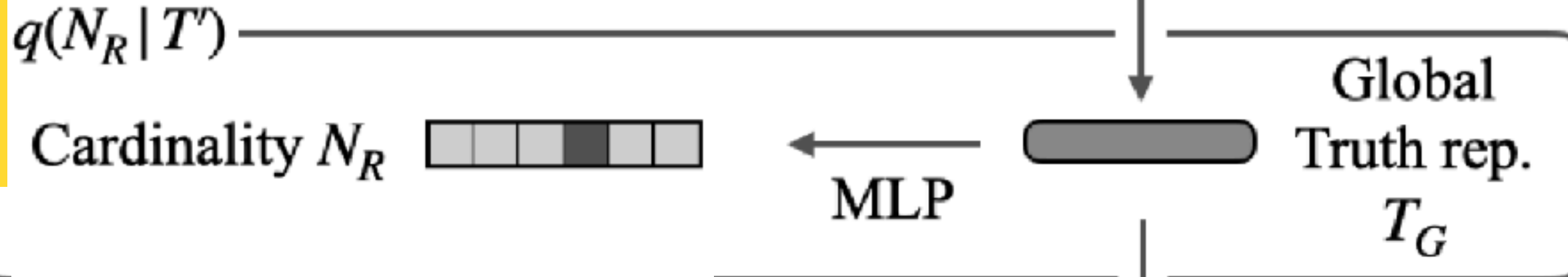
$$q_{\theta_1}(N_R | T)$$

GNN Architecture

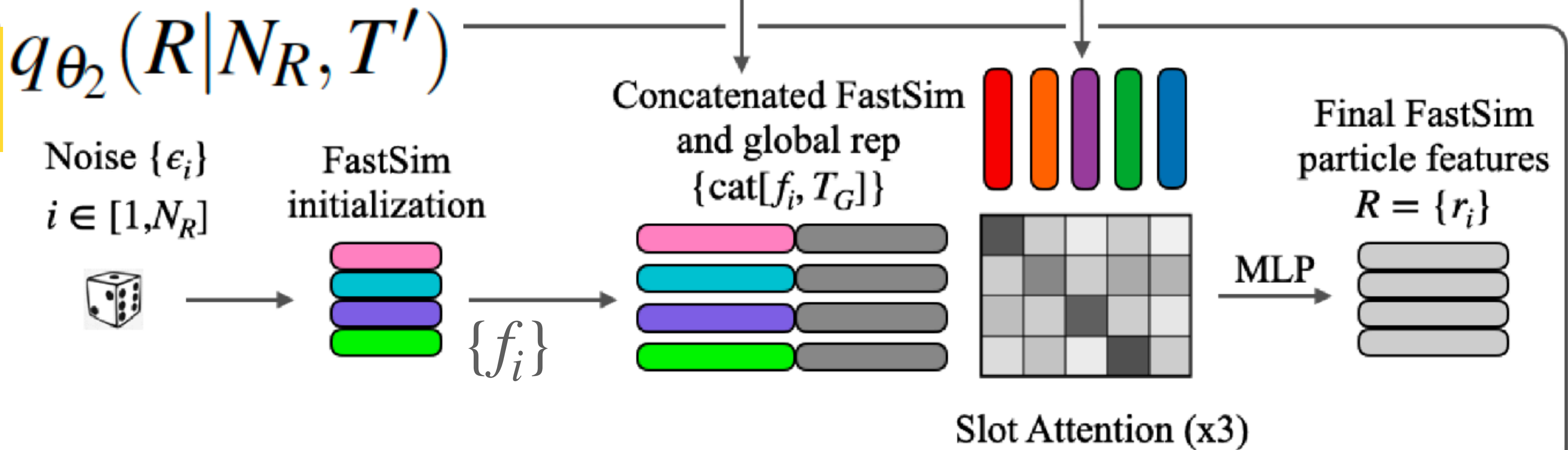
Input Set Encoding



Cardinality Prediction

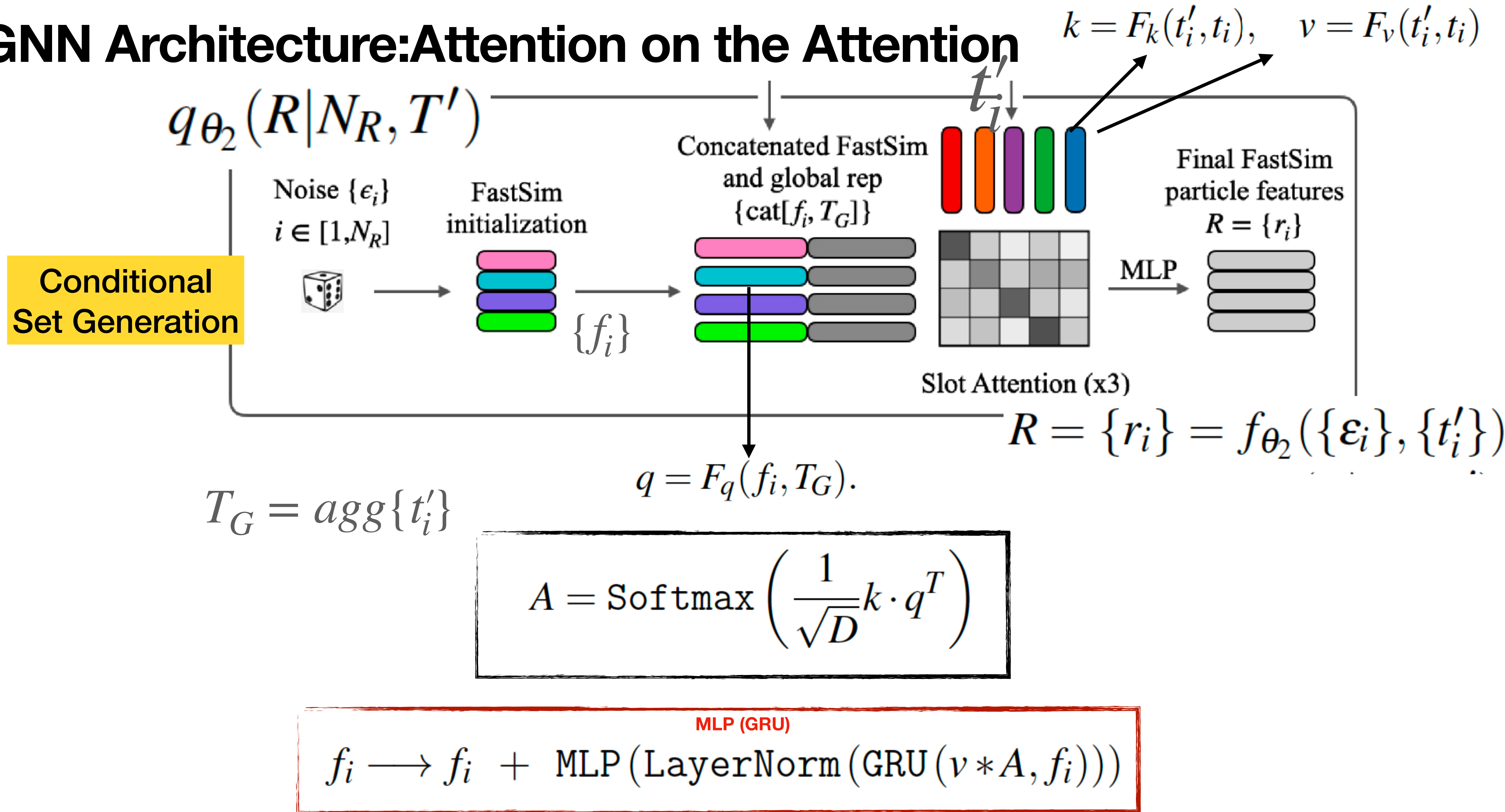


Conditional Set Generation

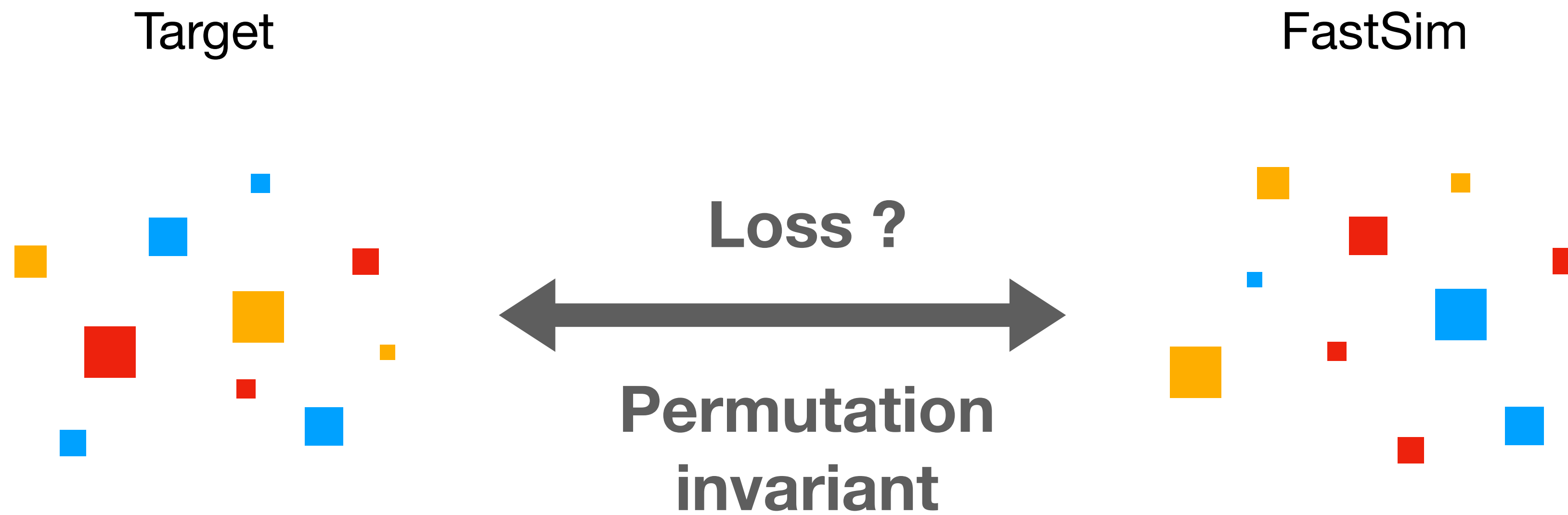


$$R = \{r_i\} = f_{\theta_2}(\{\epsilon_i\}, \{t'_i\})$$

GNN Architecture: Attention on the Attention





Set to Set problem



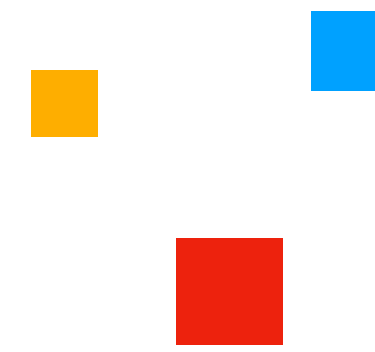
Hungarian matching

FastSim

Target

			
	0.5	0.8	0.1
	0.3	0.7	0.6
	0.3	0.4	1.5

Target



FastSim



$$\min \sum_i^n \sum_j^m C_{ij} X_{ij} \quad \text{where} \quad X_{ij} = \begin{cases} 1 & \text{if row } i \text{ is assigned to column } j \\ 0 & \text{otherwise} \end{cases}$$

$$C_{ij} = (p_{Ti} - p_{Tj})^2 + (\eta_i - \eta_j)^2 + (1 - \cos(\phi_i - \phi_j))$$

Invariant under exchange of columns/rows

“Double Hungarian”

Replicas → Set of Sets

Construct a samplebased
similarity measure between the two distributions

$$p(R | T, N)$$

$$q_\phi(R | T, N)$$

$$MMD^2(p, q) = \mathbb{E}_{x, x' \sim p} k(x, x') + \mathbb{E}_{y, y' \sim q} k(y, y') - 2\mathbb{E}_{x \sim p, y \sim q} k(x, y)$$

$$x_i = (p_{T,i}, \eta_i, \phi_i) \quad y_i = (p'_{T,i}, \eta'_i, \phi'_i)$$

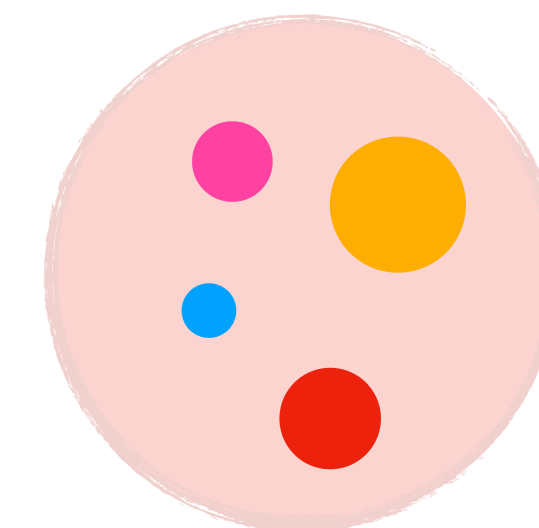
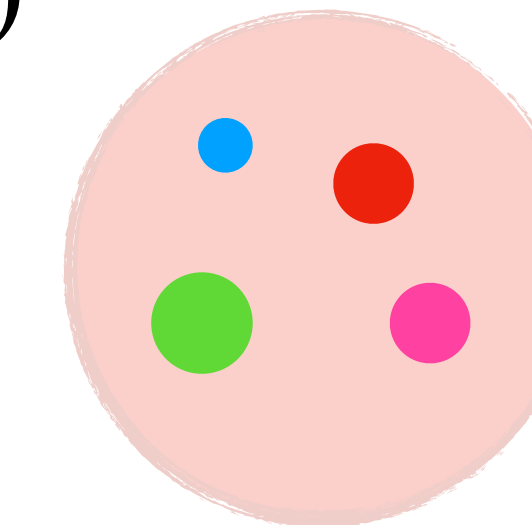
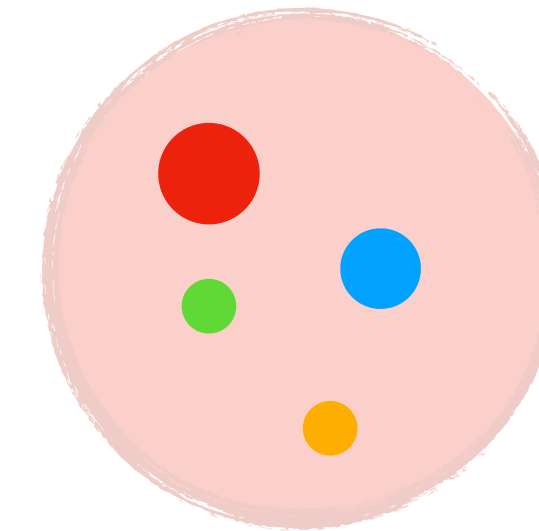
Hungarian $k(x, y) = ||x - y||^2$

MMD vanishes when $p=q$
but is time consuming

$$L_{proxy} = \min_{x_i, y_j} k(x_i, y_j)$$

$$p(R | T, N)$$

Reconstructed
Replicas



$$q_\phi(R | T, N)$$

Predicted
Replicas



“Double Hungarian”

Replicas → Set of Sets

Construct a samplebased similarity measure between the two distributions

$$p(R | T, N)$$

$$q_\phi(R | T, N)$$

$$MMD^2(p, q) = \mathbb{E}_{x, x' \sim p} k(x, x') + \mathbb{E}_{y, y' \sim q} k(y, y') - 2\mathbb{E}_{x \sim p, y \sim q} k(x, y)$$

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Hungarian $k(x, y) = ||x - y||^2$

MMD vanishes when $p=q$
but is time consuming

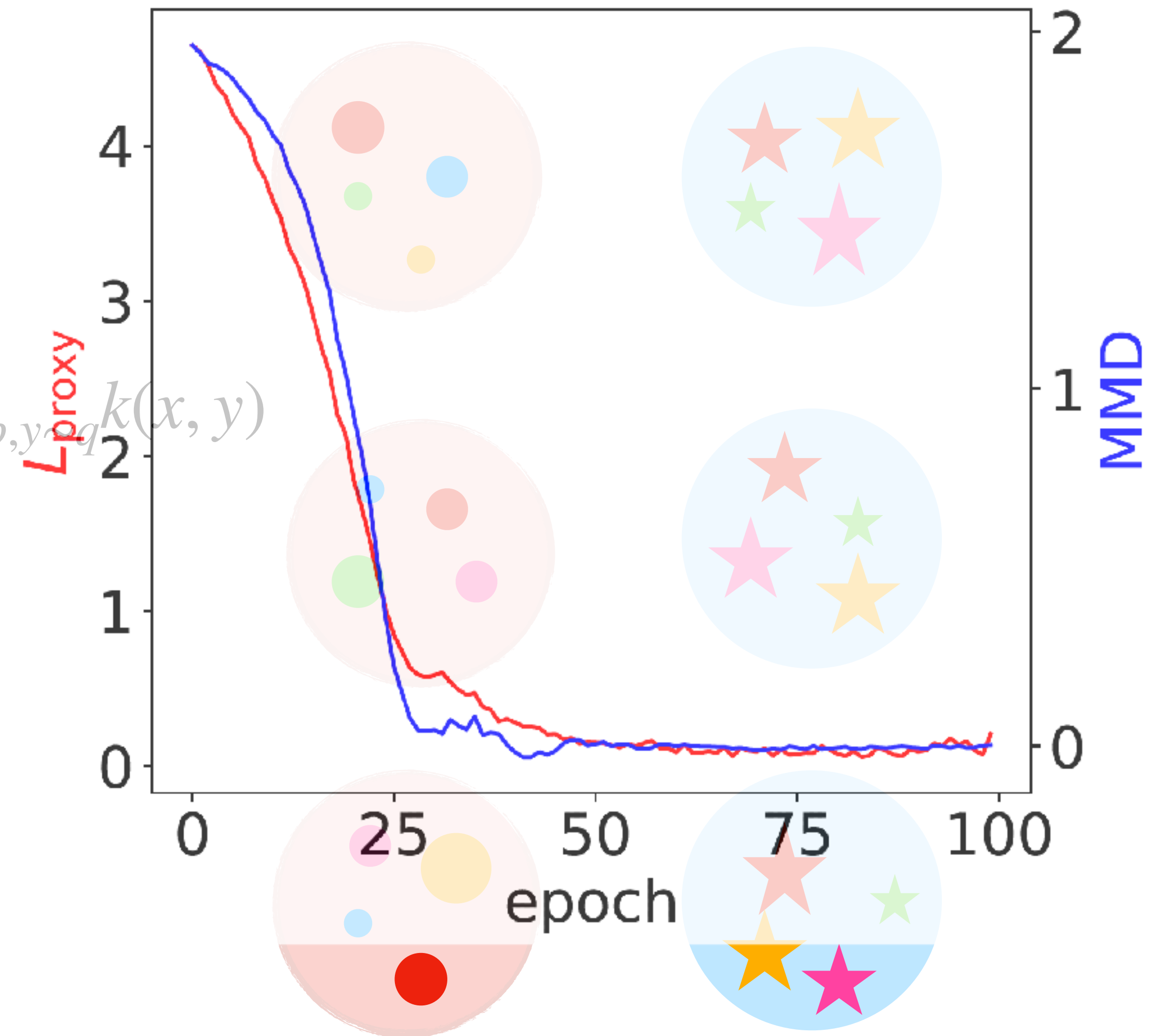
$$L_{proxy} = \min_{x_i, y_j} k(x_i, y_j)$$

$$p(R | T, N)$$

$$q_\phi(R | T, N)$$

Reconstructed
Replicas

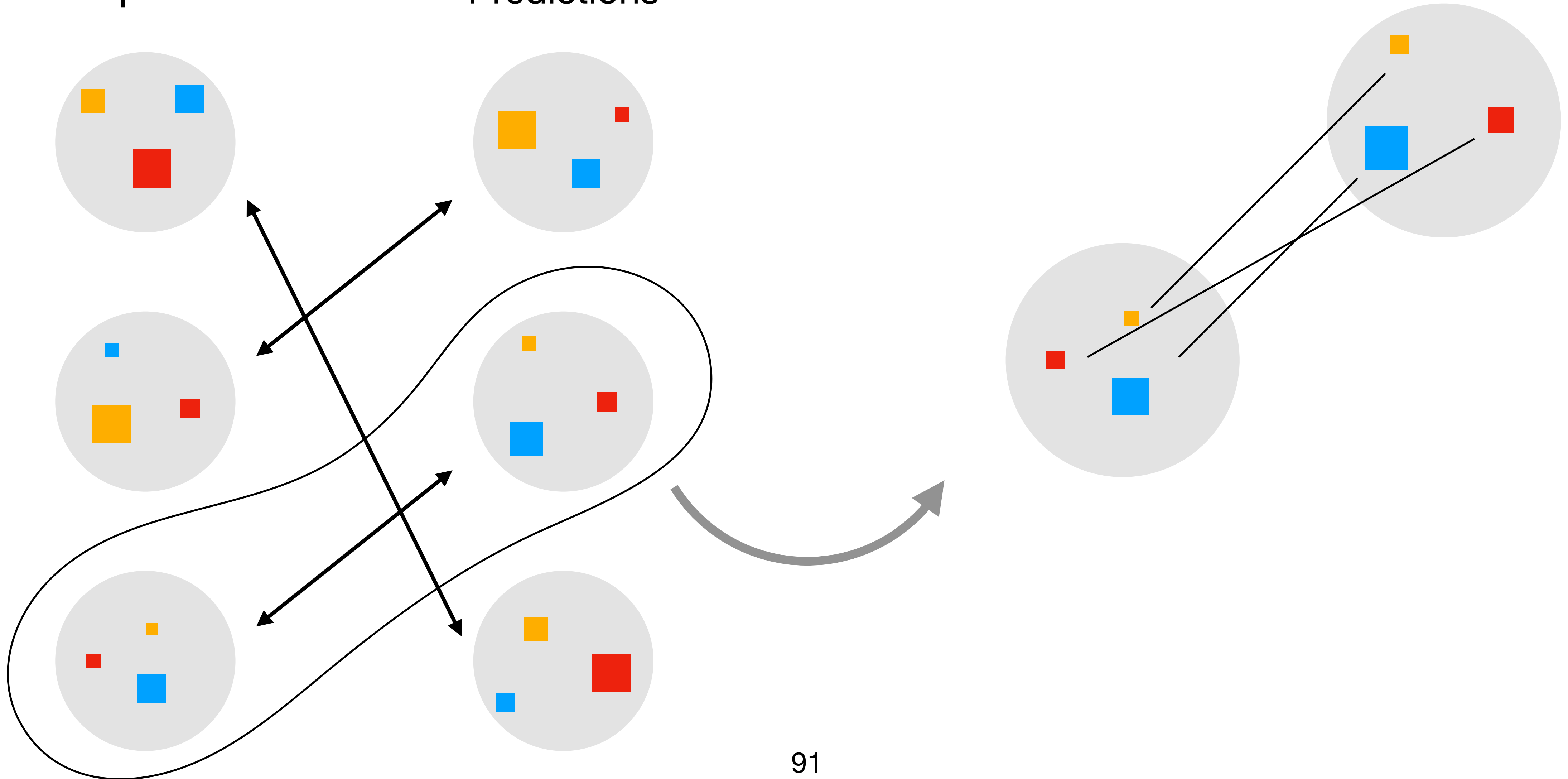
Predicted
Replicas



“Double Hungarian”

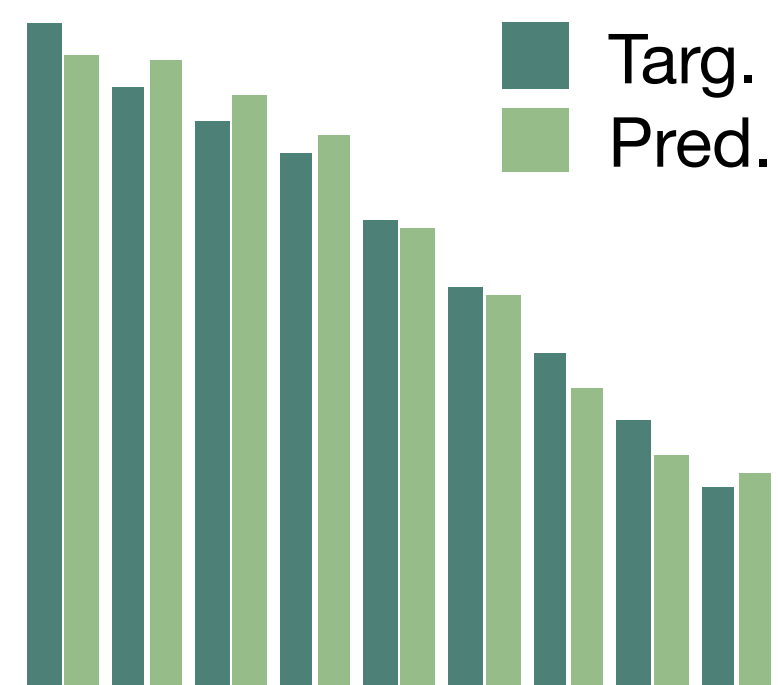
Replicas

Predictions



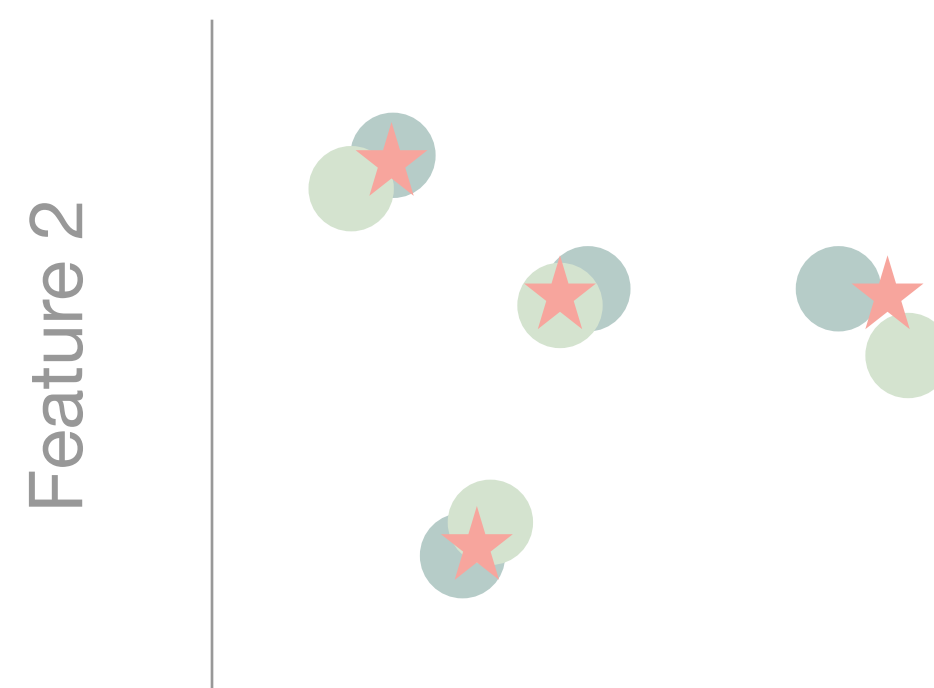
Goals

Marginal
distributions



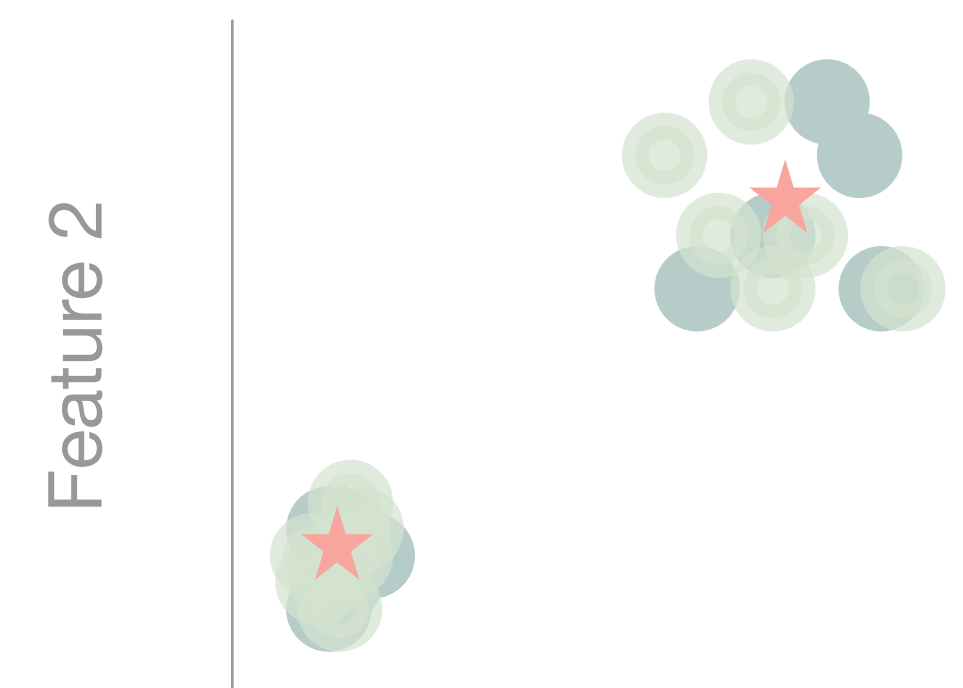
Feature

Reconstruct
constituents



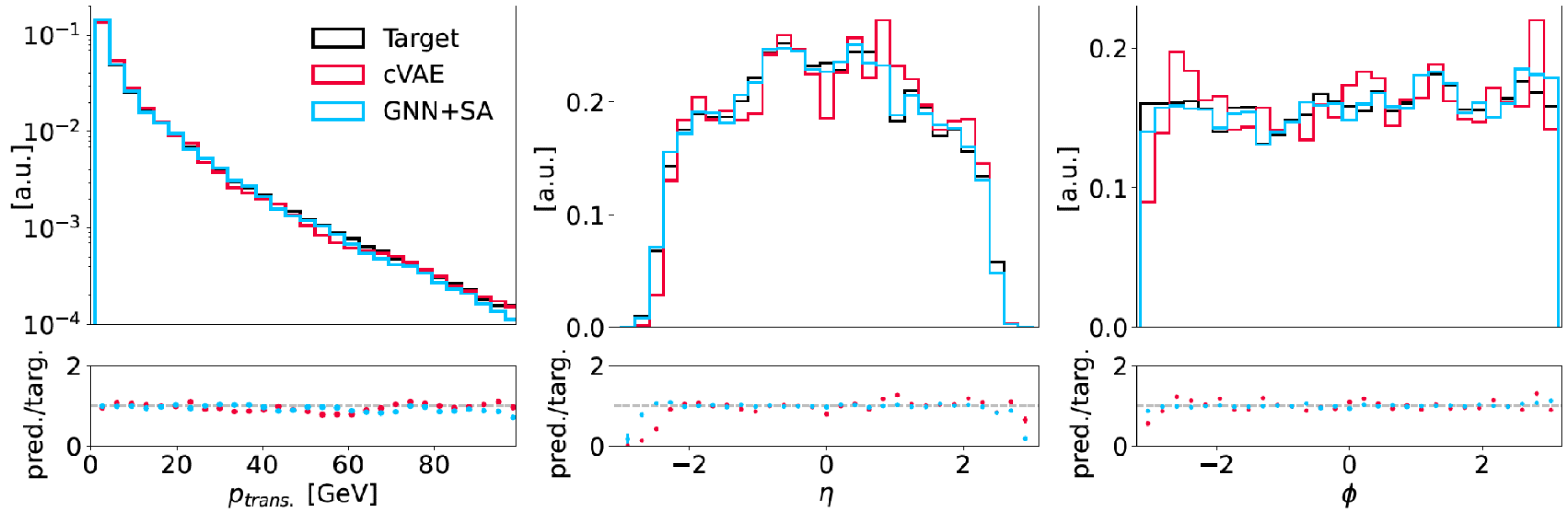
Feature 1

Resolution



Feature 1

Marginal distributions



- 1D marginal distributions similarly good for both cVAE and GNN

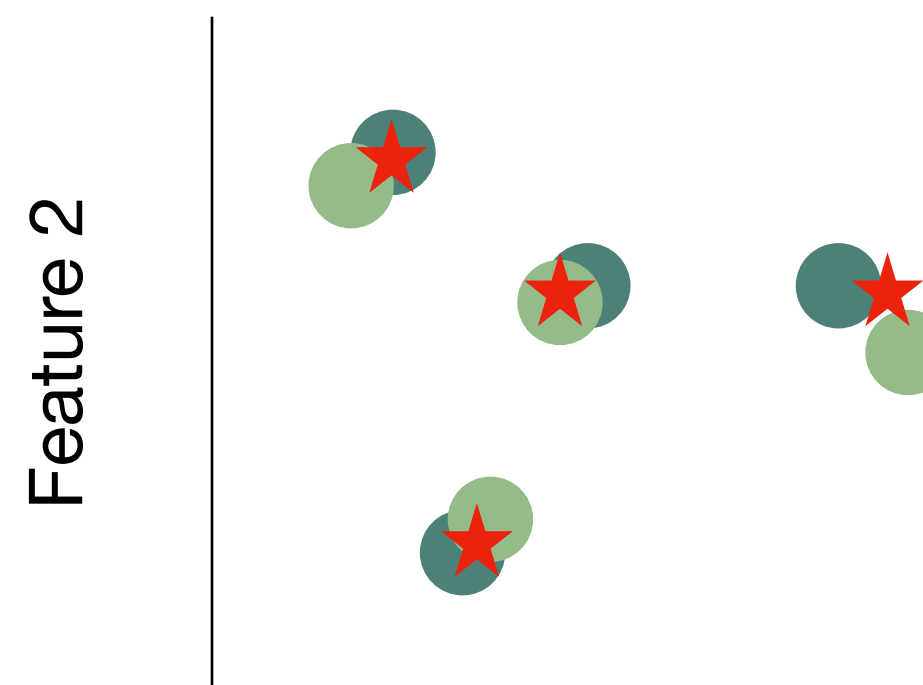
Goals

Marginal
distributions



Feature

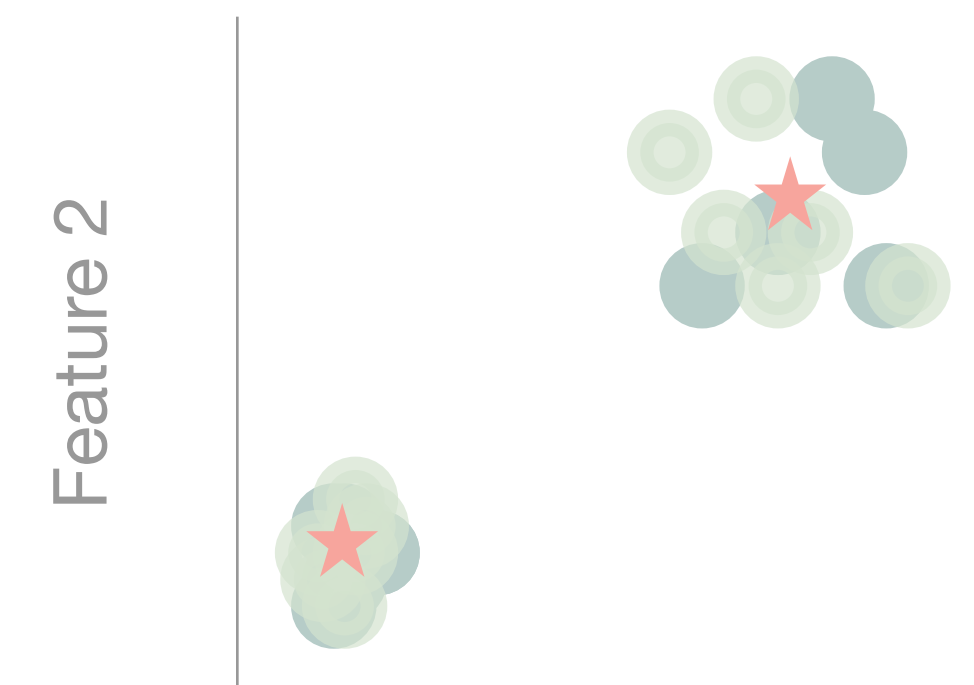
Reconstruct
constituents



Feature 1

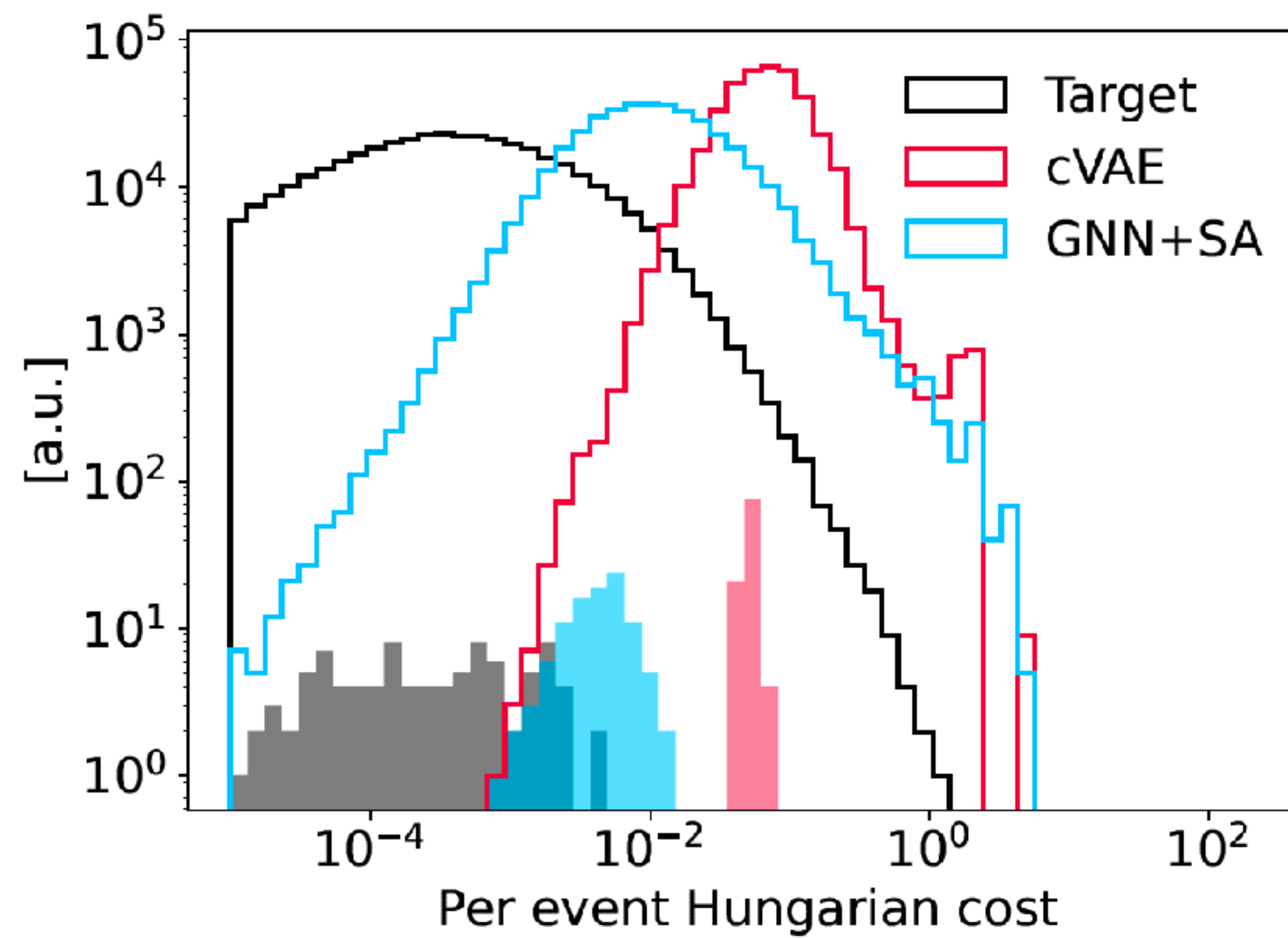
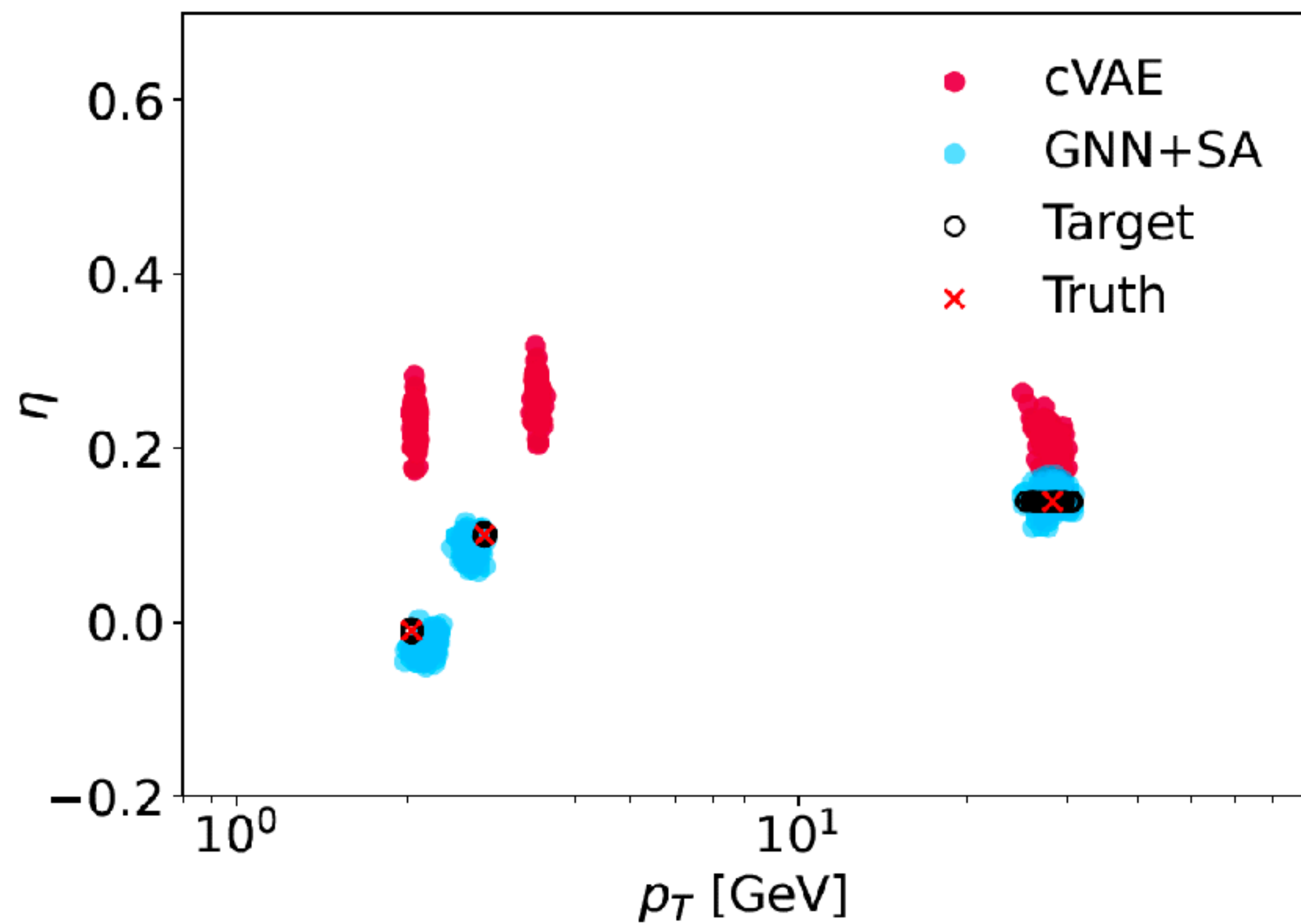
94

Resolution



Feature 1

Reconstruct Constituents



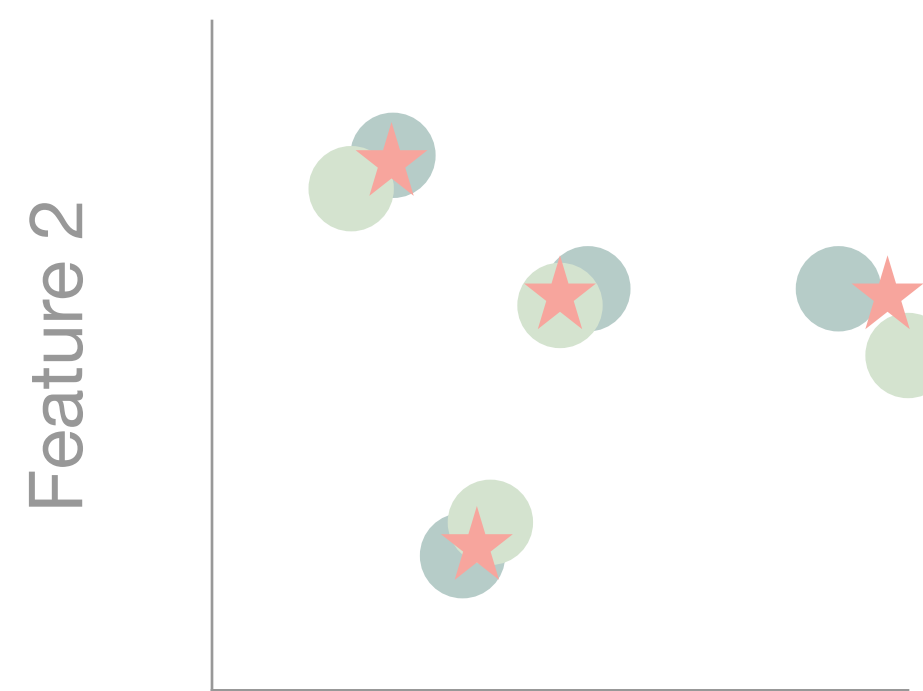
Goals

Marginal
distributions



Feature

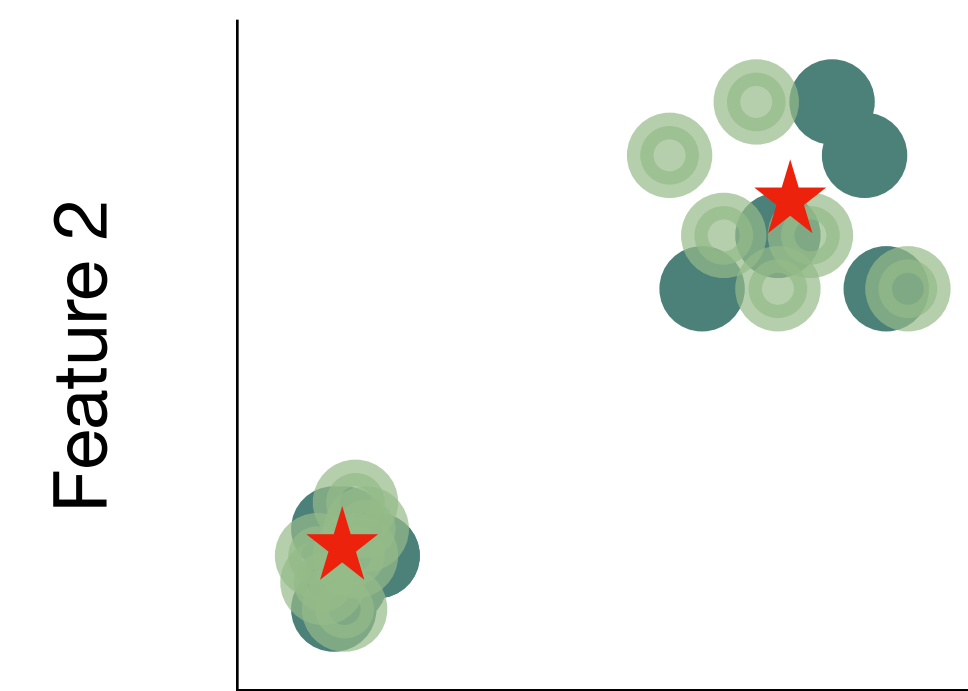
Reconstruct
constituents



Feature 1

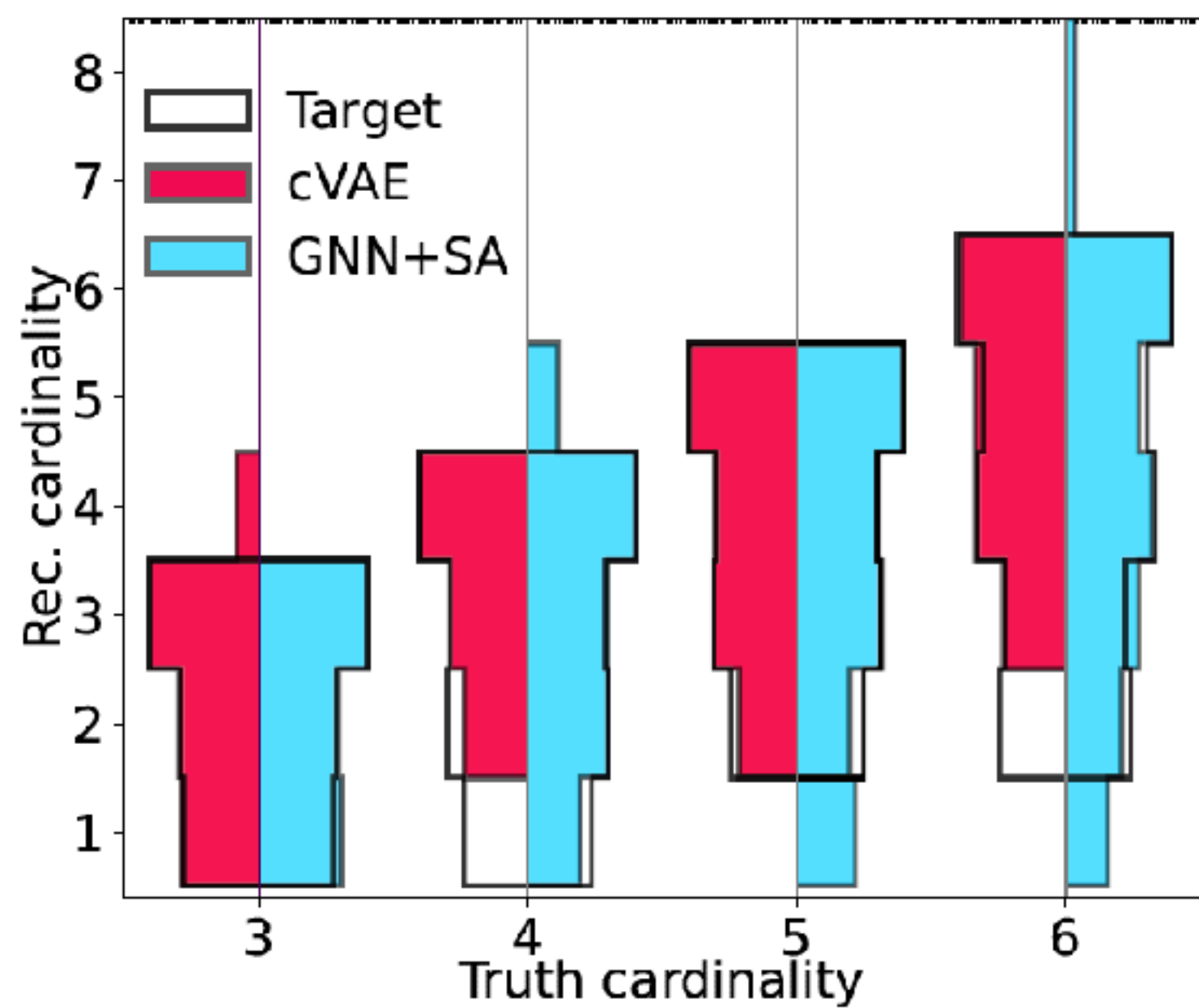
96

Resolution

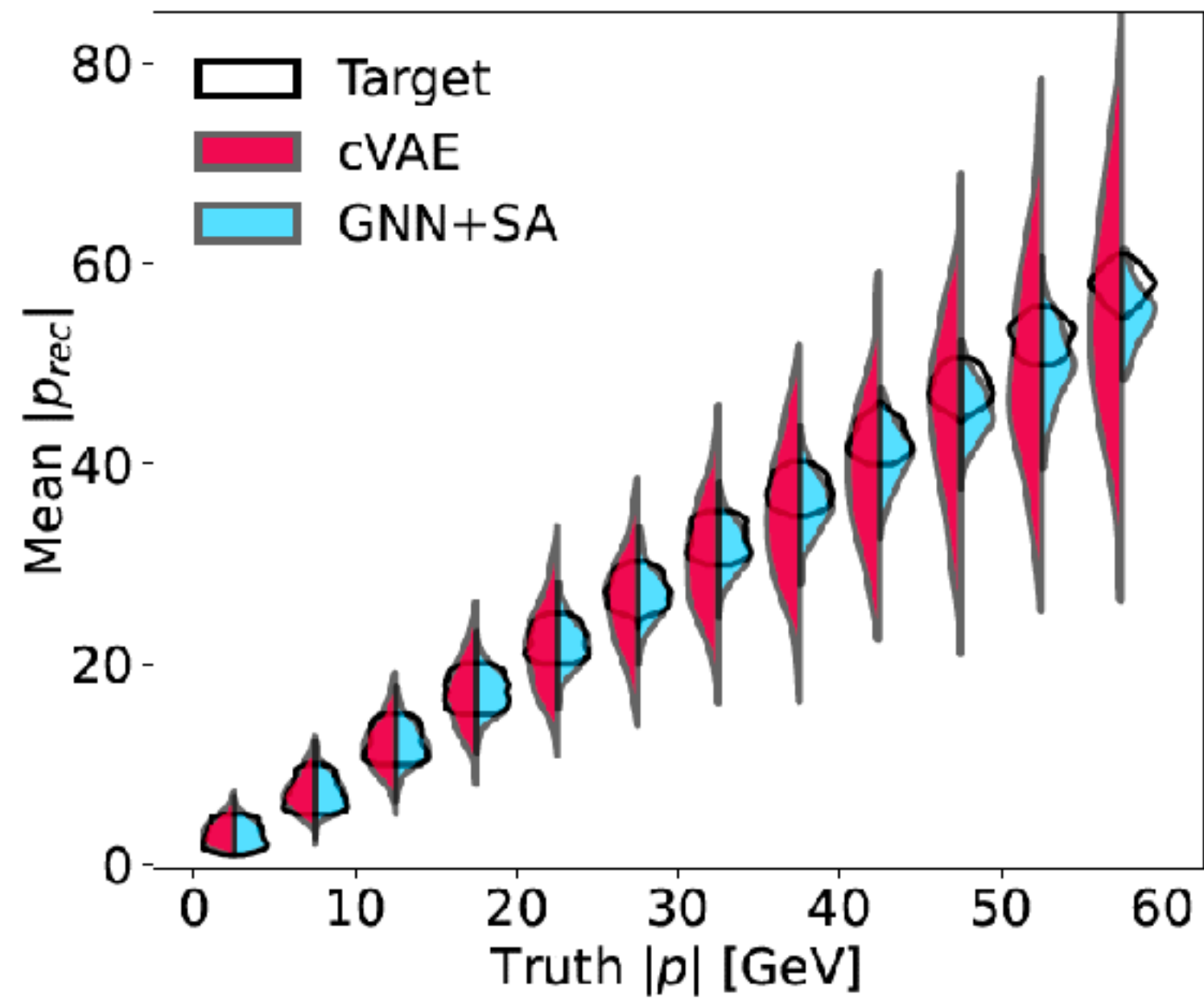


Feature 1

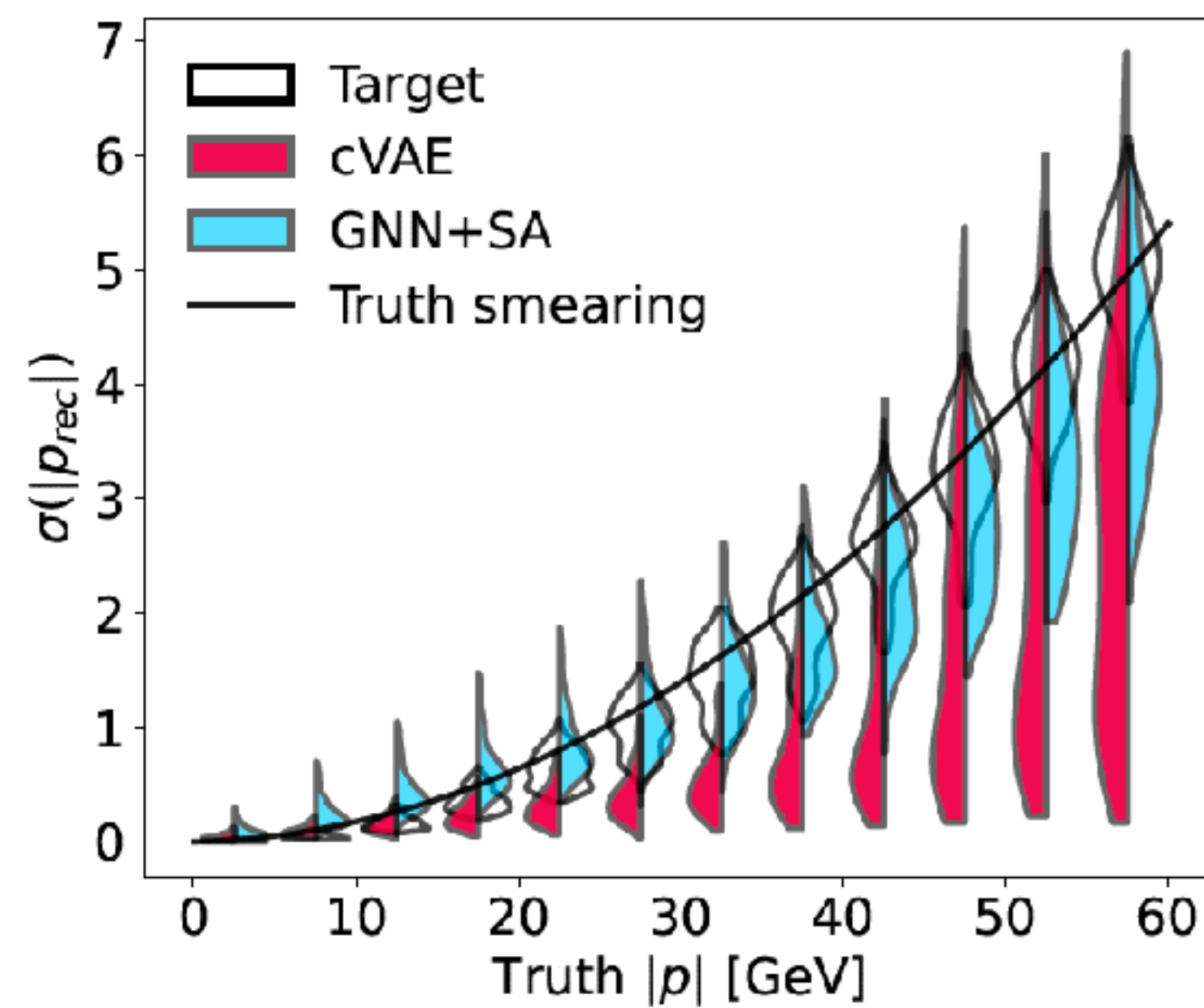
Resolution



(a) $p(N_R|N_T)$



(b) $p(\overline{|p|_R}||p|_T)$



(c) $p(\sigma(|p|_R)||p|_T)$

Conclusion

- Investigated feasibility of set generation via attention-based GNN architecture, using replicas important to learn the resolution
- Marginal distribution well-modeled by baseline (cVAE) and GNN with Slot att, however, 1D distributions can be deceptive
- The GNN+SA model outperforms the baseline model and better captures key properties of the target distribution. It performs better in predicting mean and variance of constituents

Syllabus

✓ Graph Neural Nets

✓ Set to Graph

✓ Attention is all you need

✓ Transformers, ✓ Slot Attention (SA)

✓ Set Prediction Networks with a Transformer and SA (TSPN-SA)

✓ Constrained Variational Auto Encoder (cVAE)

- Particle Flow
(Reconstructing Particles in Jets using TSPN-SA,
Hyper-Graph PFlow [HGPflow])

✓ Simulation of PF Objects (Using TSPN-SA, cVAE)