Deep Learning and Optimization

Unpacking Transformers, LLMs and Diffusion

Session 4

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slack #ensae-dl-2025

Summary of Session 3

Key ingredients to practical deep learning (activation, regularization, normalization, residual networks, etc.)

Recurrent networks struggle to learn long-term dependencies (vanishing gradients) and are slow/inefficient to train (sequential, not parallel, processing)

We learned tensor-based DL and applied it to MNIST.

	Session	Date	Content
Foundations	1	Jan, 28	Intro to DL TP: micrograd
	2	Feb, 4	Fundamentals I: inductive bias, loss functions TP: bigram, MLP for next character prediction
	3	Feb, 11	Fundamentals II: DL architectures TP: tensor-based models
Applications	4	Feb, 18	Attention & Transformers TP: GPT from scratch
	5	Feb, 25	DL for Computer vision TP: convnets on CIFAR-10
	6	Mar, 11	VAE and Diffusion TP: diffusion from scratch Quiz / Exam

The restaurant refused to serve me a ham sandwich because it only cooks vegetarian food. In the end, they just gave me two slices of bread. Their ambiance was just as good as the food and the service.

Query vector q_1
Key vector k_1

The restaurant refused to serve me a ham sandwich because it only cooks vegetarian food. In the end, they just gave me two slices of bread. Their ambiance was just as good as the food and the service.

Query vector q_2
Key vector k_2

Query vector q_1
Key vector k_1

The restaurant refused to serve me a ham sandwich because it only cooks vegetarian food. In the end, they just gave me two slices of bread. Their ambiance was just as good as the food and the service.

Query vector q_2
Key vector k_2

Attention of “restaurant” *onto* “their ambiance”

$q_1 \cdot k_2$

Attention and Transformers

Value vector v_1

Query vector q_1

Key vector k_1

The restaurant refused to serve me a ham sandwich because it only cooks vegetarian food. In the end, they just gave me two slices of bread. Their ambiance was just as good as the food and the service.

Query vector q_2

Key vector k_2

Attention of “restaurant” *onto* “their ambiance”

$q_1 \cdot k_2$

$softmax(q_1 \cdot k_2) \cdot v_1$

Value vector v_1

Query vector q_1

Key vector k_1

The restaurant refused to serve me a ham sandwich because it only cooks vegetarian food. In the end, they just gave me two slices of bread. Their ambiance was just as good as the food and the service.

Query vector q_2

Key vector k_2

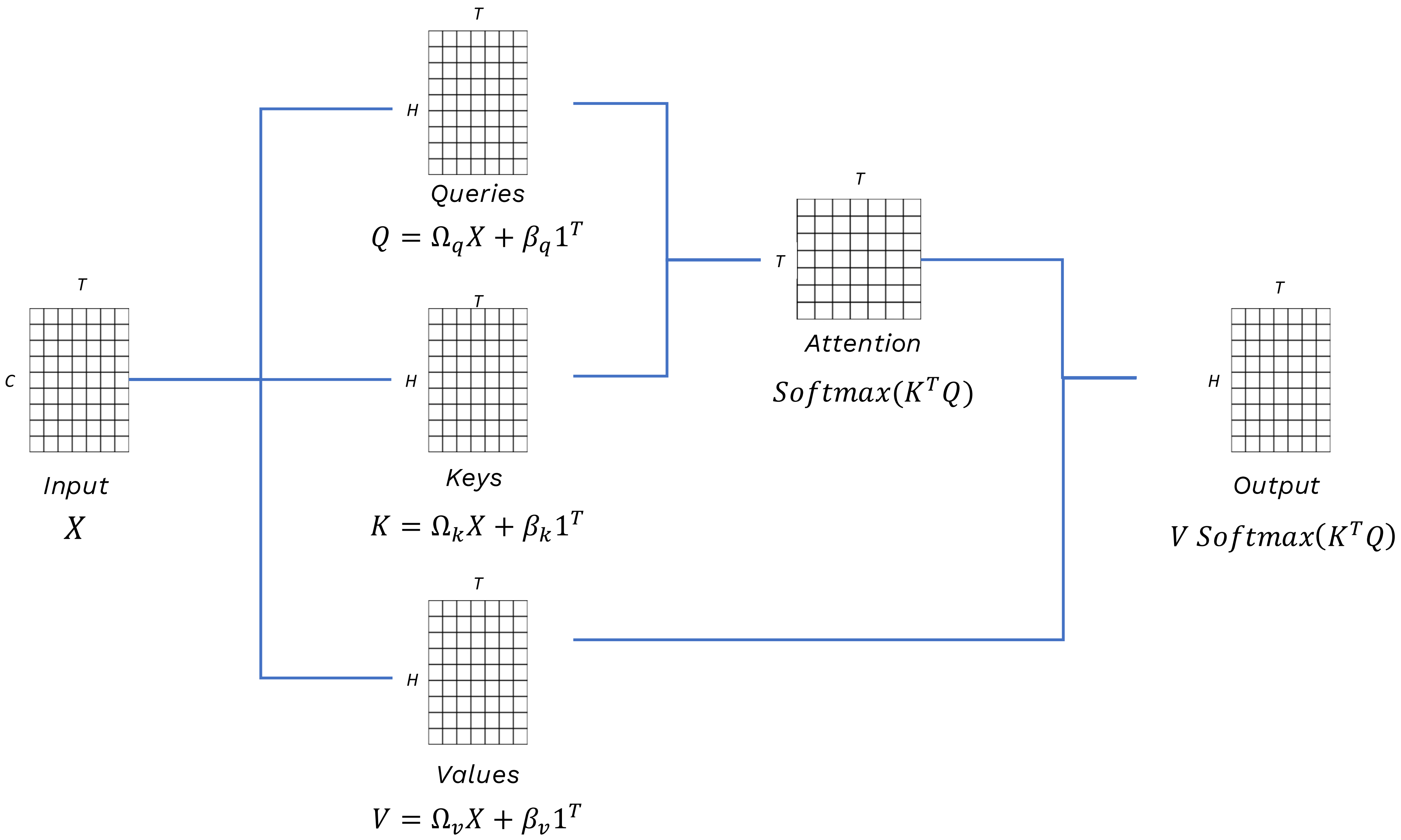
Attention of "restaurant" *onto* "their ambiance"

$q_1 \cdot k_2$

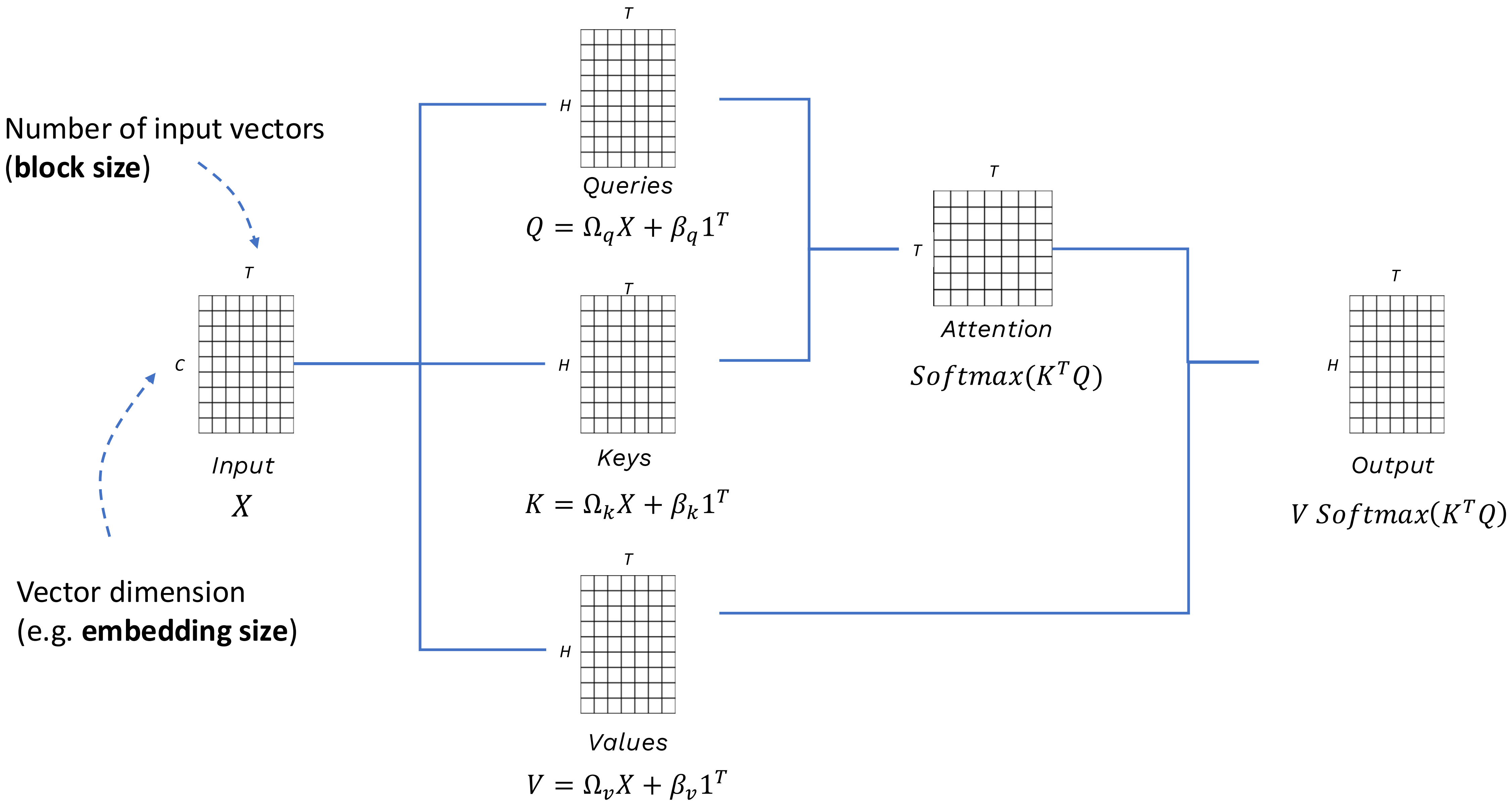
$softmax(q_1 \cdot k_2) \cdot v_1$

Attention is then feed into traditional architectures

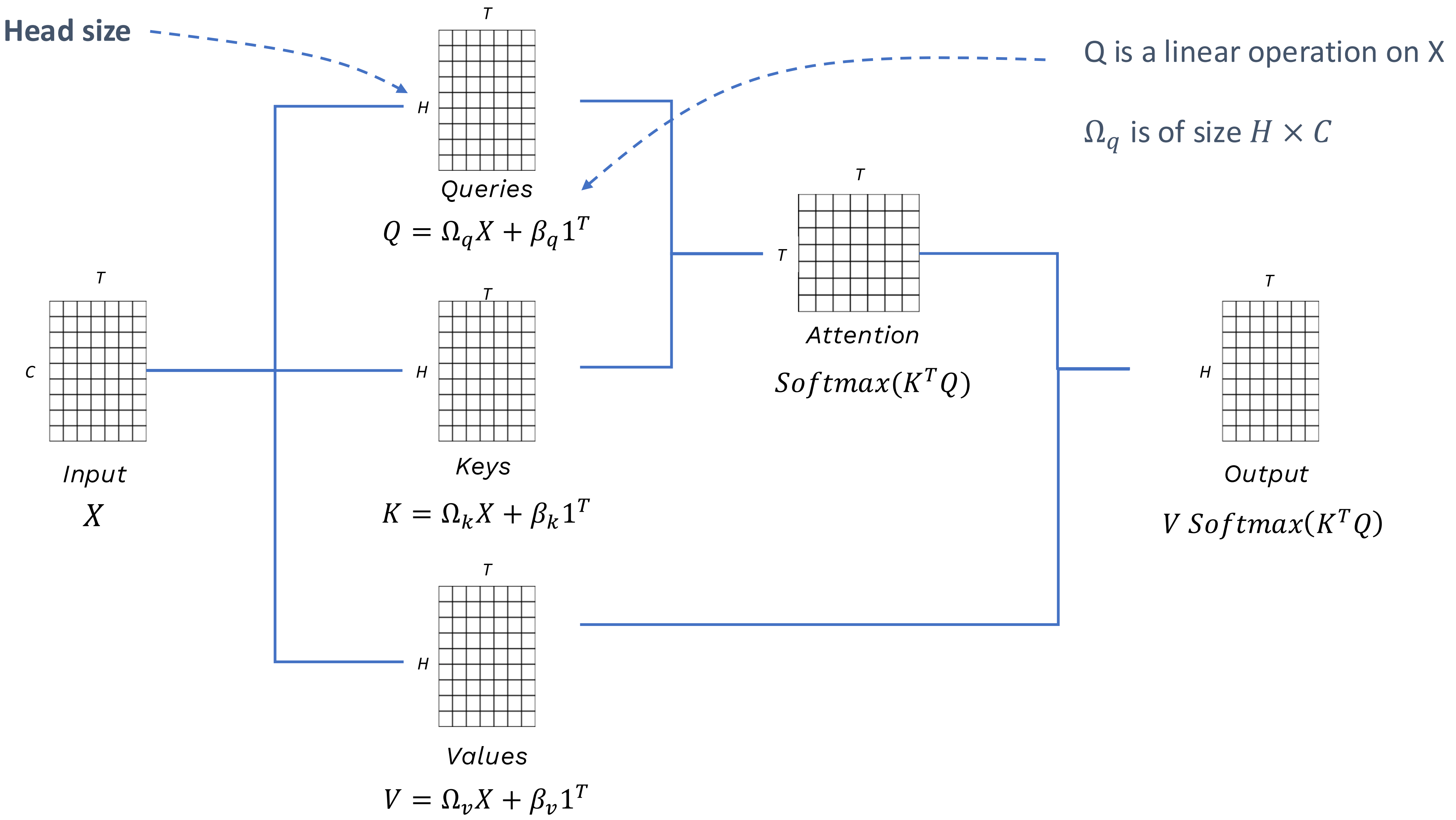
Attention and Transformers



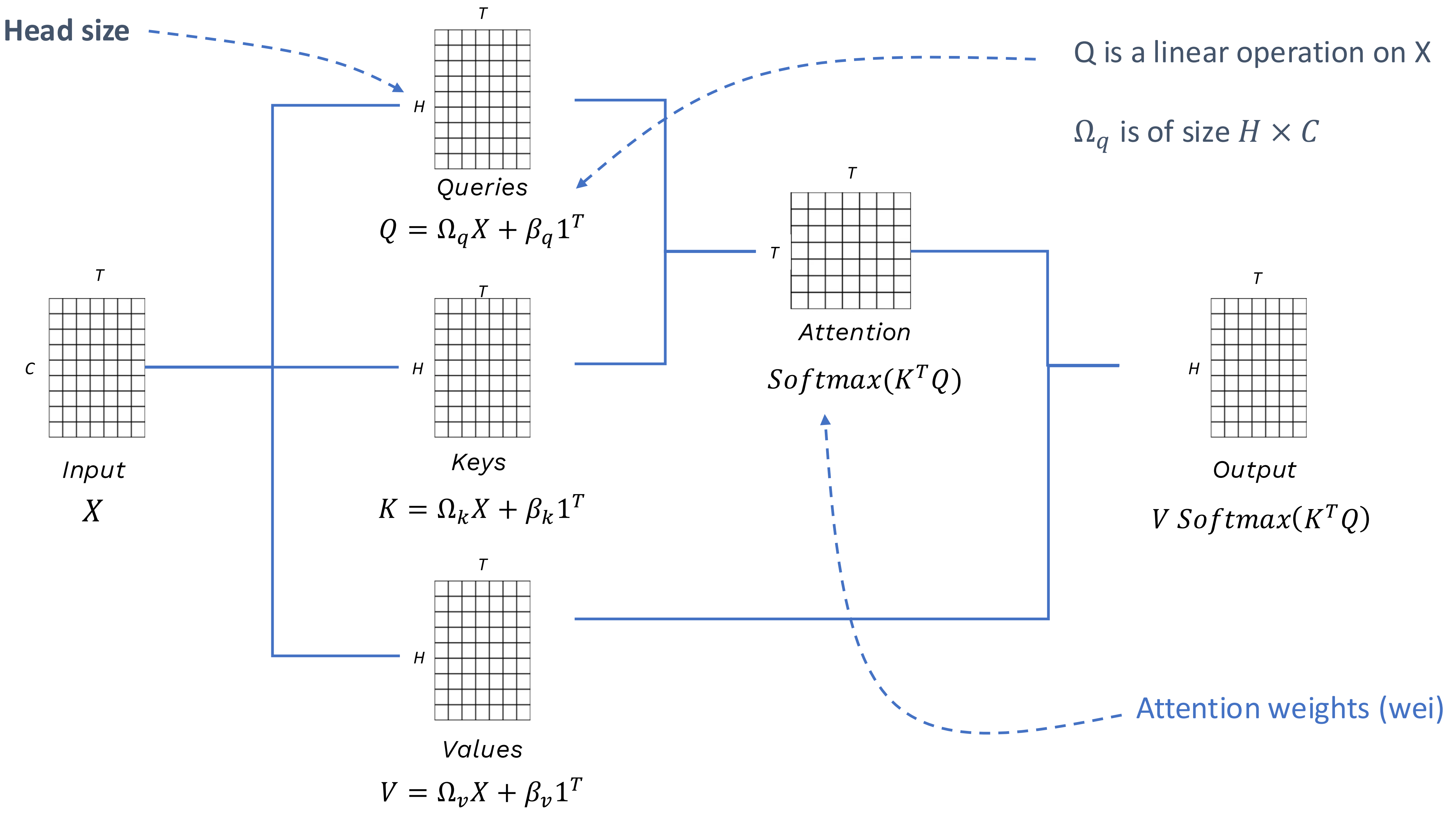
Attention and Transformers

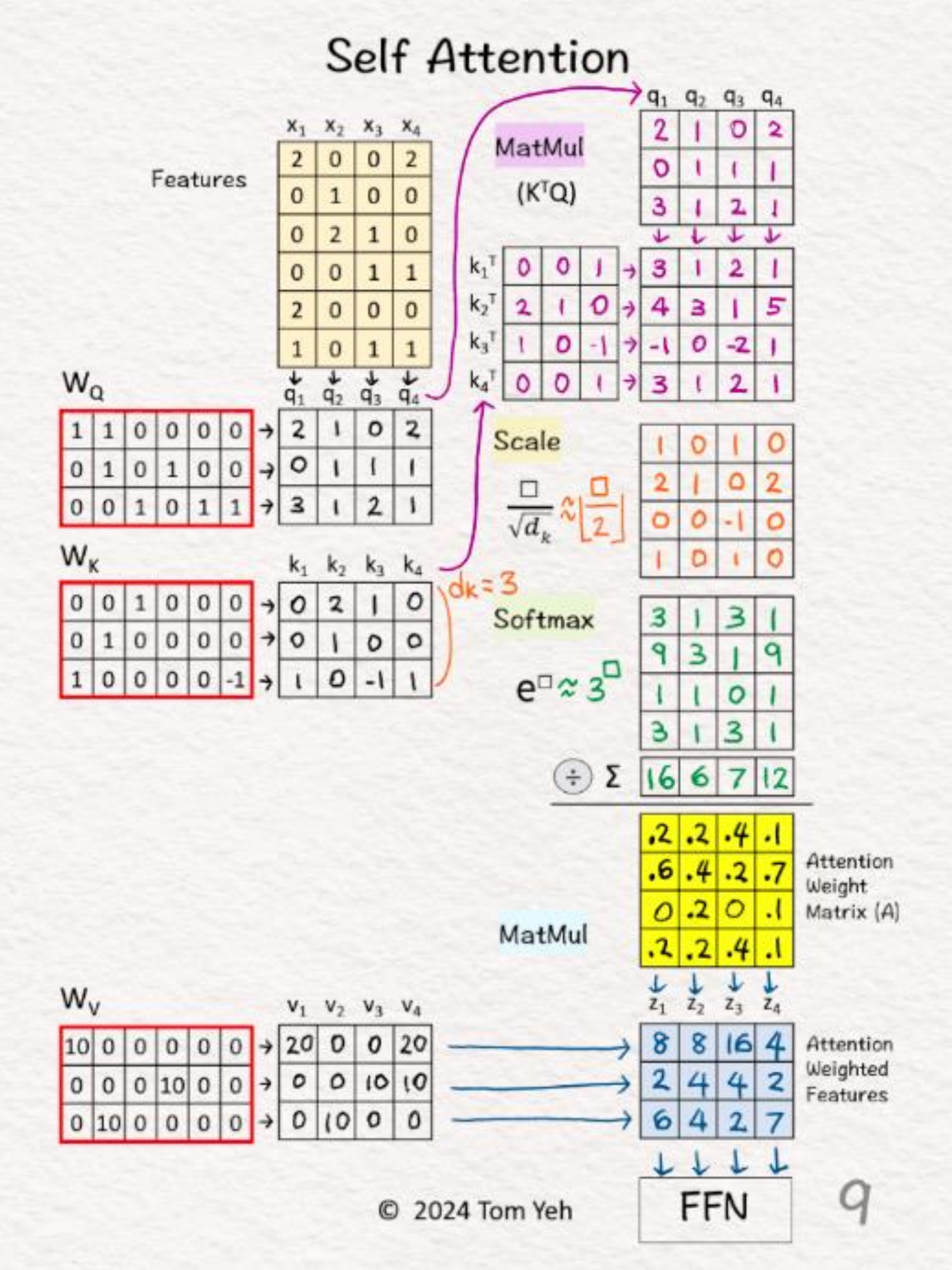


Attention and Transformers



Attention and Transformers





Source: Tom Yeh, 2024

Scaled Dot-Product Self-Attention

$$Sa[X] = V \cdot Softmax\left[\frac{K^T Q}{\sqrt{D_q}}\right]$$

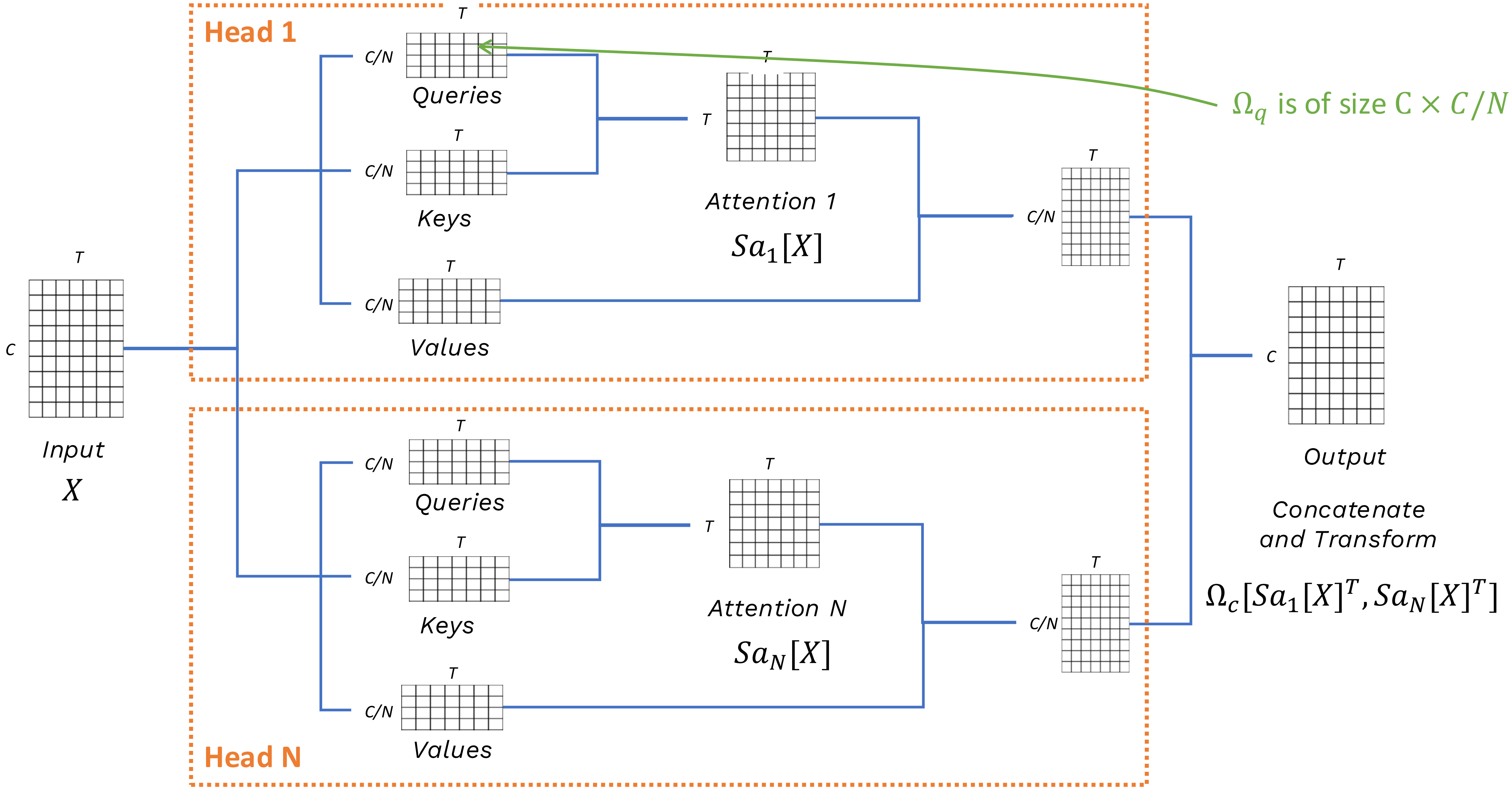
Scaled Dot-Product Self-Attention

$$Sa[X] = V \cdot Softmax\left[\frac{K^T Q}{\sqrt{D_q}}\right]$$

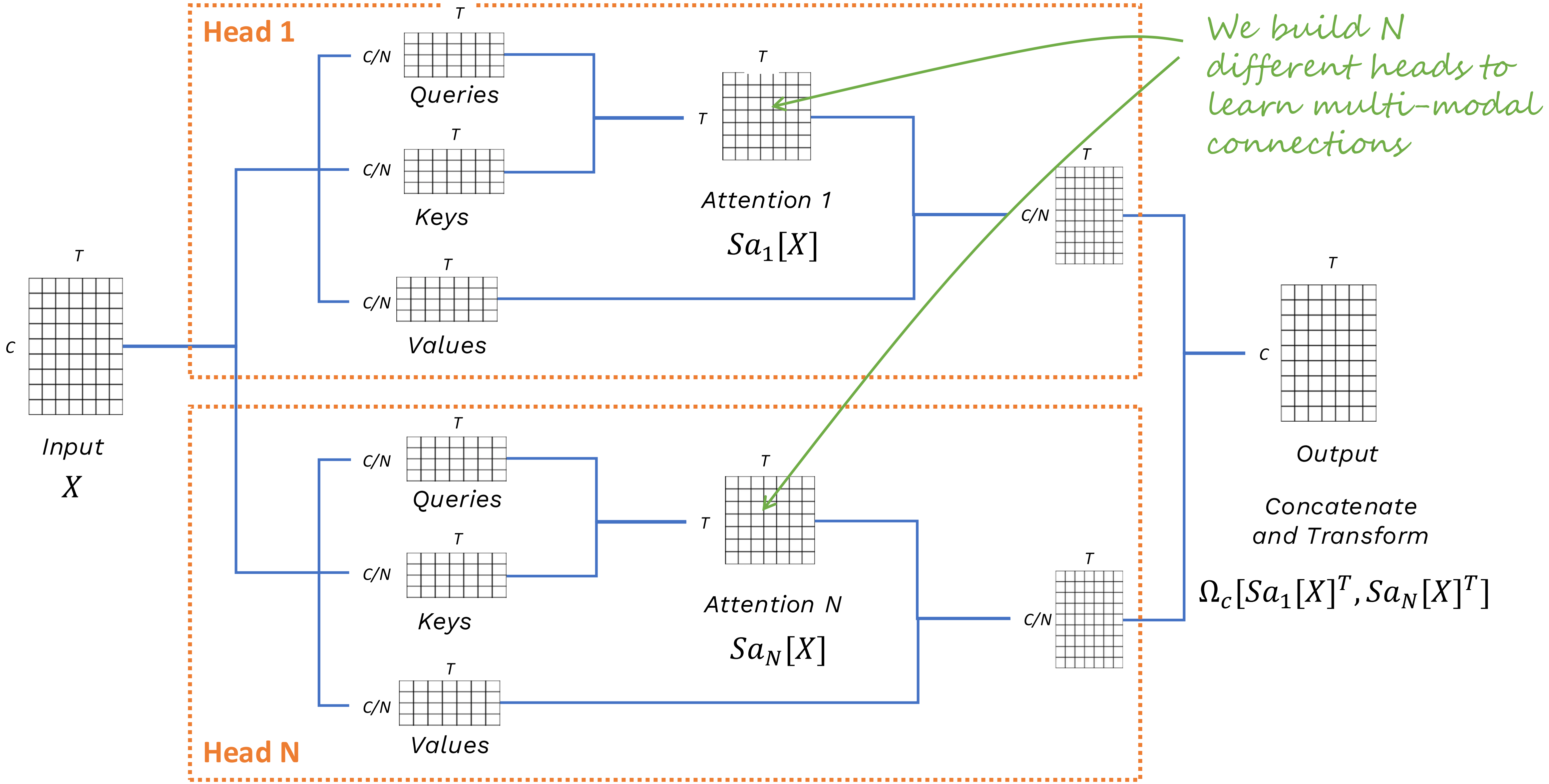
Quadratic in X!

$$Sa[X] = V \cdot Softmax\left[\frac{X^T \Omega_K^T \Omega_Q X}{\sqrt{D_q}}\right]$$

Multi-head attention (for N heads)



Multi-head attention (for N heads)



Multi-head attention (for N heads)

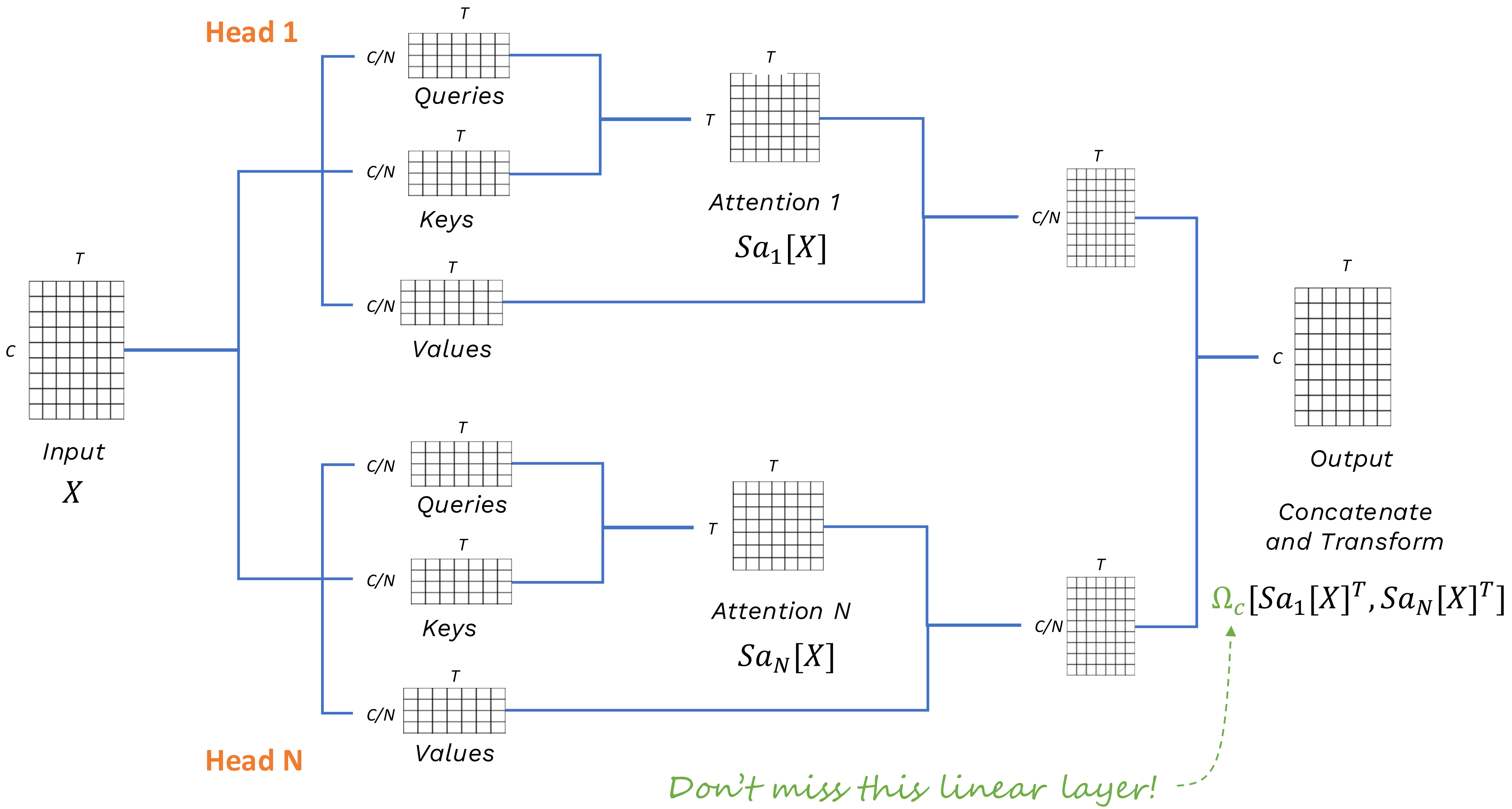
"The cat sat on the mat"

Head 0: syntactic — "sat" attends to "cat" (subject-verb)

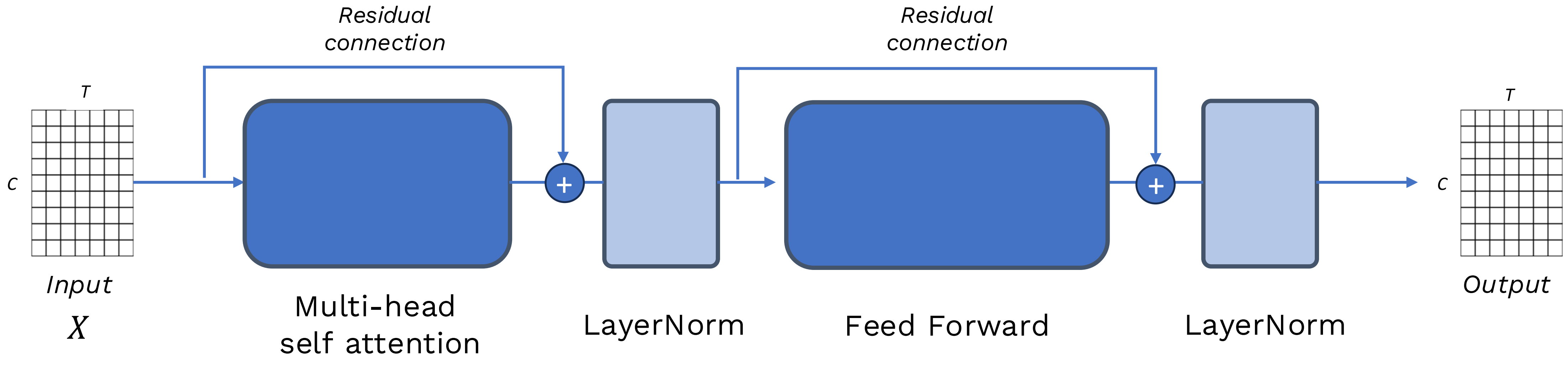
Head 1: positional — "sat" attends to nearby words

Head 2: semantic — "sat" attends to "mat" (related concepts)

Multi-head attention (for N heads)

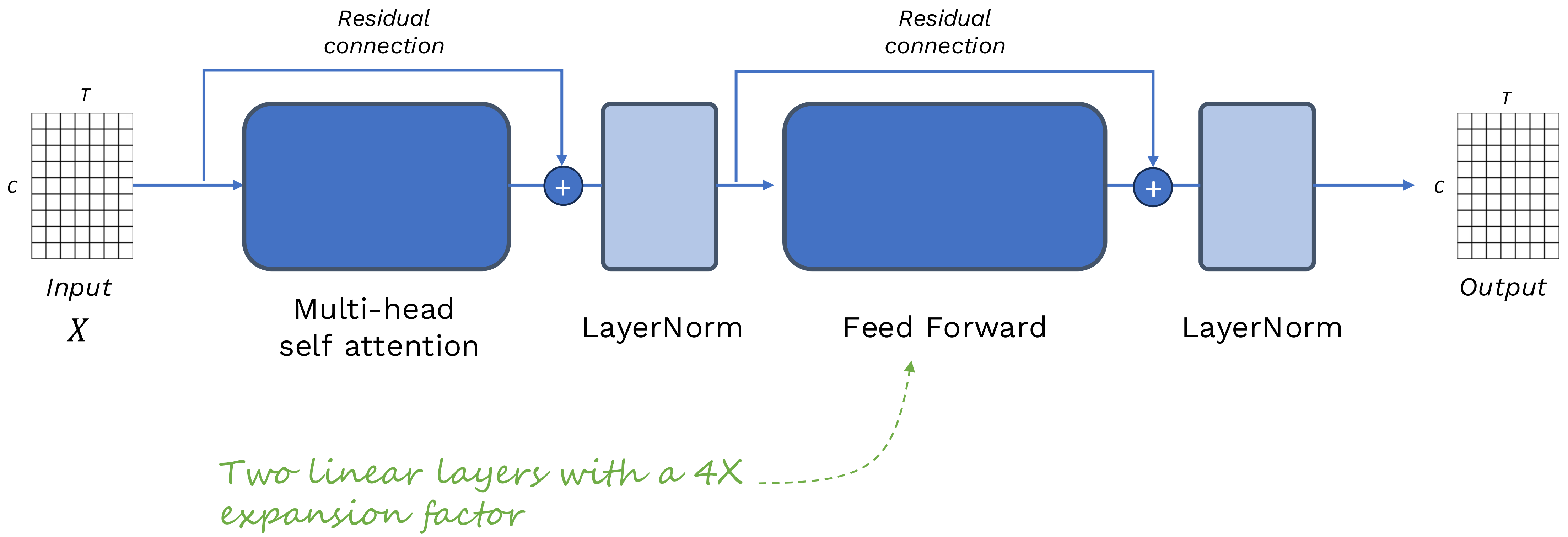


Attention and Transformers



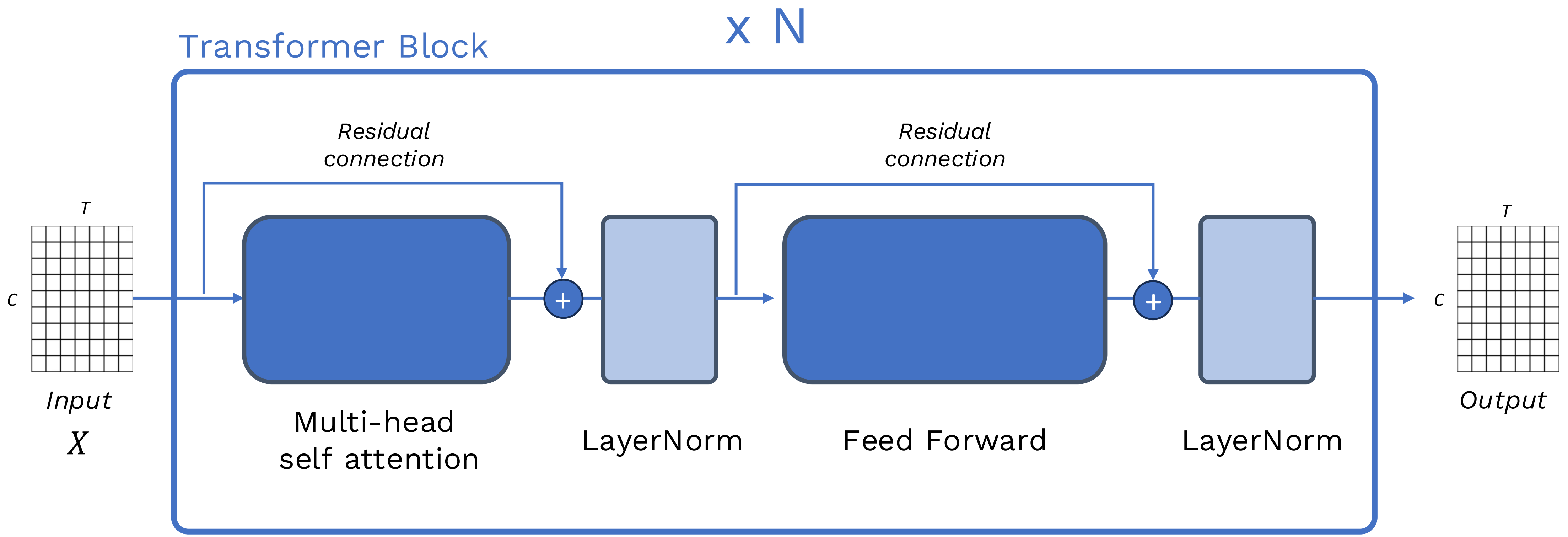
Attention Is All You Need, A. Vaswani et al, NeurIPS 2017

Attention and Transformers



Attention Is All You Need, A. Vaswani et al, NeurIPS 2017

Attention and Transformers



Attention Is All You Need, A. Vaswani et al, NeurIPS 2017

Tokenizing the input

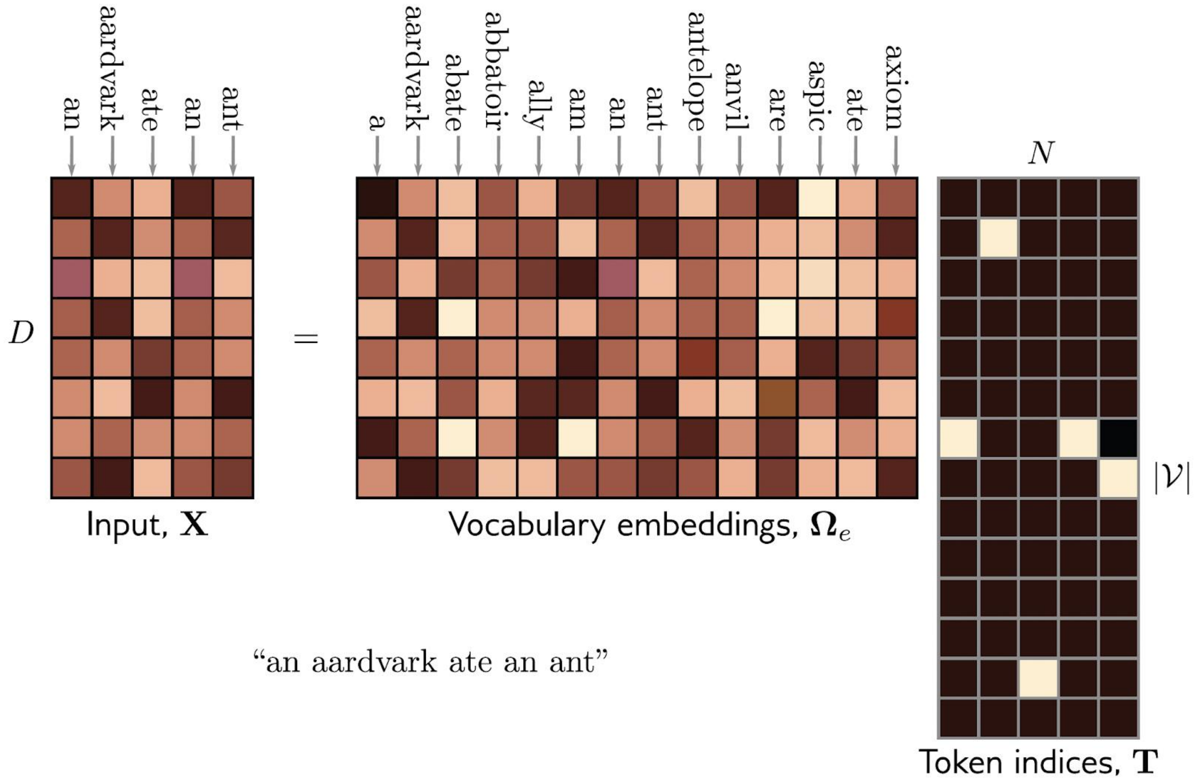
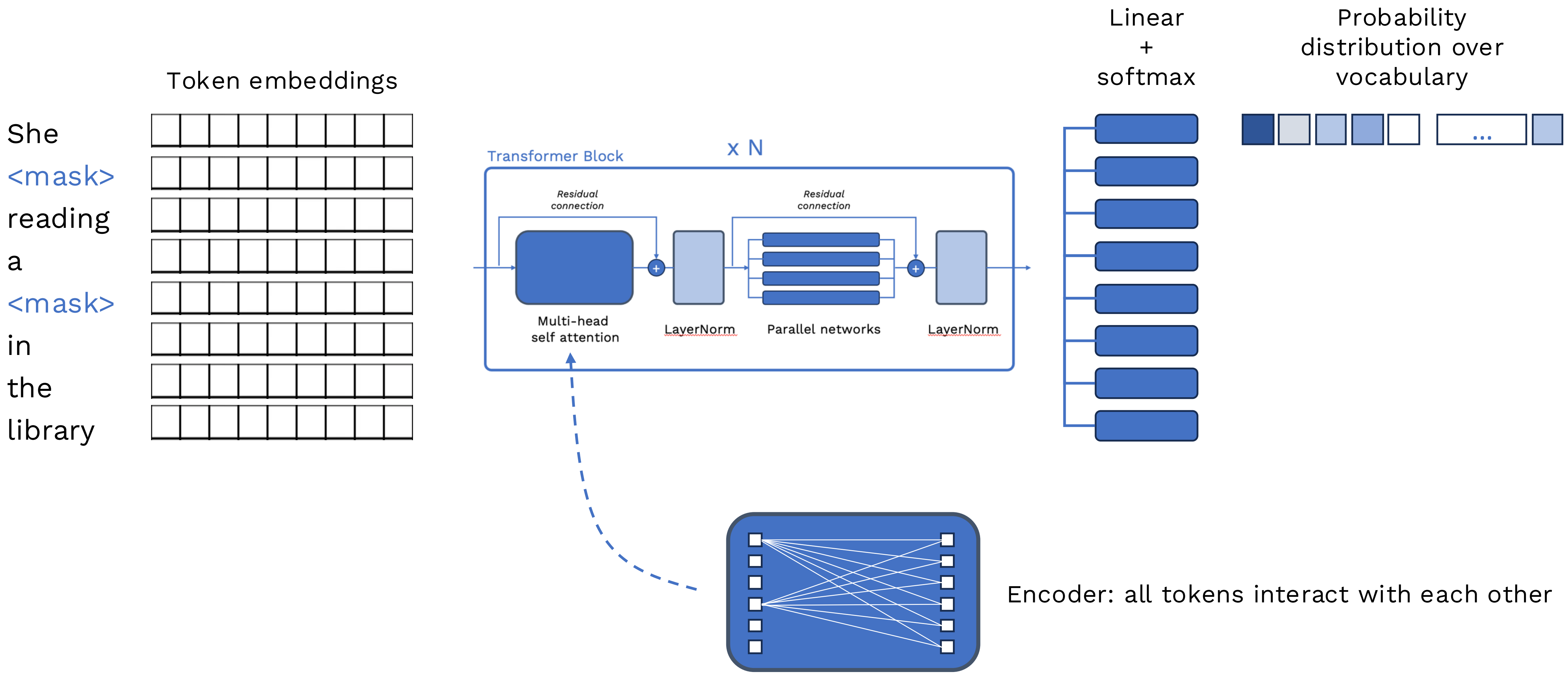


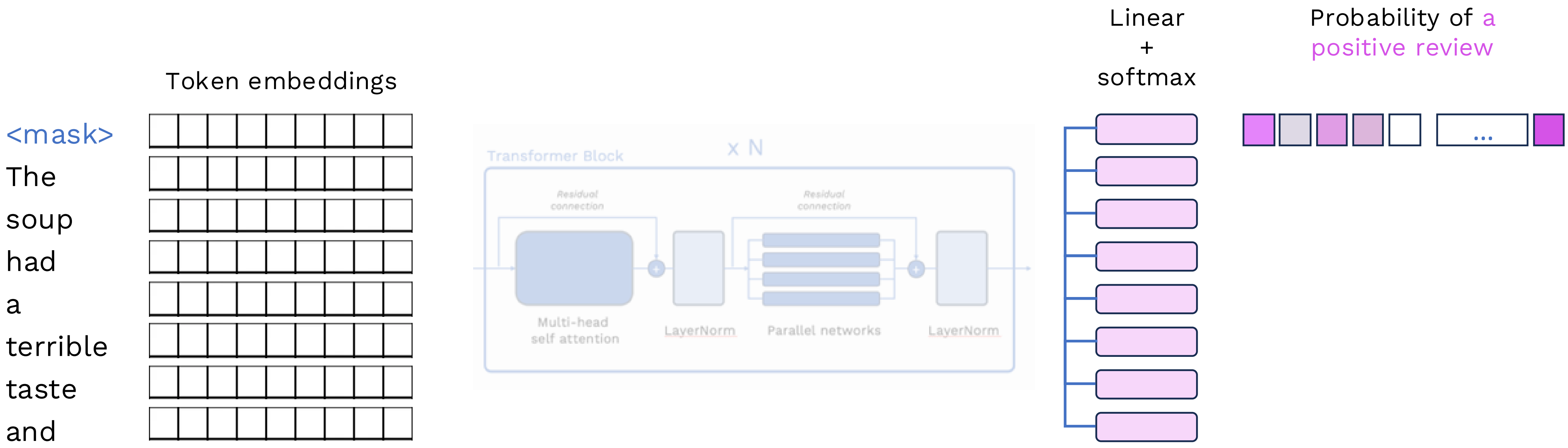
Figure 12.9 The input embedding matrix $\mathbf{X} \in \mathbb{R}^{D \times N}$ contains N embeddings of length D and is created by multiplying a matrix $\boldsymbol{\Omega}_e$ containing the embeddings for the entire vocabulary with a matrix containing one-hot vectors in its columns that correspond to the word or sub-word indices. The vocabulary matrix $\boldsymbol{\Omega}_e$ is considered a parameter of the model and is learned along with the other parameters. Note that the two embeddings for the word an in $\mathbf{X}$ are the same.

Source: Understanding Deep Learning, S. Prince, 2023

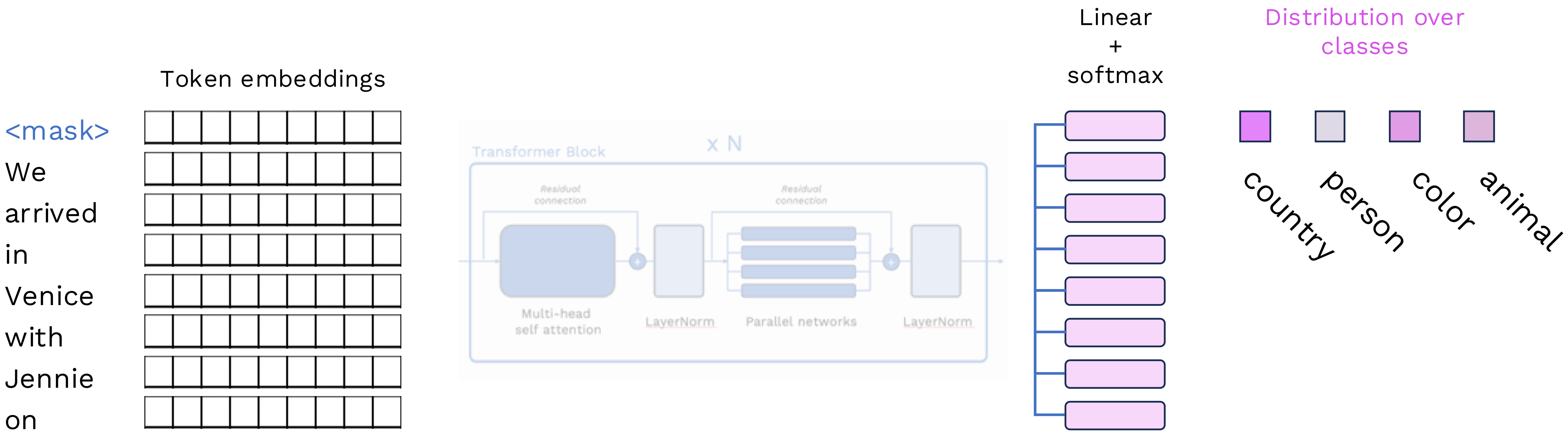
Pretraining for BERT-like encoder



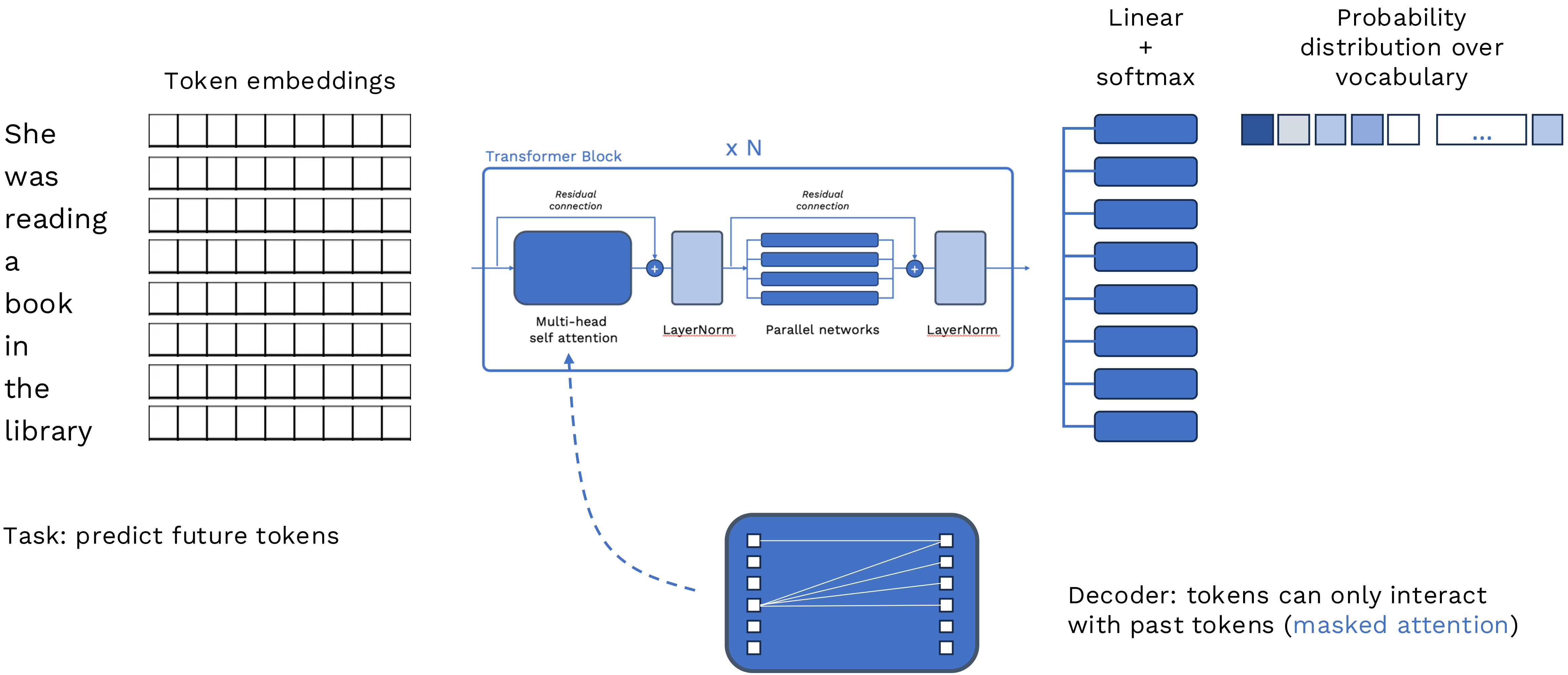
Fine-tuning to specific tasks: review prediction



Fine-tuning to specific tasks: text classification



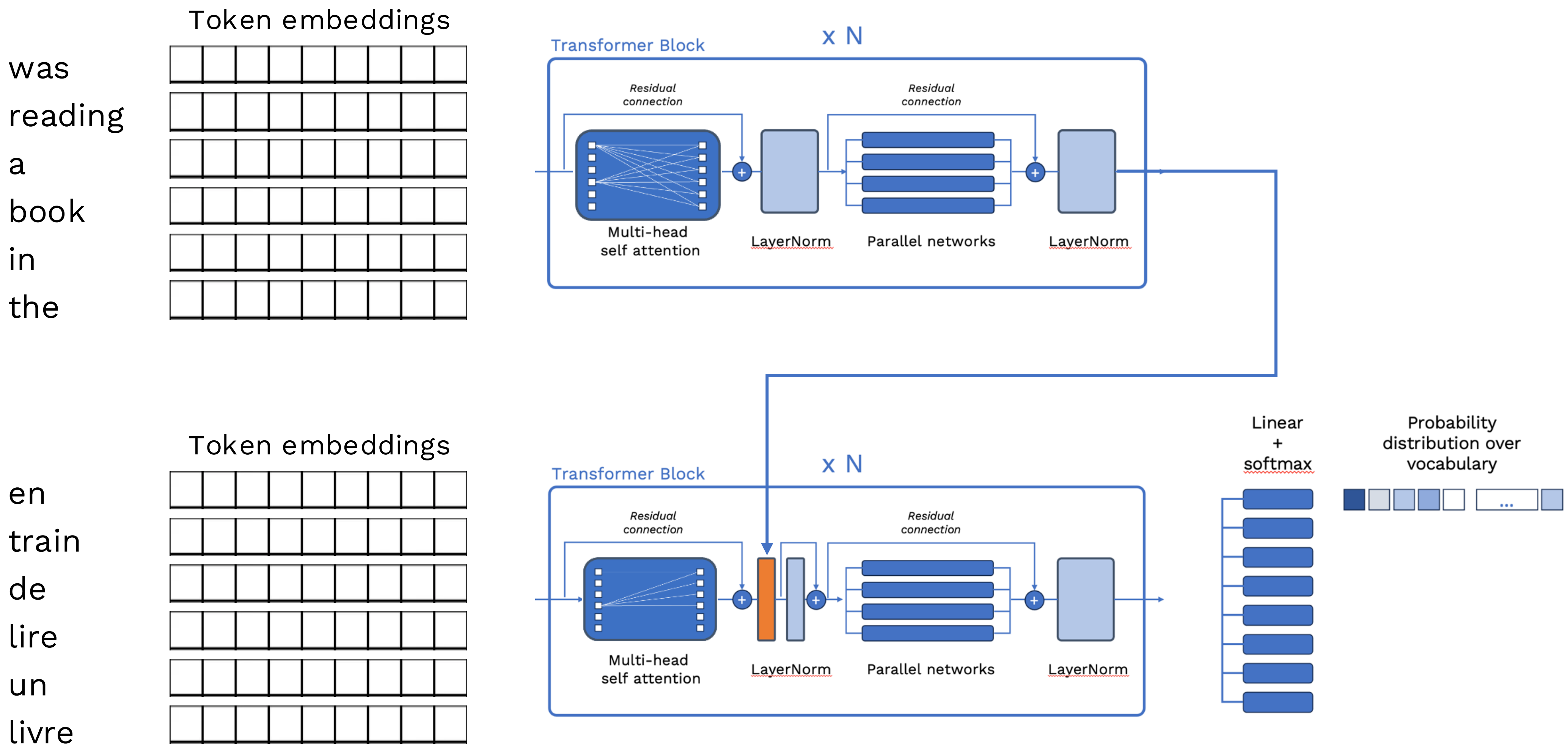
Pretraining for GPT-like decoder



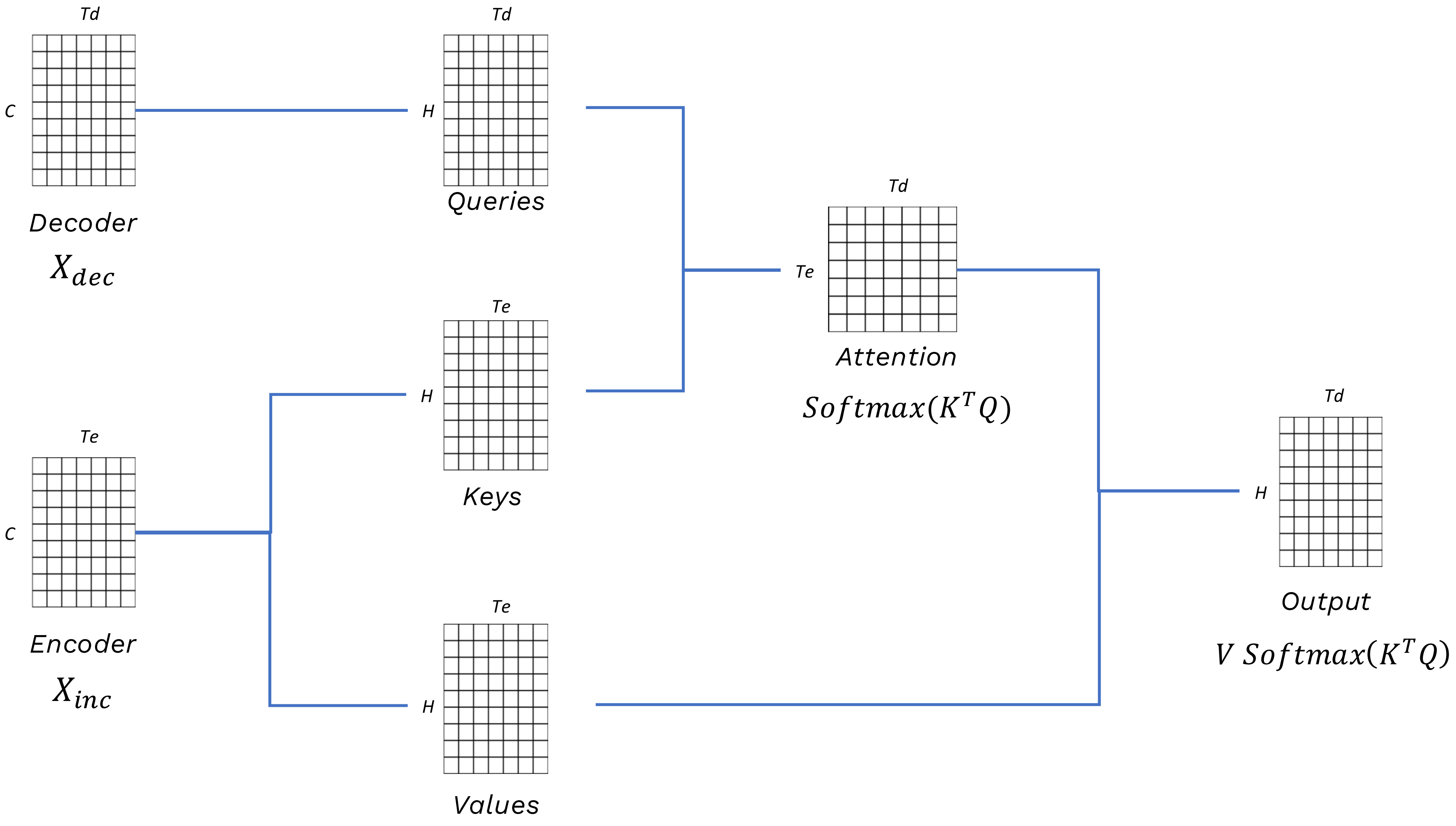
Task: predict future tokens

Decoder: tokens can only interact with past tokens (masked attention)

Encoder-decoder architecture for translation with cross-attention



Cross-attention



The original Transformer architecture

Encoder

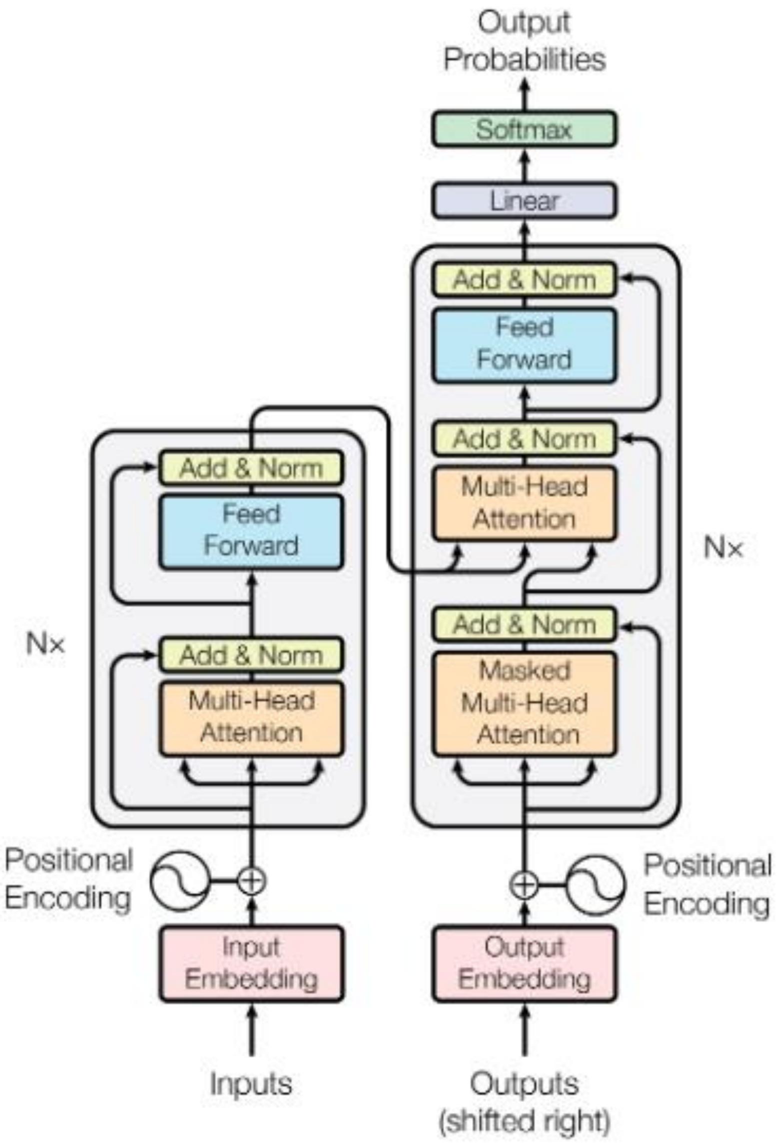


Figure 1: The Transformer - model architecture.

Decoder

Source: Attention is All you Need

Positional encoding

Encodes the relative position of tokens in the block

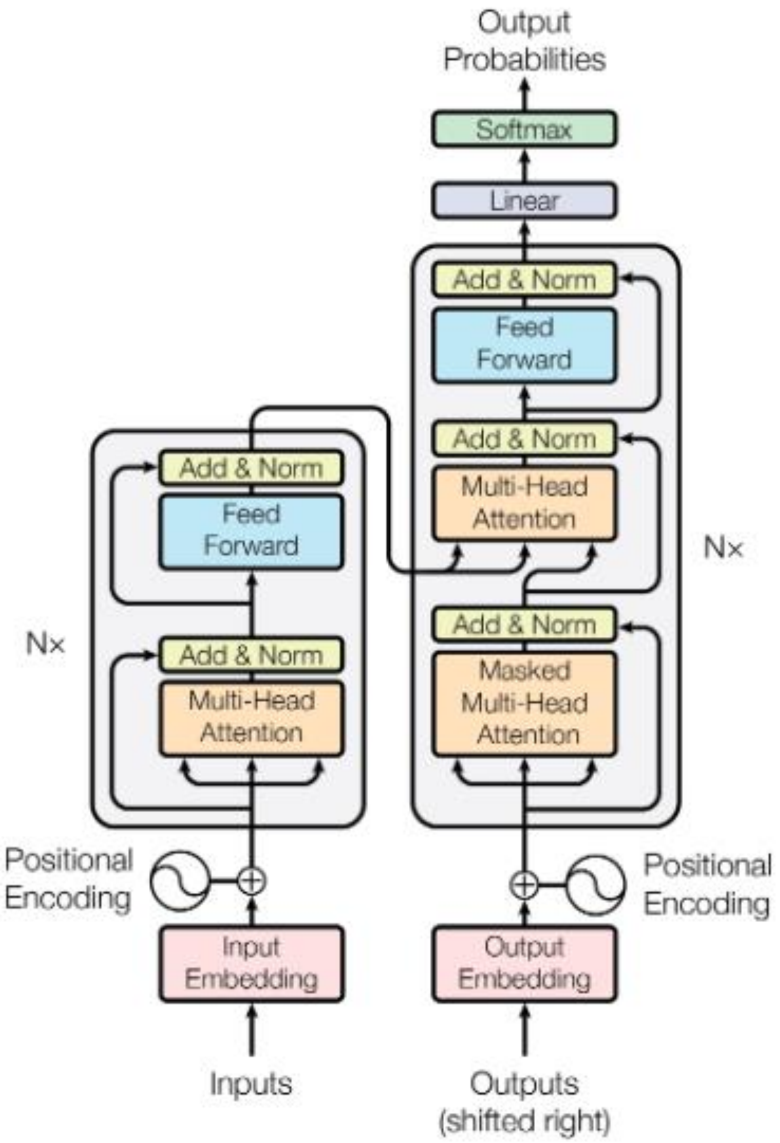
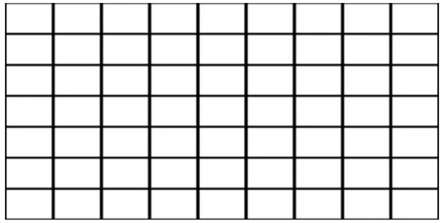


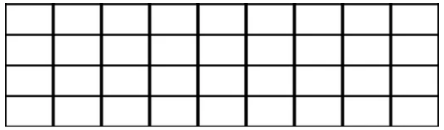
Figure 1: The Transformer - model architecture.

Vocabulary embedding table



embedding size x vocab size

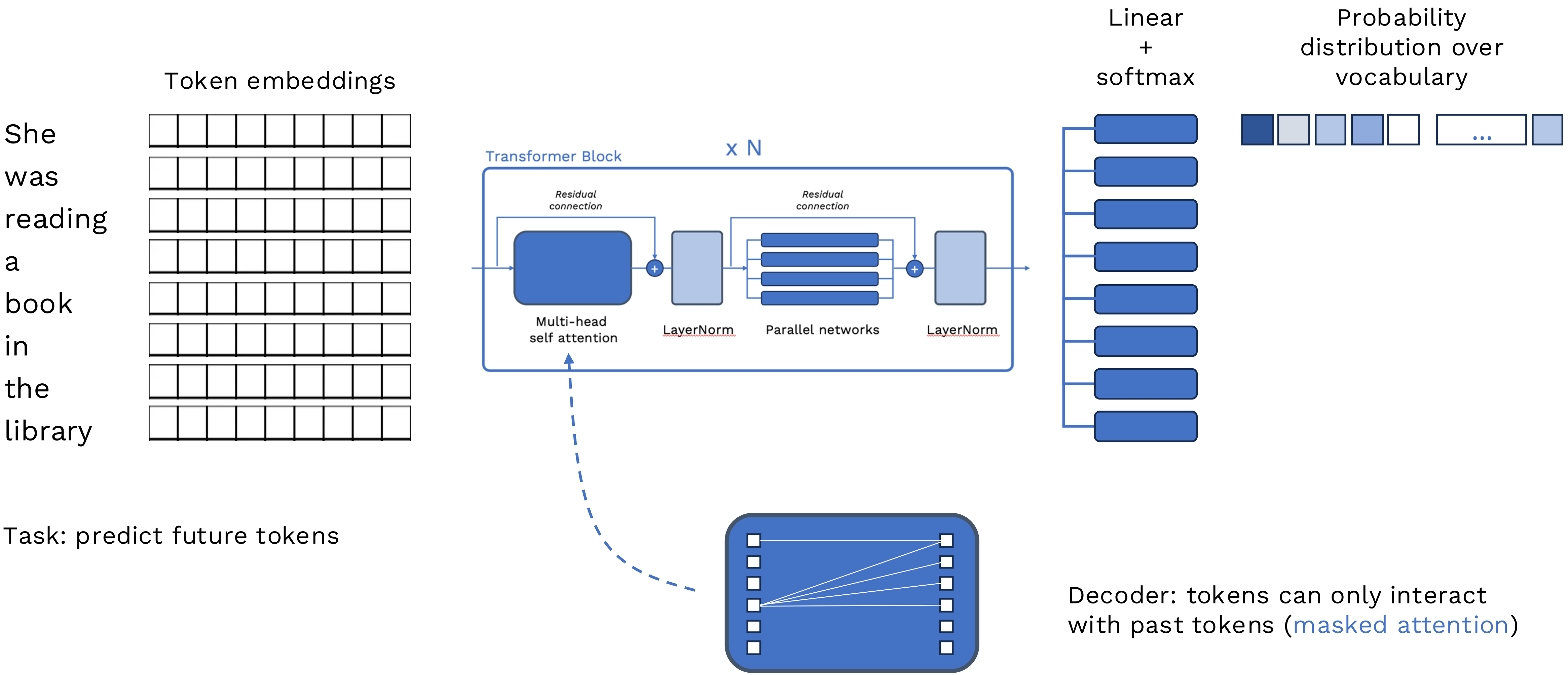
Position embedding table



embedding size x block size

Source: Attention is All you Need

Practical 4: Let’s build a GPT-like encoder!



Task: predict future tokens

Decoder: tokens can only interact with past tokens (masked attention)

Dataset generation

First, you know Caius Marcius is chief enemy to the people.

18 47 56 57 22 13

Dataset generation

	18	47	56	57	22	13
	22	31	82	16	46	81
Batch	46	36	32	82	10	11
	74	59	82	91	60	38
	27	21	37	26	42	18

Dataset generation

	X						Y					
	18	47	56	57	22	13	47	56	57	22	13	42
	22	31	82	16	46	81	31	82	16	46	81	32
Batch	46	36	32	82	10	11	36	32	82	10	11	69
	74	59	82	91	60	38	59	82	91	60	38	41
	27	21	37	26	42	18	21	37	26	42	18	77

Dataset generation

Example 1

	X						Y					
	$\boxed{18}$	47	56	57	22	13	$\boxed{47}$	56	57	22	13	42
	22	31	82	16	46	81	31	82	16	46	81	32
Batch	46	36	32	82	10	11	36	32	82	10	11	69
	74	59	82	91	60	38	59	82	91	60	38	41
	27	21	37	26	42	18	21	37	26	42	18	77

Dataset generation

Example 2

Batch	X						Y					
	$\boxed{18 \quad 47}$		56	57	22	13	47	$\boxed{56}$	57	22	13	42
	22	31	82	16	46	81	31	82	16	46	81	32
	46	36	32	82	10	11	36	32	82	10	11	69
	74	59	82	91	60	38	59	82	91	60	38	41
	27	21	37	26	42	18	21	37	26	42	18	77

Dataset generation

Example 3

	X						Y					
	$\boxed{18 \quad 47 \quad 56}$			57	22	13	47	56	$\boxed{57}$	22	13	42
	22	31	82	16	46	81	31	82	16	46	81	32
Batch	46	36	32	82	10	11	36	32	82	10	11	69
	74	59	82	91	60	38	59	82	91	60	38	41
	27	21	37	26	42	18	21	37	26	42	18	77

Dataset generation

Example 7

	X						Y					
	18	47	56	57	22	13	47	56	57	22	13	42
	22	31	82	16	46	81	31	82	16	46	81	32
Batch	46	36	32	82	10	11	36	32	82	10	11	69
	74	59	82	91	60	38	59	82	91	60	38	41
	27	21	37	26	42	18	21	37	26	42	18	77

Dataset generation

	X						Y					
	18	47	56	57	22	13	47	56	57	22	13	42
	22	31	82	16	46	81	31	82	16	46	81	32
Batch	46	36	32	82	10	11	36	32	82	10	11	69
	74	59	82	91	60	38	59	82	91	60	38	41
	27	21	37	26	42	18	21	37	26	42	18	77

Example 30

Dataset generation

X

	18	47	56	57	22	13
	22	31	82	16	46	81
Batch	46	36	32	82	10	11
	74	59	82	91	60	38
	27	21	37	26	42	18

Dataset generation

X

	18	47	56	57	22	13
	22	31	82	16	46	81
Batch	46	36	32	82	10	11
(B)	74	59	82	91	60	38
	27	21	37	26	42	18

Time (T) →

Embedding (”channel”)

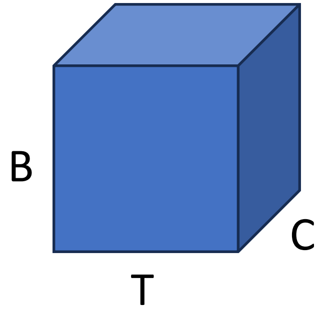
(C)

Dataset generation

X

	18	47	56	57	22	13
	22	31	82	16	46	81
Batch	46	36	32	82	10	11
(B)	74	59	82	91	60	38
	27	21	37	26	42	18

Time (T)



A batch is a 3D tensor

Embedding ("channel")

(C)

Tensor computation

```
ones = torch.zeros(2, 2) + 1

twos = torch.ones(2, 2) * 2

threes = (torch.ones(2, 2) * 7 - 1) / 2

fours = twos ** 2

sqrt2s = twos ** 0.5
```

Tensor computation

```
powers2 = twos ** torch.tensor([[1, 2], [3, 4]])

fives = ones + fours

dozens = threes * fours
```

```
tensor([[ 2.,  4.],
        [ 8., 16.]])
```

Tensor computation

```
a = torch.rand((2,4,3))

a.transpose()
```

Tensor computation

```
a = torch.rand((2,4,3))

a.transpose()
```

TypeError: transpose() received an invalid combination of arguments

Tensor computation

```
a = torch.rand((2,4,3))

a.transpose(-2, -1)

a.shape
```

```
torch.Size([2, 3, 4])
```

Tensor computation

```
a = torch.rand(2, 3)
b = torch.rand(3, 2)

print(a * b)
```

Tensor computation

```
a = torch.rand(2, 3)
b = torch.rand(3, 2)

print(a * b)
```

RuntimeError: The size of tensor a (3) must match the size of tensor b (2) at non-singleton dimension 1

Tensor computation

```
a = torch.rand(2, 3)
b = torch.rand(3, 2)

print(a @ b)
```

This works!

@ is for matrix multiplication

* is for element-wise multiplication

Tensor broadcasting

```
a = torch.rand(2, 3)
b = torch.rand(1, 3)

print(a * b)
```

This works!

Tensor broadcasting

```
a = torch.tensor([[1, 2, 1], [2, 5, 1]])
b = torch.ones(1, 3) + 1

print(a * b)

tensor([[ 2.,  4.,  2.],
        [ 4., 10.,  2.]])
```

Tensor broadcasting

Brodcasting rules:

Comparing the dimension sizes of the two tensors, going from last to first:

- Each dimension must be equal, or
- One of the dimensions must be of size 1, or
- The dimension does not exist in one of the tensors

Tensor computation

```
a = torch.rand(5, 4, 3)
b = torch.rand(1, 3, 6)

print(a @ b)
```

Tensor computation

```
a = torch.rand(5, 4, 3)
b = torch.rand(1, 3, 6)

print(a @ b)
```

This works!

Tensor computation

```
a = torch.rand(1, 5, 4, 3)
b = torch.rand(3, 1, 3, 6)

print(a @ b)
```

Tensor computation

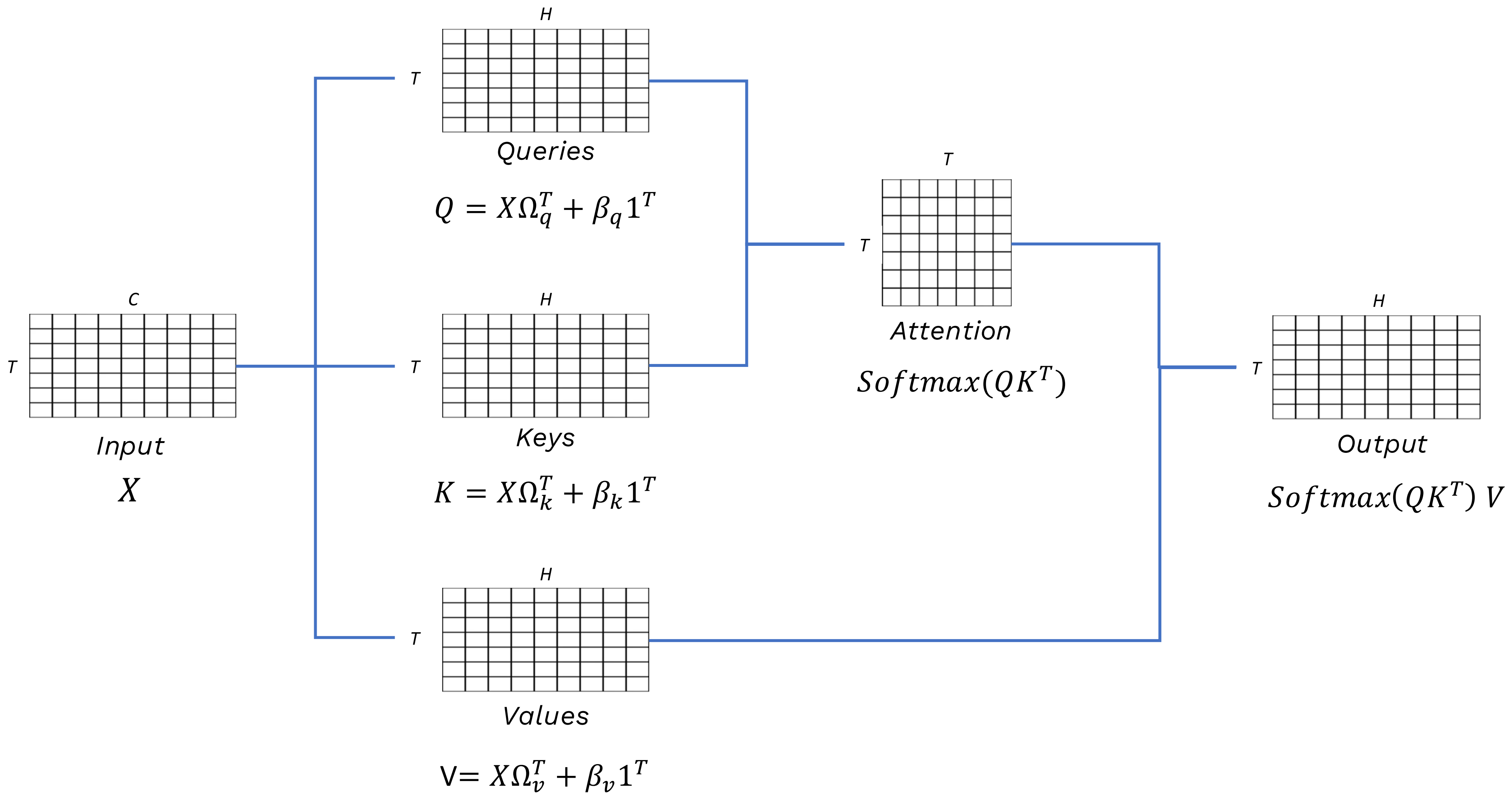
```
a = torch.rand(1, 5, 4, 3)
b = torch.rand(3, 1, 3, 6)

print(a @ b)
```

This works!

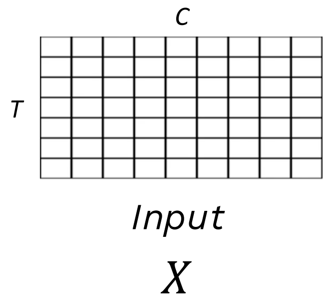
Tensor computation

```
xbow = wei @ x  # (B, T, T) x (B, T, C) --> (B, T, C)
```

In a pytorch implementation, the last two dimensions are inverted!

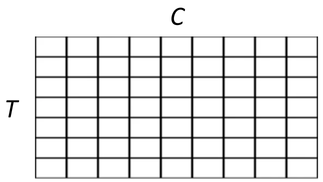


In a pytorch implementation, the last two dimensions are inverted!



This is because pytorch is channel-last for memory optimization.

In a pytorch implementation, the last two dimensions are inverted!



Input

X

A linear layer nn.Linear(in, out) implements:

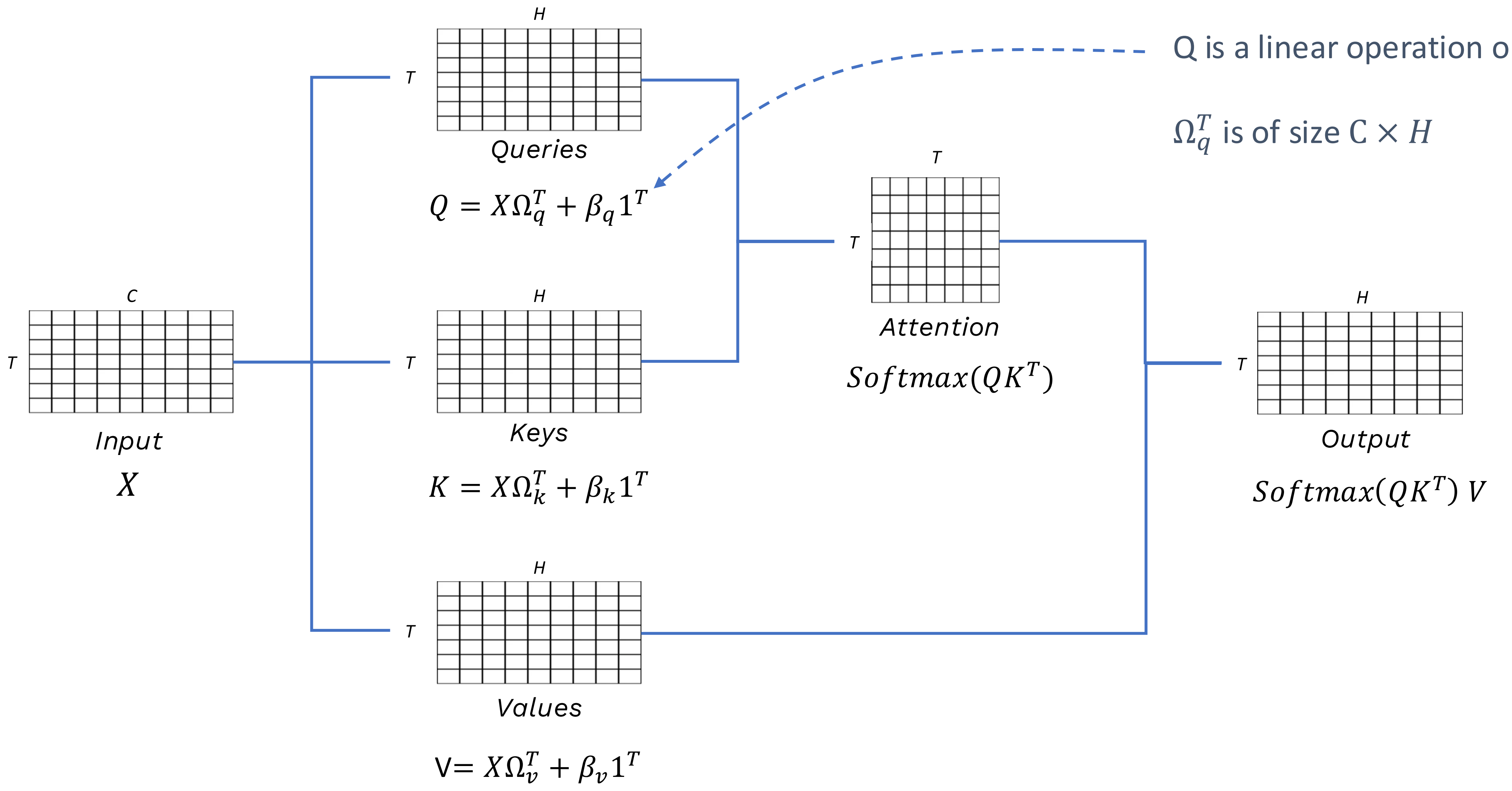
$$y = x.A^T + b$$

and not

$$y = A.x + b$$

Therefore the shape of A is (out, in)

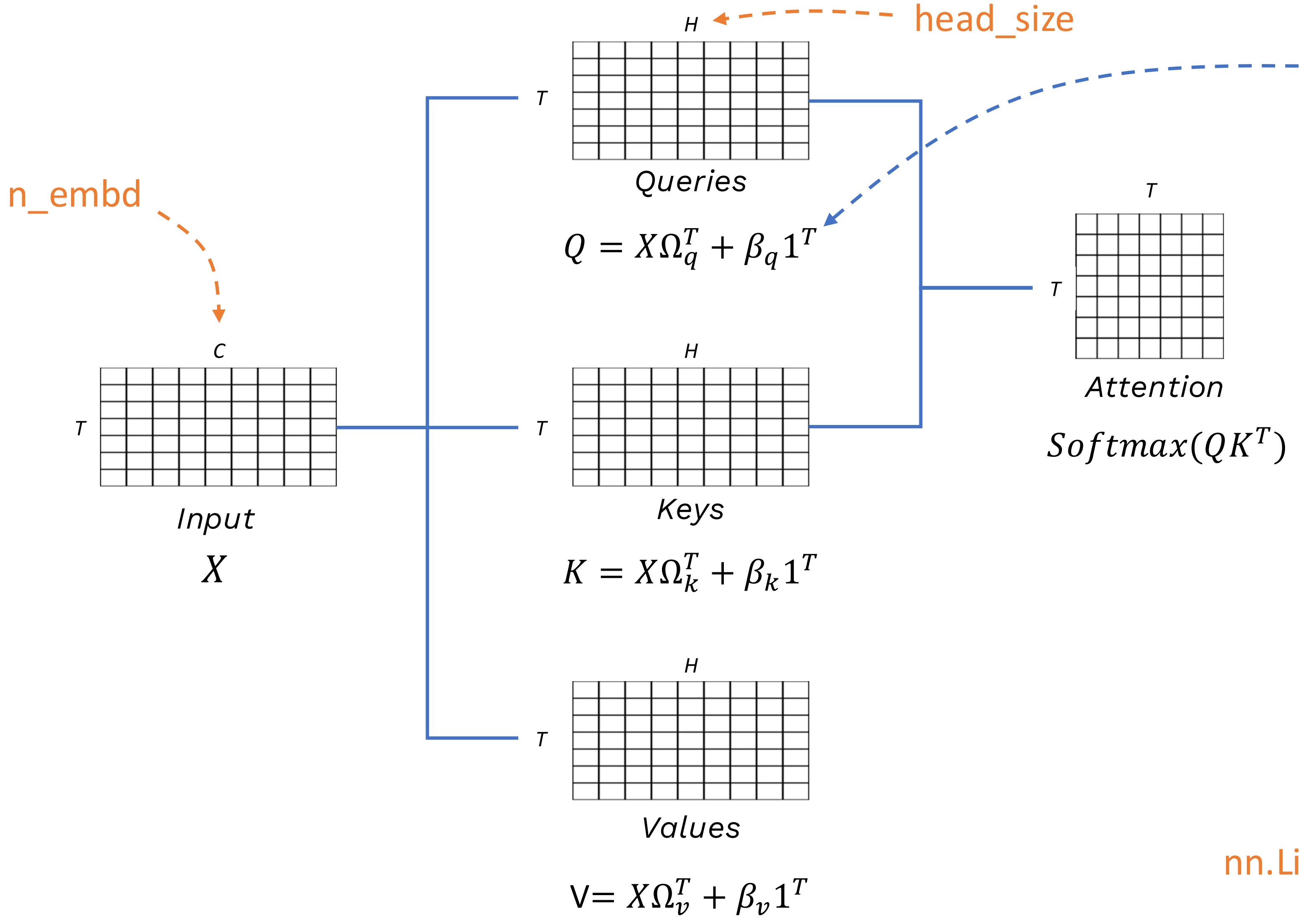
In a pytorch implementation, the last two dimensions are inverted!



Q is a linear operation on X

Ω_q^T is of size $\mathrm{C} \times H$

In a pytorch implementation, the last two dimensions are inverted!



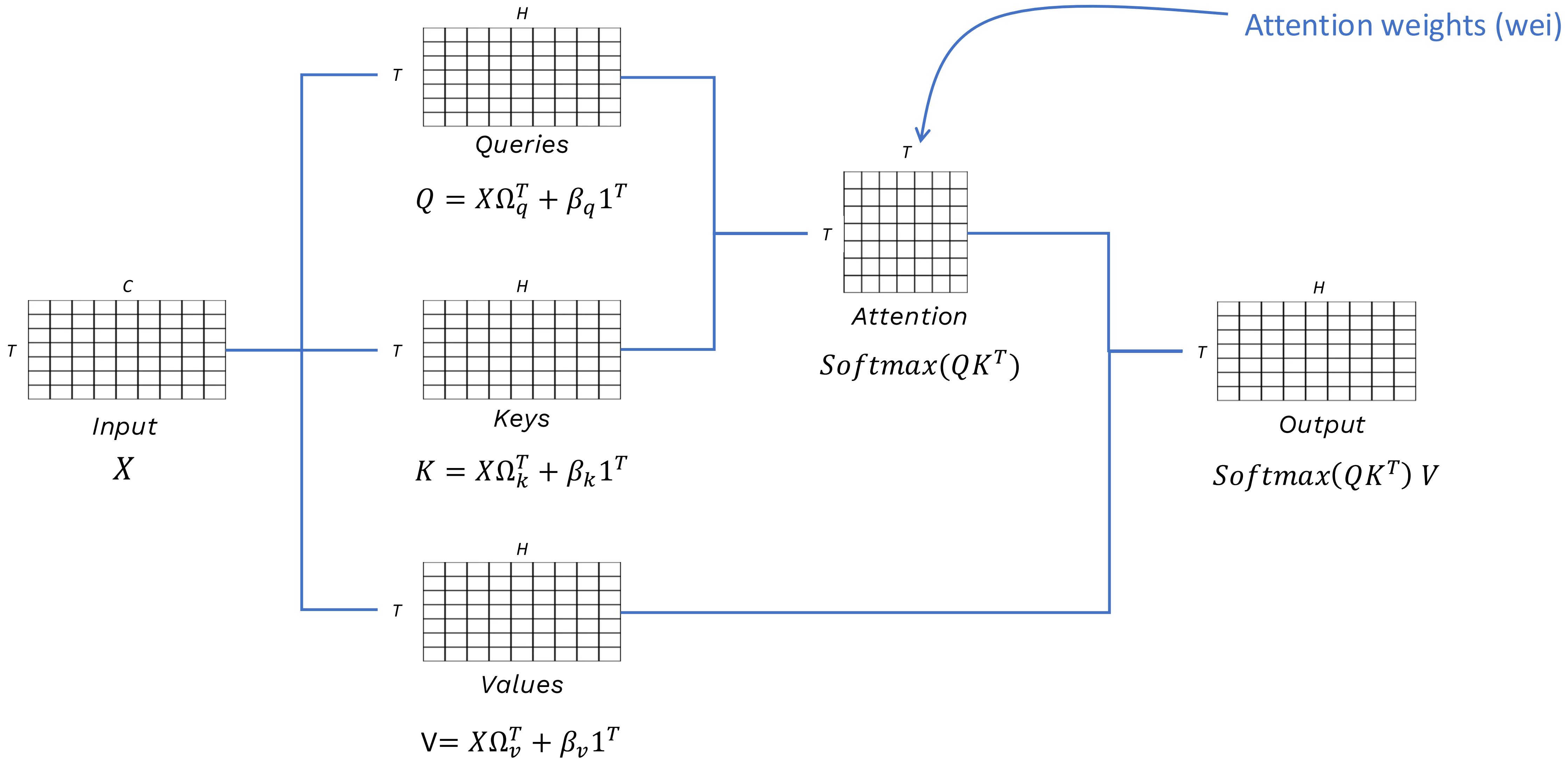
Q is a linear operation on X

Ω_q^T is of size C $\times$ H

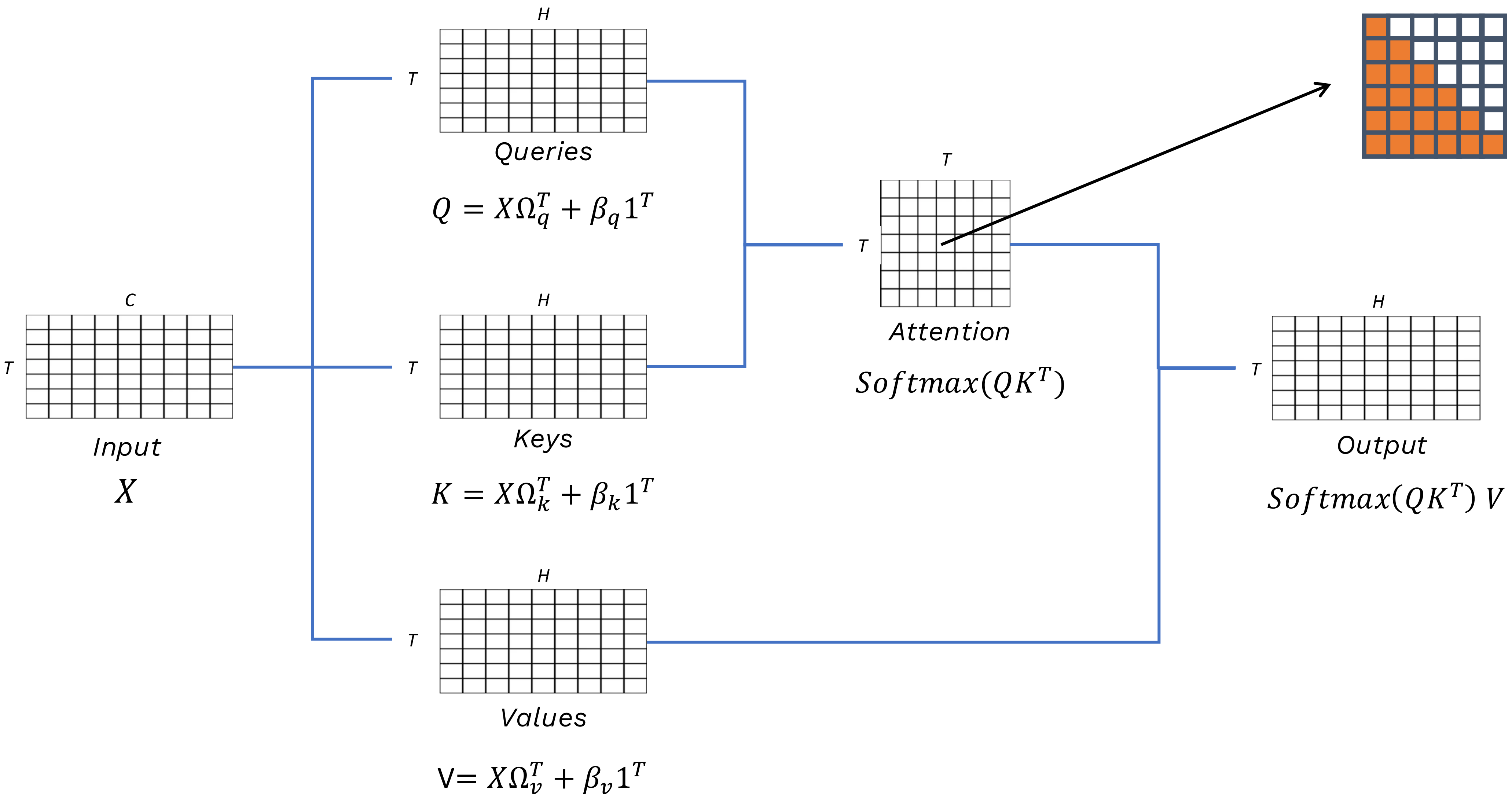
nn.Linear(C, H)

nn.Linear(n_embd, head_size)

Masked self-attention



Masked self-attention



Masked self-attention

```
tril = torch.tril(torch.ones(T,T))
```

```
tensor([[1., 0., 0.],
        [1., 1., 0.],
        [1., 1., 1.]])
```

Masked self-attention

```
tril = torch.tril(torch.ones(T,T))

wei = torch.zeros((T,T))

wei = wei.masked_fill(tril == 0, float('-inf'))

tensor([[0., -inf, -inf],
        [0., 0., -inf],
        [0., 0., 0.]])
```

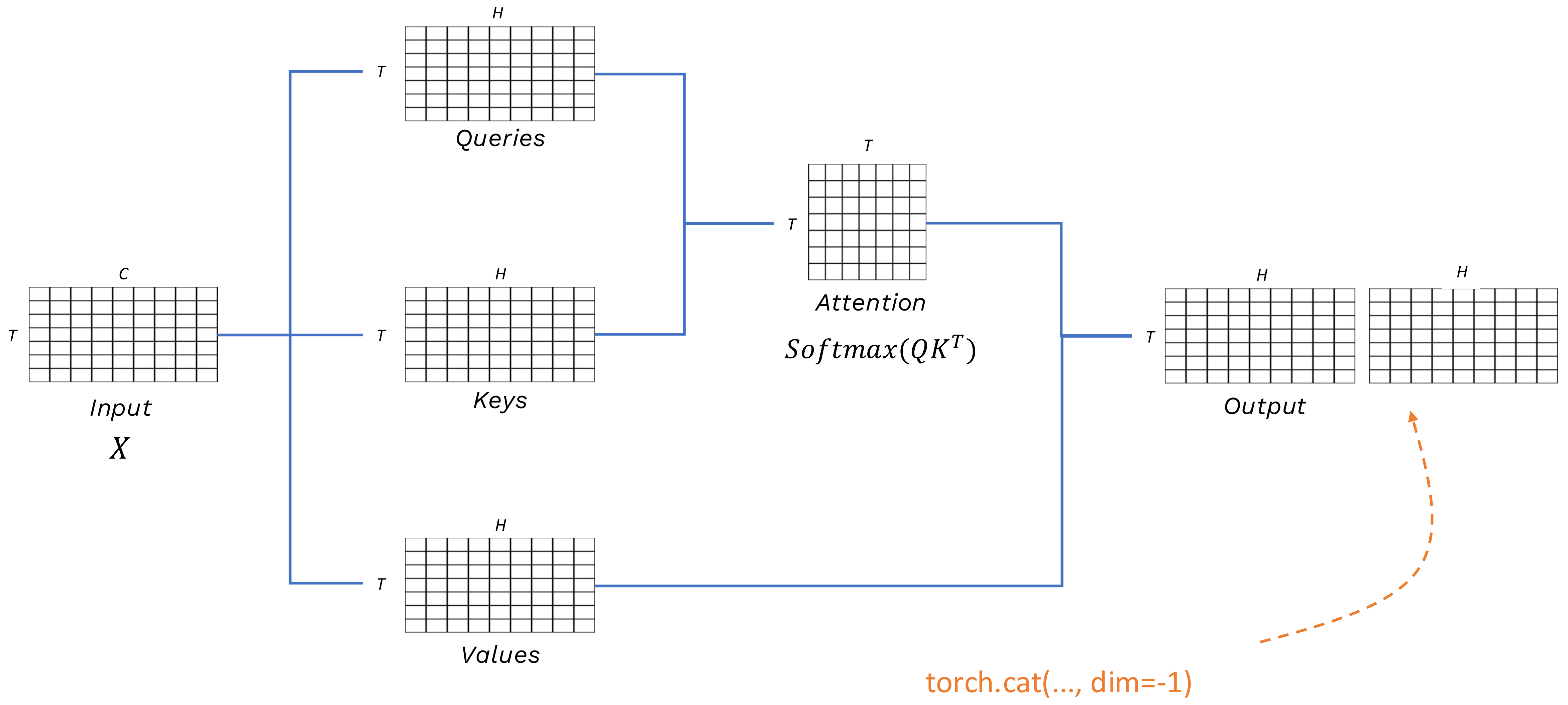
Masked self-attention

```
tril = torch.tril(torch.ones(T,T))

wei = torch.zeros((T,T))

wei = wei.masked_fill(tril == 0, float('-inf'))

tensor([[0., -inf, -inf],
        [0., 0., -inf],
        [0., 0., 0.]])

wei = F.softmax(wei, dim=-1)
```

Masked self-attention

```
tril = torch.tril(torch.ones(T,T))

wei = torch.zeros((T,T))

wei = wei.masked_fill(tril == 0, float('-inf'))

tensor([[0., -inf, -inf],
        [0., 0., -inf],
        [0., 0., 0.]])

wei = F.softmax(wei, dim=-1)

tensor([[1.0000, 0.0000, 0.0000],
        [0.5000, 0.5000, 0.0000],
        [0.3333, 0.3333, 0.3333]])
```

Beware of concatenation in multi-head



Getting started

```
class Head(nn.Module):
    """ one head of self-attention """

    def __init__(self, head_size):
        super().__init__()
        self.key = nn.Linear(..., ..., bias=False)
        ...

    def forward (self, x):
        B, T, C = x.shape
        k = self.key(x) # (B,T,C)
        ...
```

Getting started

```
class Head(nn.Module):
  """ one head of self-attention """

  def __init__(self, head_size):
    super().__init__()
    self.key = nn.Linear(..., ..., bias=False)
    ...

  def forward (self, x):
    B, T, C = x.shape
    k = self.key(x) # (B,T,C)
    q = ...
    # compute self attention scores (affinities)
    wei = ...
    wei = wei.masked_fill(self.tril[:T, :T] == 0, float('-inf’))
    wei = F.softmax(wei, dim=-1)
    ...
```

Practical 4 summary

1. Self-attention by hand
2. Self-attention in pytorch
3. GPT piece-by-piece
4. GPU goes rrr!

Dataset: Shakespeare’s corpus (input.txt)