CS11-711 Advanced NLP

Transformers

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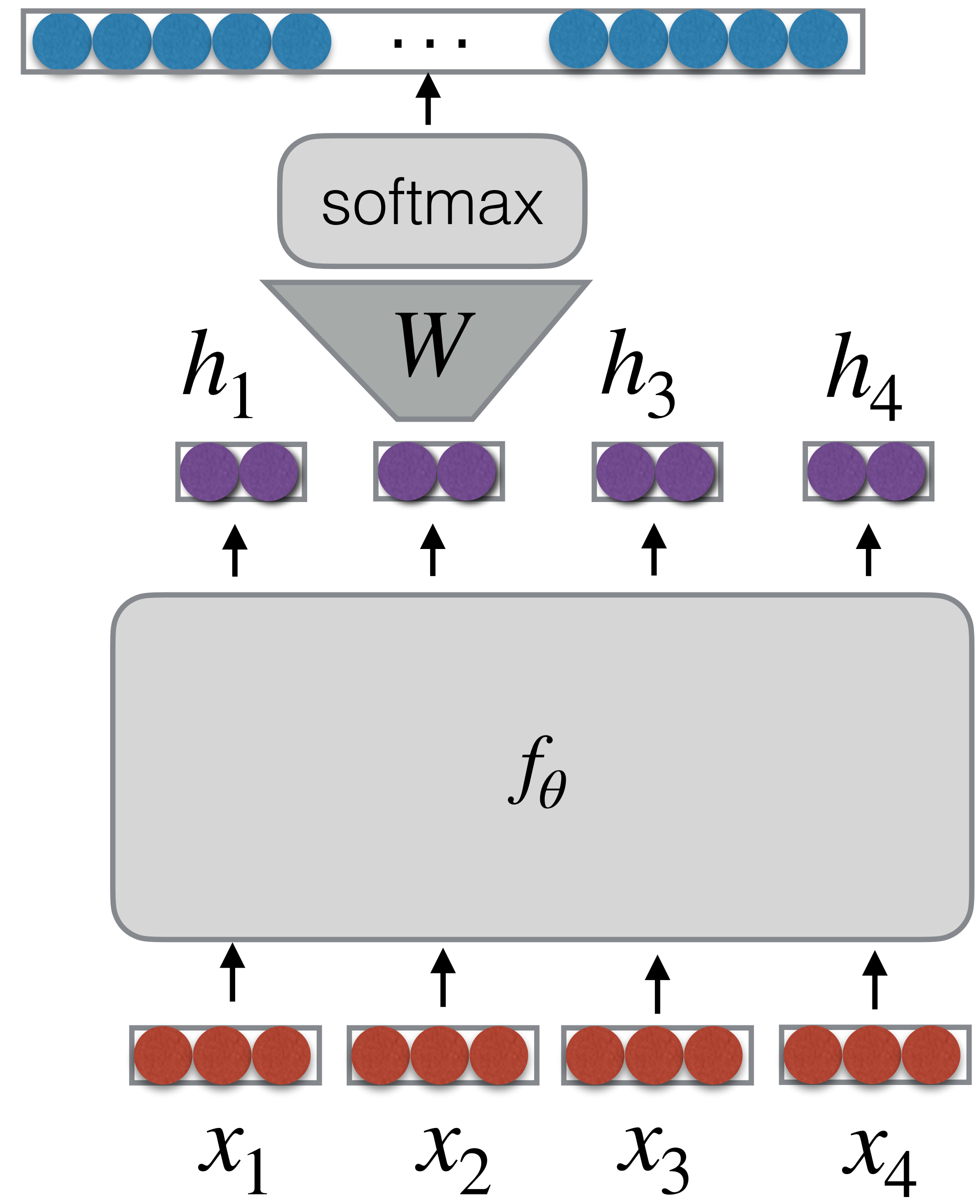
https://cmu-l3.github.io/anlp-fall2025/

https://github.com/cmu-l3/anlp-fall2025-code

Slides adapted from Graham Neubig's Fall 2024 course

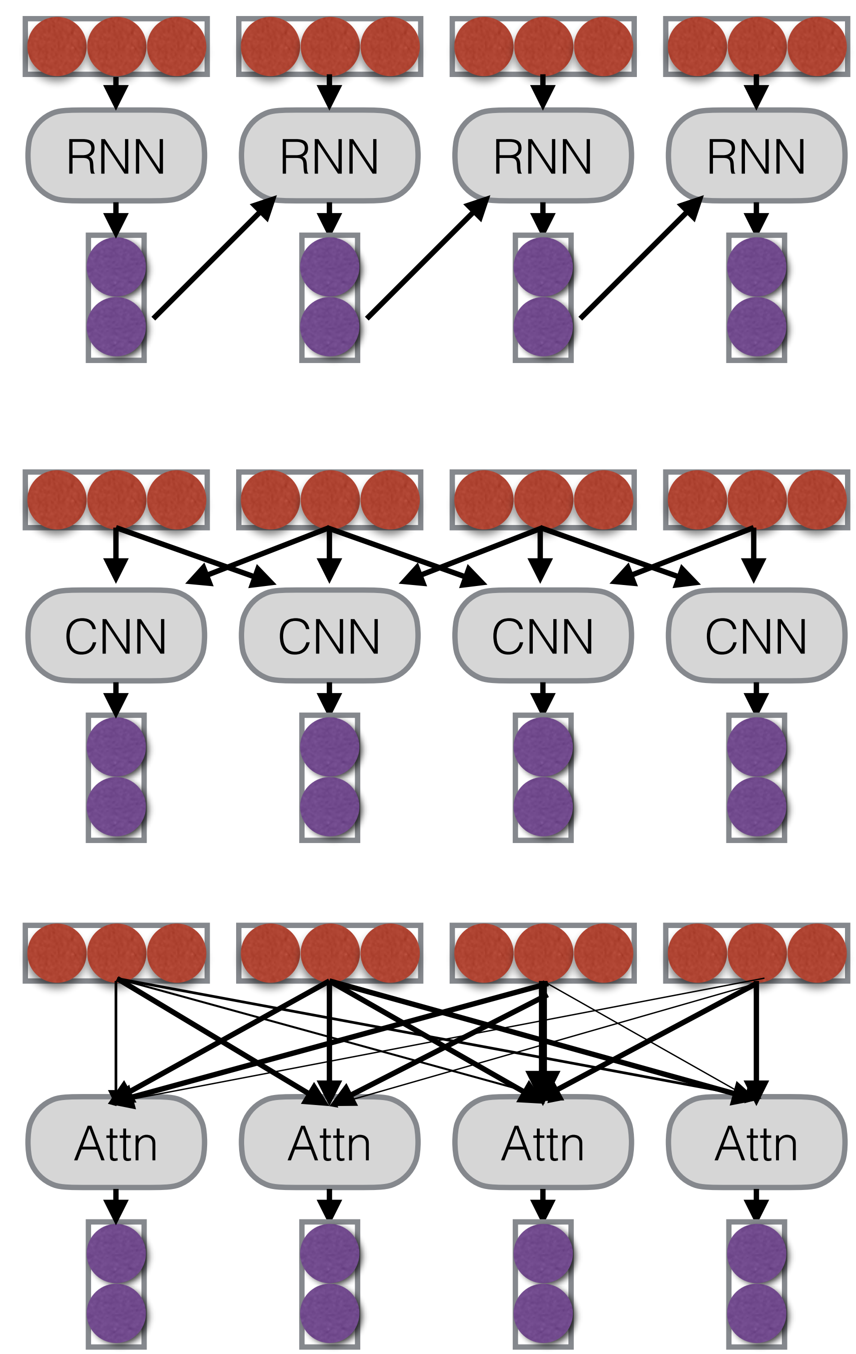
Recap: sequence model

- $f_\theta(x_1, \ldots, x_{|x|}) \rightarrow h_1, \ldots, h_{|x|}$
  - $h_t \in \mathbb{R}^d$: hidden state
- Language modeling:
  - $p_\theta(\cdot \mid x_{<t}) = \text{softmax}\left(Wh_t^\top\right)$



Three types of sequence models

- **Recurrence:** Condition representations on an encoding of the history
- **Convolution:** Condition representations on local context
- **Attention:** Condition representations on a weighted average of all tokens



Today's lecture

- **Transformer**: a sequence model based on attention
- Roadmap:
    - Attention
    - Transformer architecture
    - Improved transformer architecture

Attention

Basic Idea

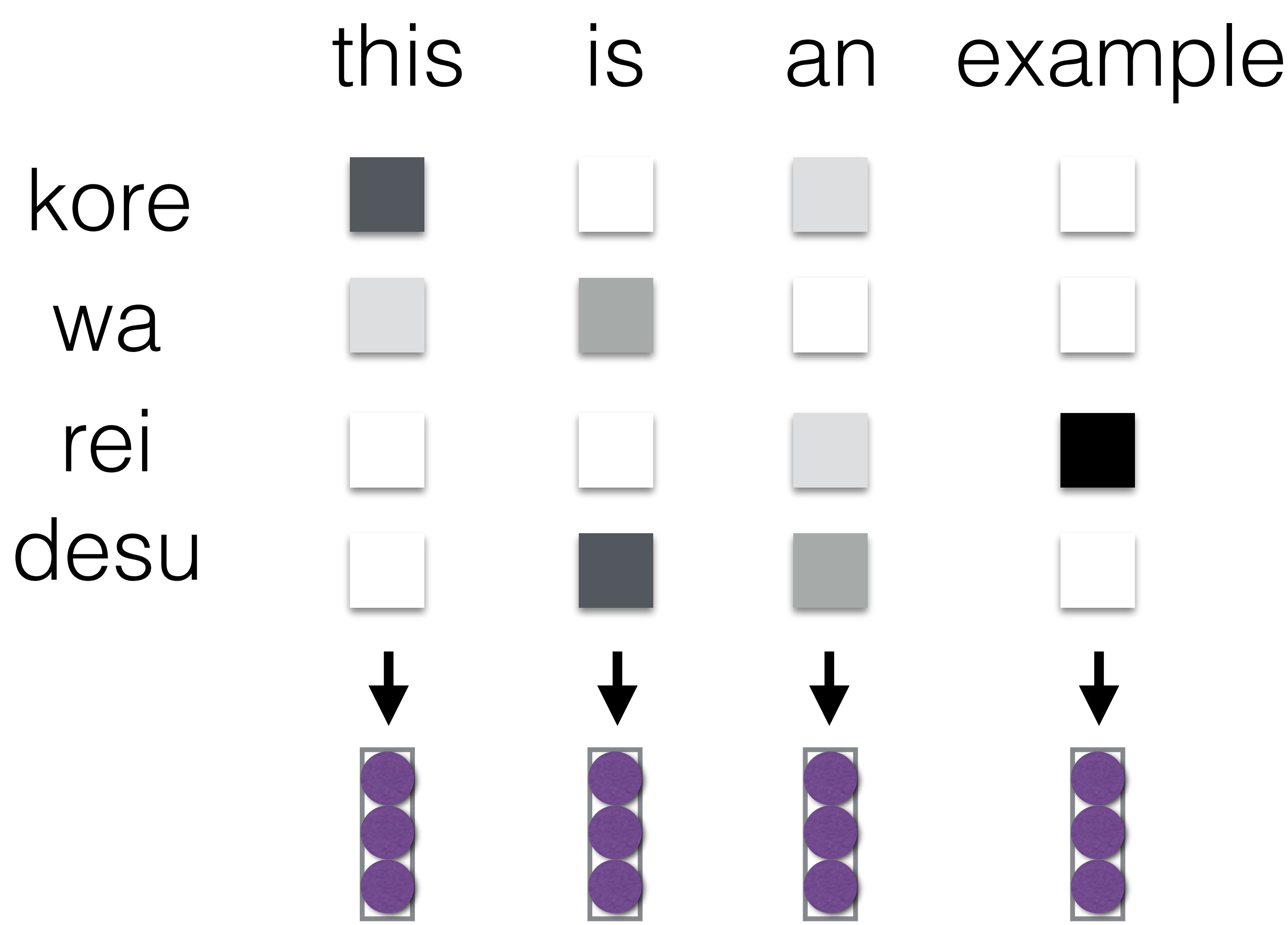
(Bahdanau et al. 2015)

- Encode each token in the sequence into a vector
- When decoding, perform a linear combination of these vectors, weighted by “attention weights”

Cross Attention

(Bahdanau et al. 2015)

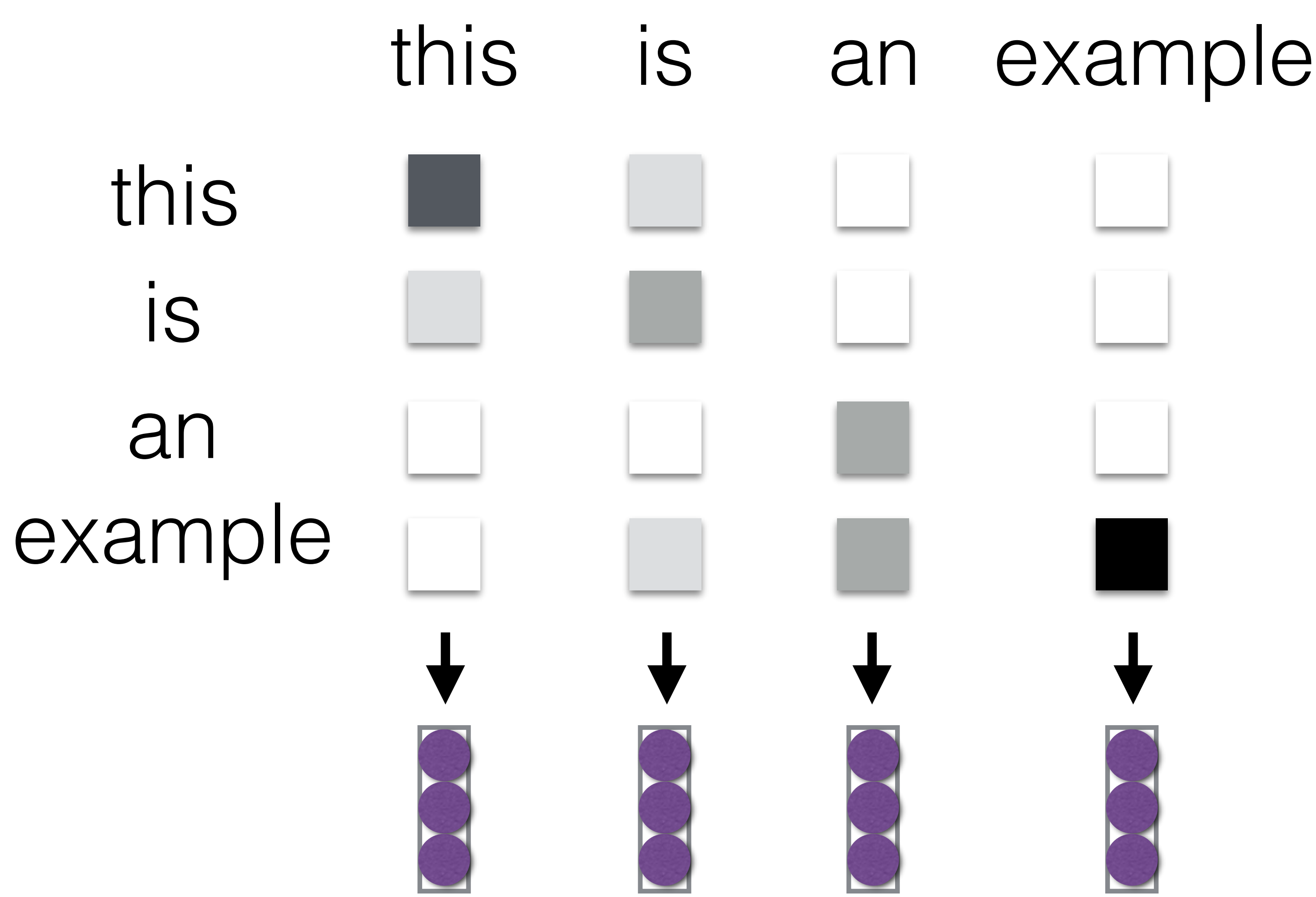
- Each element in a sequence attends to elements of another sequence



Self Attention

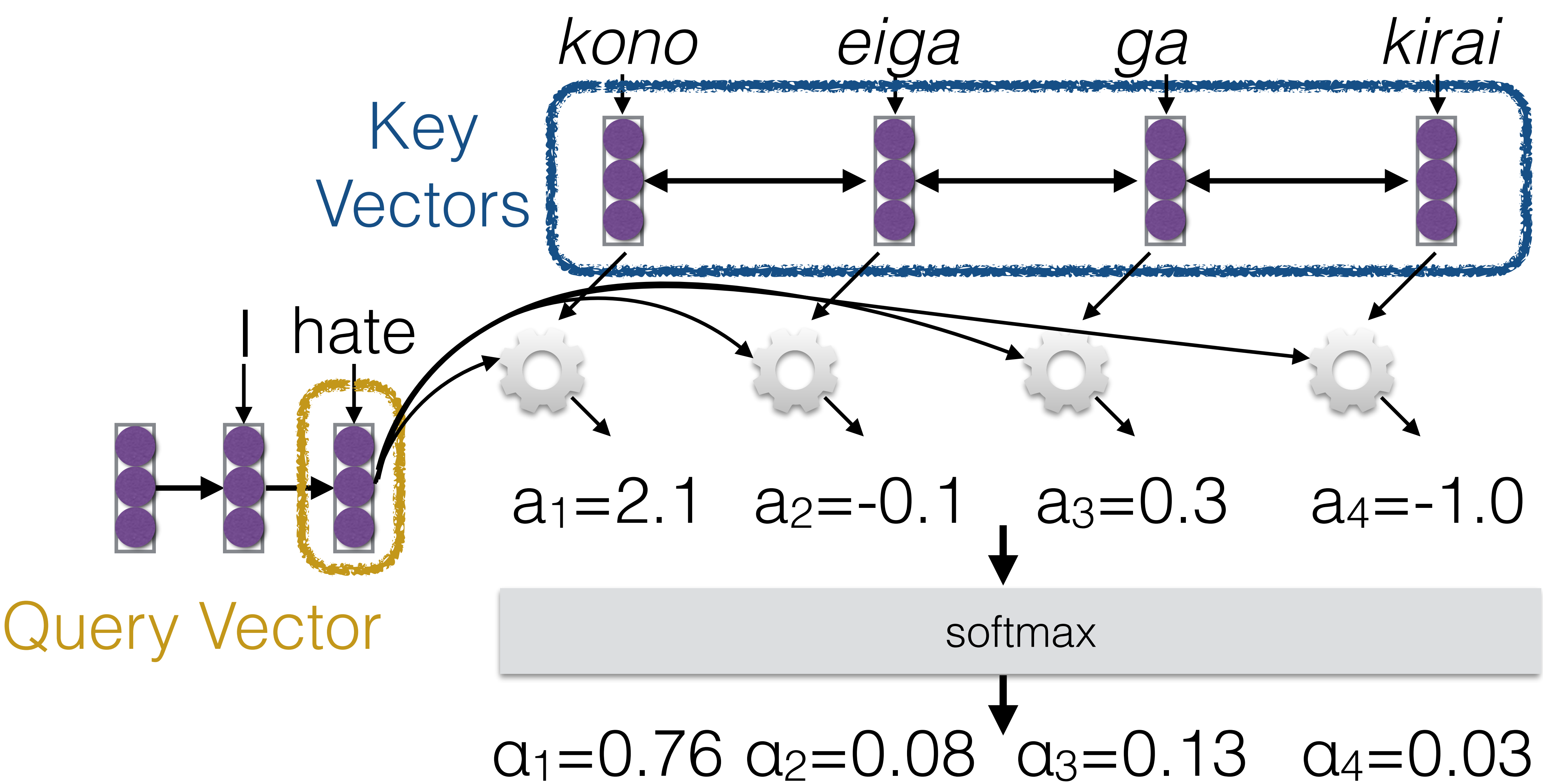
(Cheng et al. 2016, Vaswani et al. 2017)

- Each element in the sequence attends to elements of that sequence



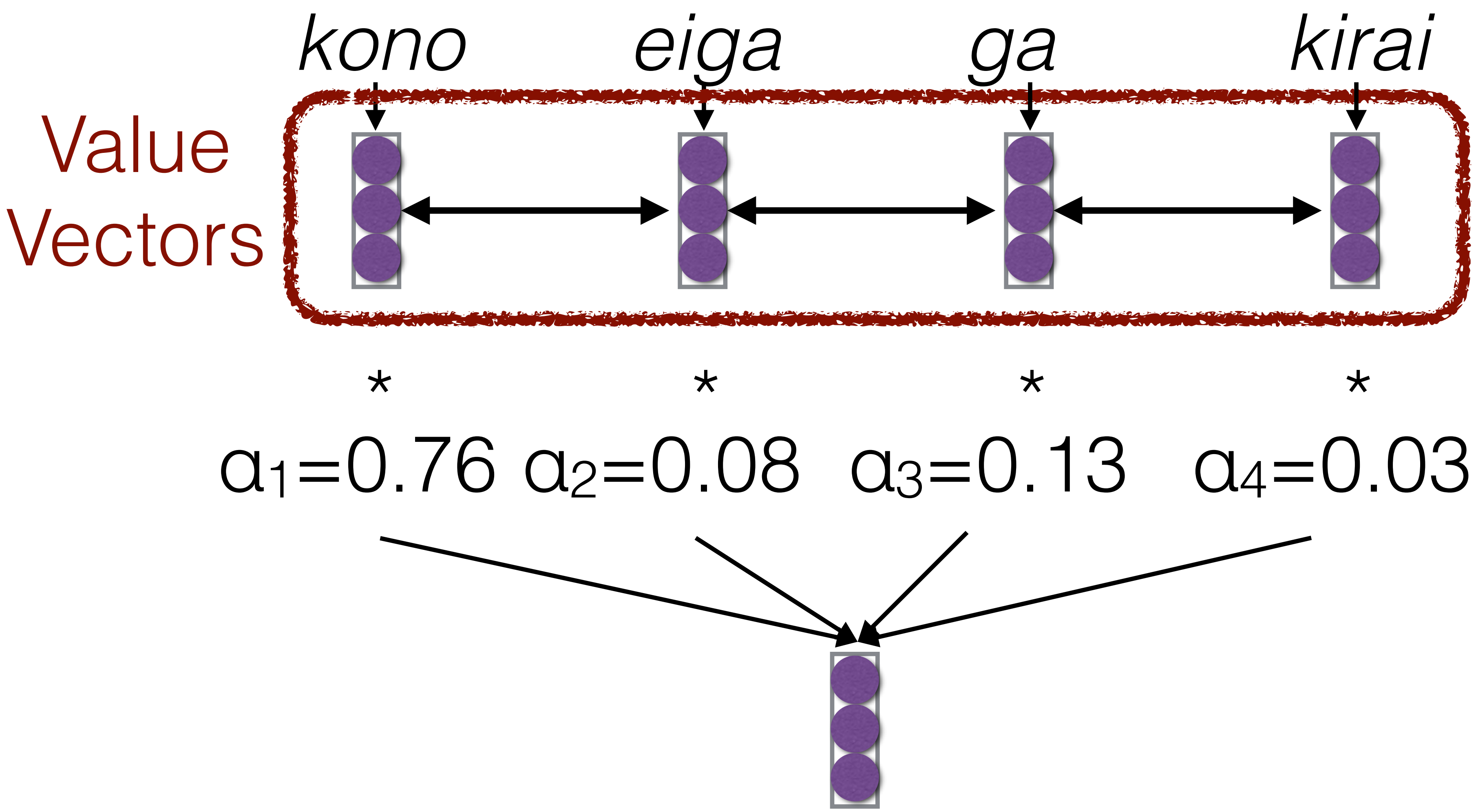
Calculating Attention (1)

- Use "query" vector (decoder state) and "key" vectors (all encoder states)
- For each query-key pair, calculate weight
- Normalize to add to one using softmax



Calculating Attention (2)

- Combine together value vectors (usually encoder states, like key vectors) by taking the weighted sum



- Use this in any part of the model you like

Query-key-value framework

- Keys $k_1, \ldots, k_N$
  - $k_i = W_K h_i$
- Values $v_1, \ldots, v_N$
  - $v_i = W_V h_i$
- Query q_t
  - $q_t = W_Q h_t$
- $c_t = \sum_{i=1}^{N} \alpha_{t,i} v_i$ where
  - $\alpha_{t,i} = \frac{\exp(a(q_t, k_i))}{\sum_{j=1}^{N} \exp(a(q_t, k_j))}$
  - $a(q, k)$ is a weighting/compatibility function, e.g. $a(q, k) = q^\top k$

Cross-attention example

- Keys: based on encoder states h_i
- Values: based on encoder states h_i
- Query: based on decoder state $\tilde{h}_t$

Self-attention example

- Keys: based on decoder states h_i
- Values: based on decoder states h_i
- Query: based on decoder state h_t

A Graphical Example

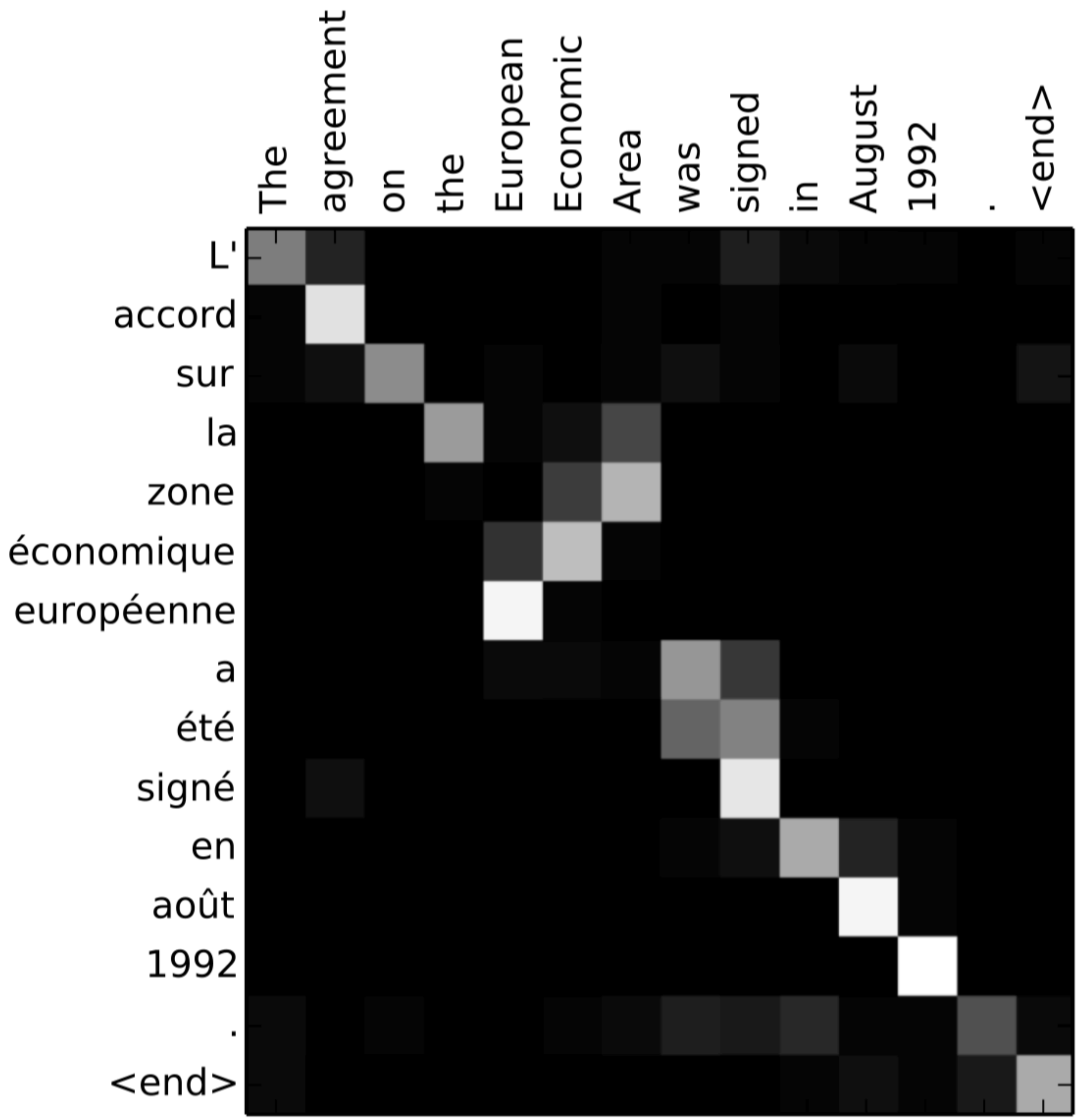


Image from Bahdanau et al. (2015)

Attention Score Functions

- **Dot Product** (Luong et al. 2015)

$$a(\boldsymbol{q}, \boldsymbol{k}) = \boldsymbol{q}^{\intercal} \boldsymbol{k}$$

- **Scaled Dot Product** (Vaswani et al. 2017)
  - *Problem:* scale of dot product increases as dimensions get larger
  - *Fix:* scale by size of the vector

$$a(\boldsymbol{q}, \boldsymbol{k}) = \frac{\boldsymbol{q}^{\intercal} \boldsymbol{k}}{\sqrt{|\boldsymbol{k}|}}$$

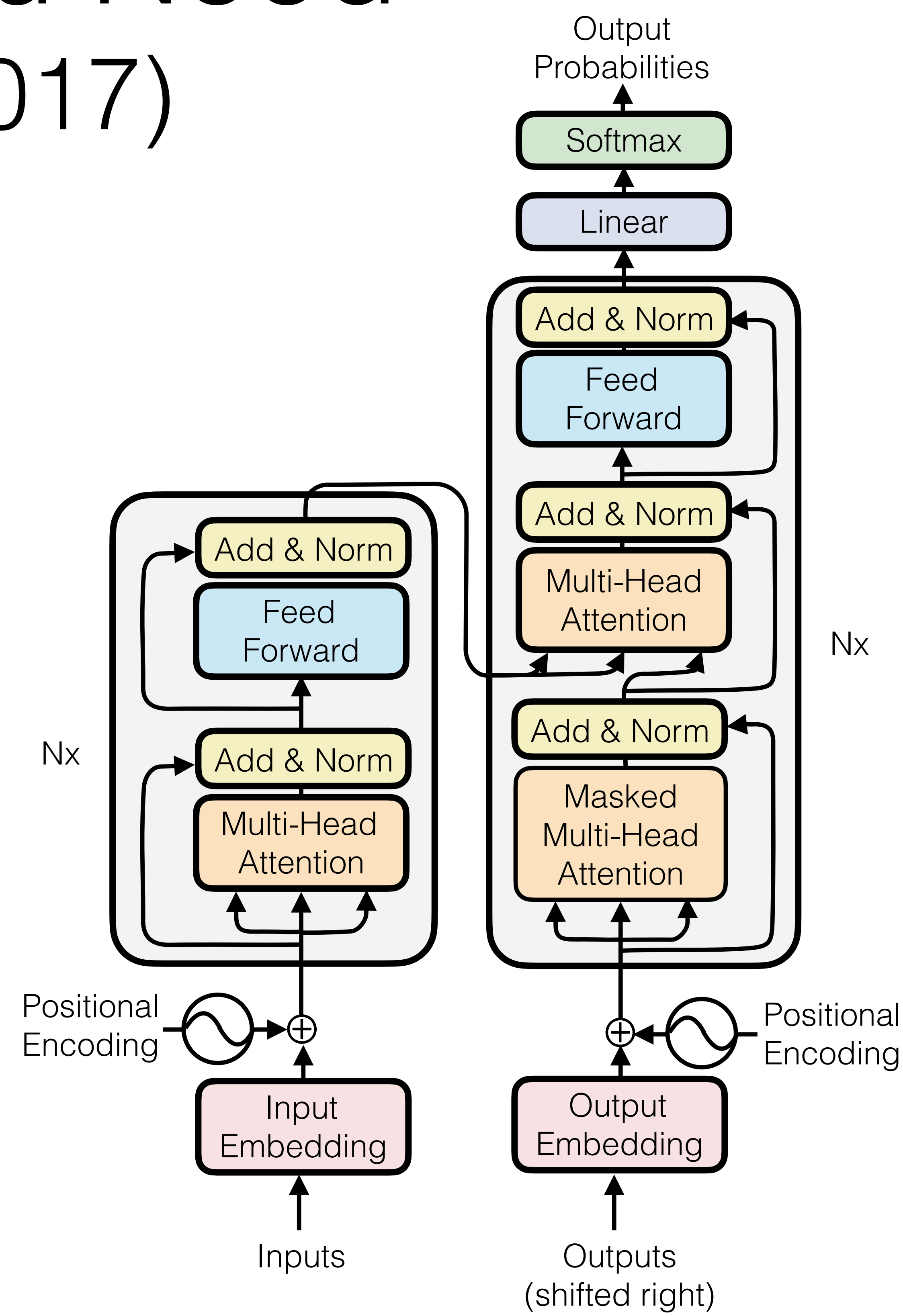
Today's lecture

- Roadmap:
  - Attention
  - **Transformer architecture**
  - Improved transformer architecture

Transformers

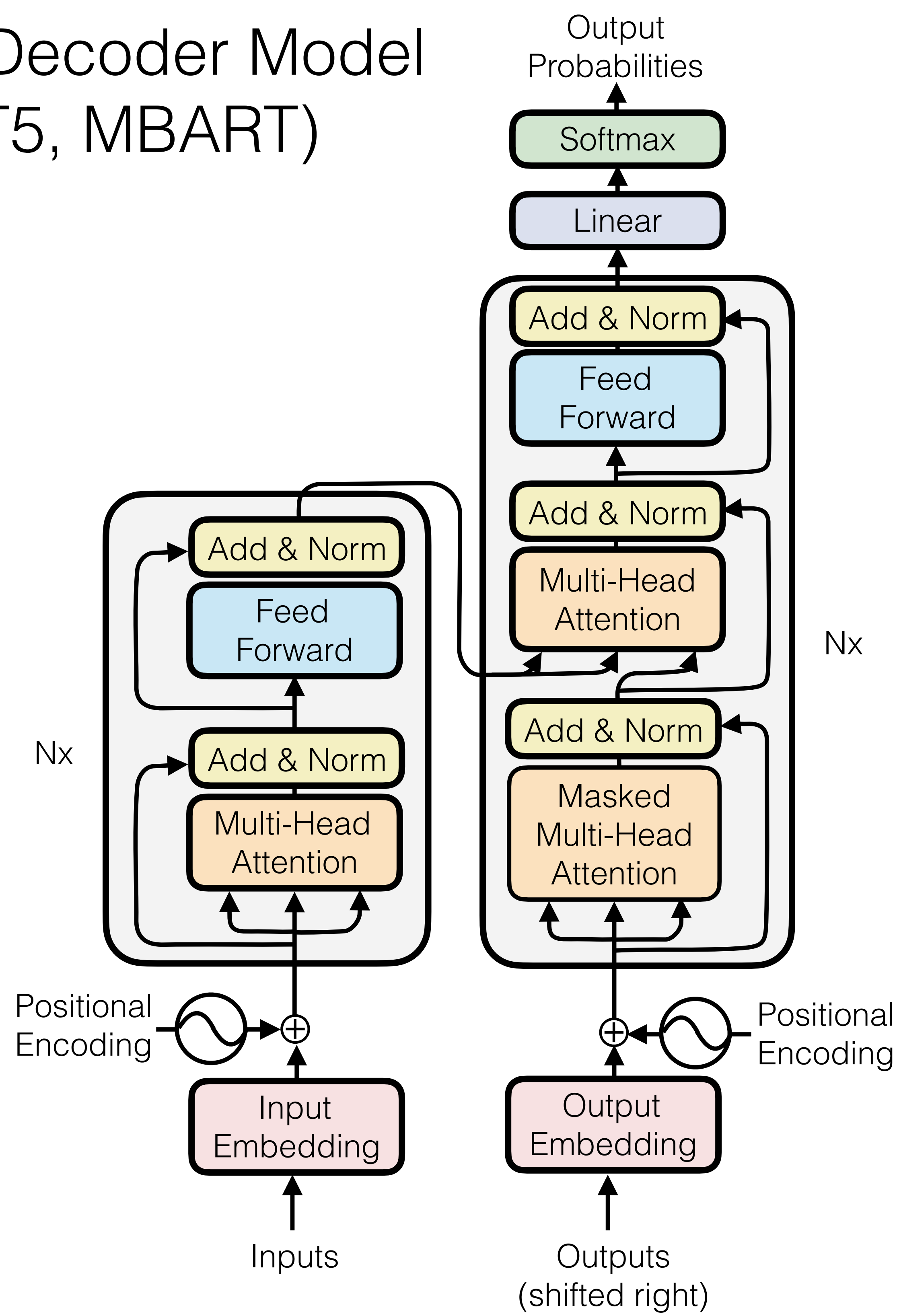
"Attention is All You Need" (Vaswani et al. 2017)

- A sequence-to-sequence architecture based entirely on attention
- Strong results on machine translation
- Fast: leverages parallelism from matrix multiplications

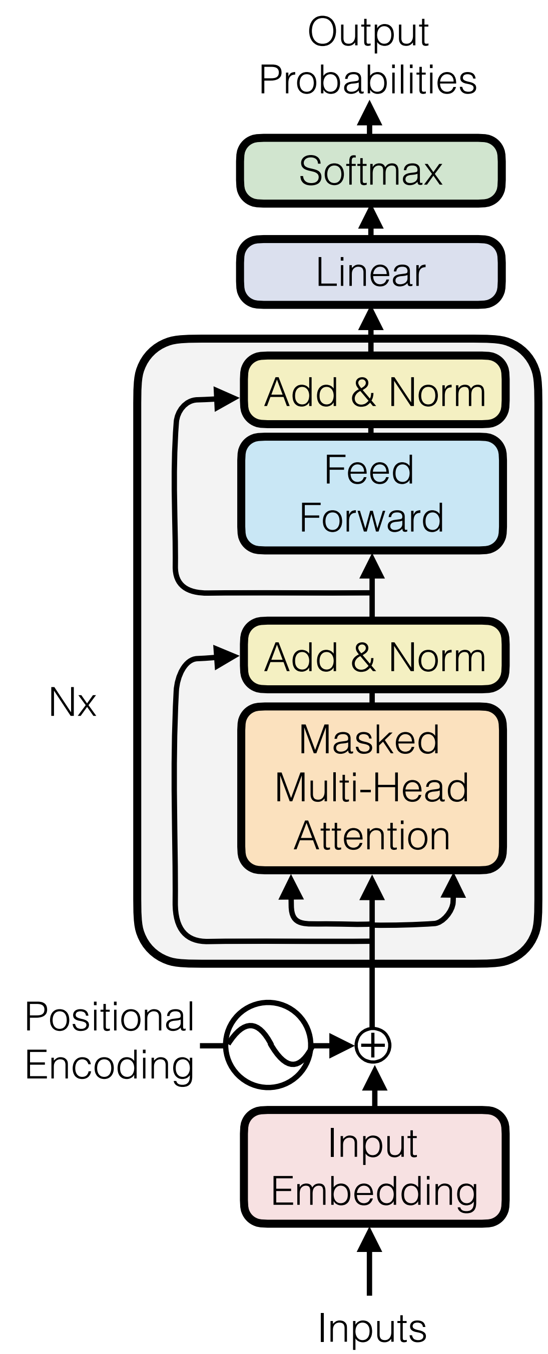


Two Types of Transformers

Encoder-Decoder Model (e.g. T5, MBART)

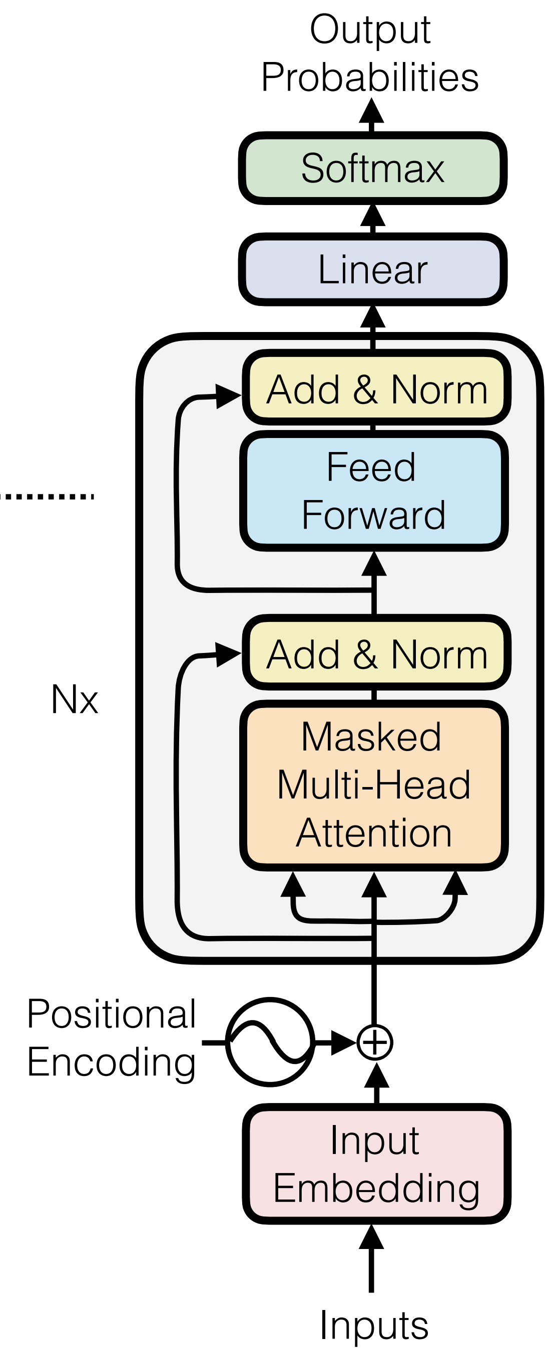


Decoder Only Model (e.g. GPT, LLaMa)



Basic idea

- Stack "transformer layers"
- 5 key concepts in the layer design and how we embed inputs



Core Transformer Concepts

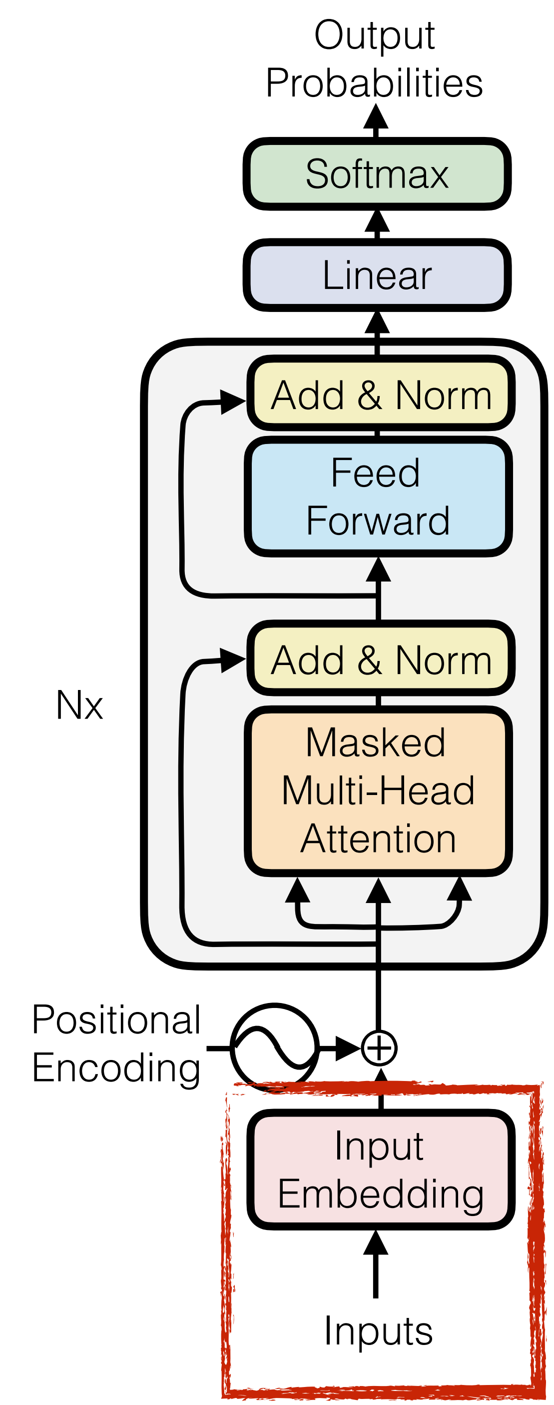
- Positional encodings
- Scaled dot product self-attention
- Multi-headed attention
- Residual + layer normalization
- Feed-forward layer

(Review)
Inputs and Embeddings

- **Inputs:** Generally split using subwords

the books were improved
the book _s were **improv _ed**

- **Input Embedding:** Looked up, like in previously discussed models



Positional Encoding

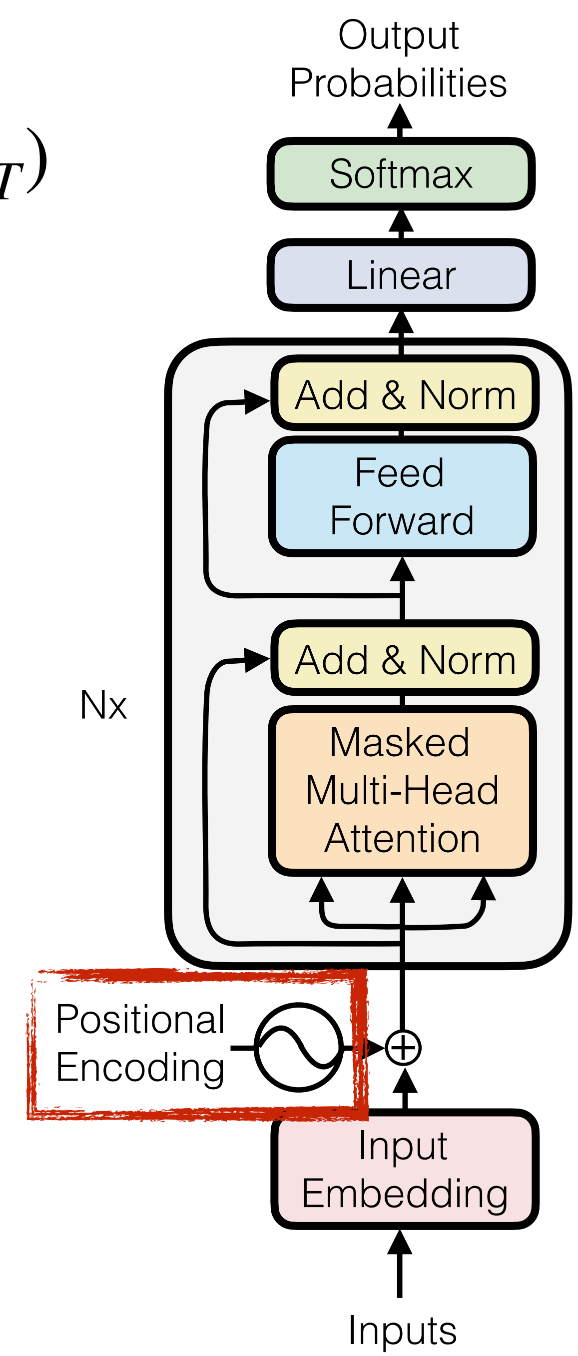
- The transformer model is purely attentional
  - Permutation equivariant: $f(\pi \circ (x_1, \ldots, x_T)) = \pi \circ f(x_1, \ldots x_T)$
- We need a way to identify the position of each token

A big dog and a very big cat

A big cat and a very big dog

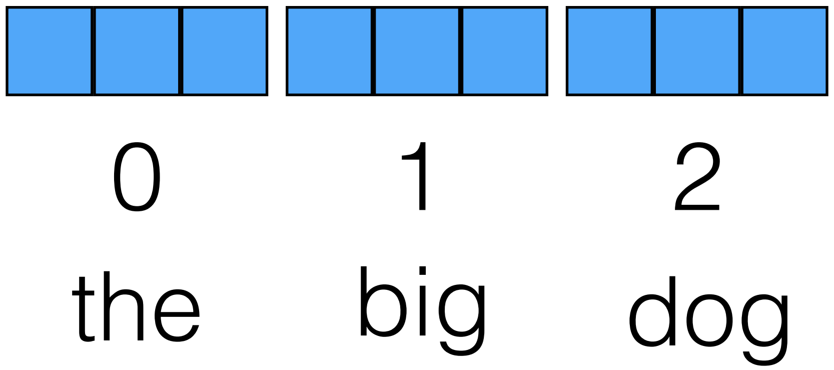
- Positional encodings add an embedding based on the word position

$W_{big} + W_{pos2}$ $W_{big} + W_{pos7}$



Example: Learned Positional Encoding
(Shaw+ 2018)

- Just create a learnable embedding
  - $W_{position} \in \mathbb{R}^{T_{max} \times d}$
  - Each position $t \in \{1, \ldots, T_{max}\}$ has a learned vector representation.



- **Advantages:** flexibility
- **Disadvantages:** cannot extrapolate to longer sequences

S: other positional encoding techniques

Core Transformer Concepts

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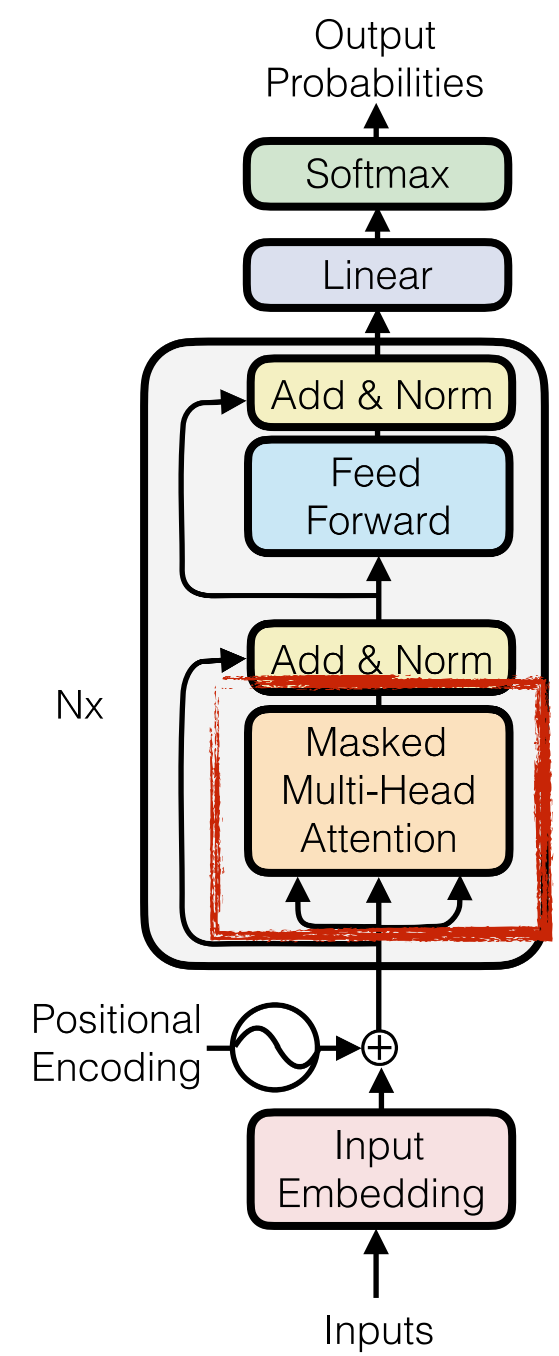
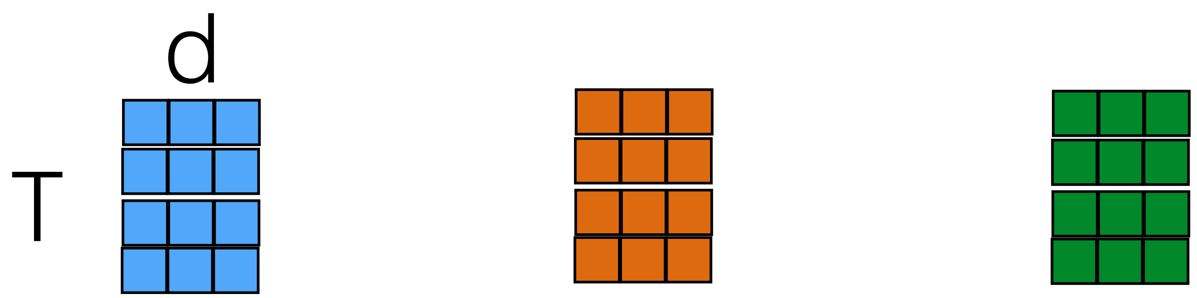


Scaled dot product attention

- As we saw on the previous slide: $a(\boldsymbol{q}, \boldsymbol{k}) = \dfrac{\boldsymbol{q}^\top \boldsymbol{k}}{\sqrt{|\boldsymbol{k}|}}$
- Full version, efficient matrix version:

$$Q \in \mathbb{R}^{T \times d} \quad K \in \mathbb{R}^{T \times d} \quad V \in \mathbb{R}^{T \times d}$$



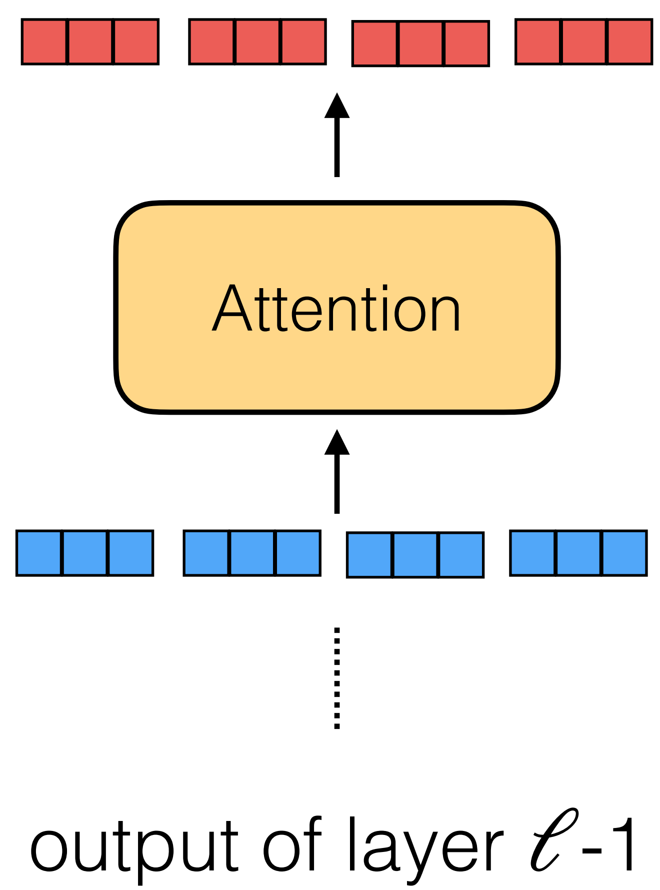
$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^\top}{\sqrt{d_k}}\right)V$$

S: dimensions of (i) softmax output, (ii) attention output

Scaled dot product self-attention

- Apply attention to the output of the previous layer:
  - $Q = H^{(\ell-1)}W_Q$
  - $K = H^{(\ell-1)}W_K$
  - $V = H^{(\ell-1)}W_V$
- Where $H^{(\ell-1)} \in \mathbb{R}^{T \times d}$ is the output of the previous transformer layer
- W_Q, W_K, W_V are learned weights

$$\text{Attention}(Q, K, V) \rightarrow \tilde{H}^{\ell}$$



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- **Multi-headed attention**
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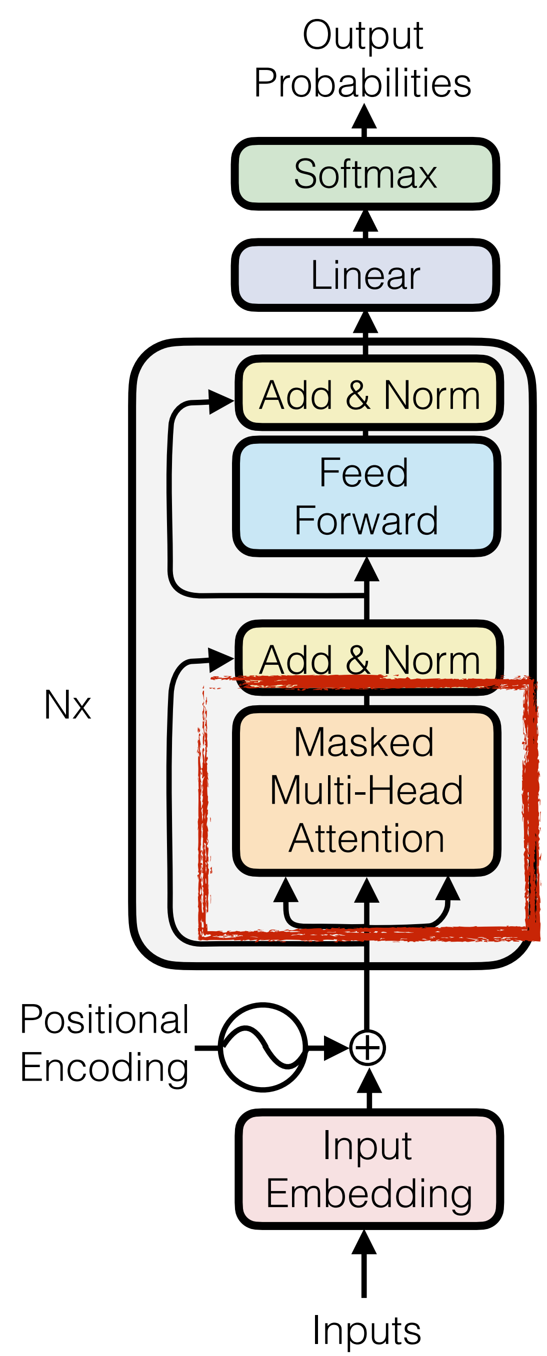


Intuition for Multi-heads

- **Intuition:** Information from different parts of the sentence can be useful to disambiguate in different ways

I **run** a small business

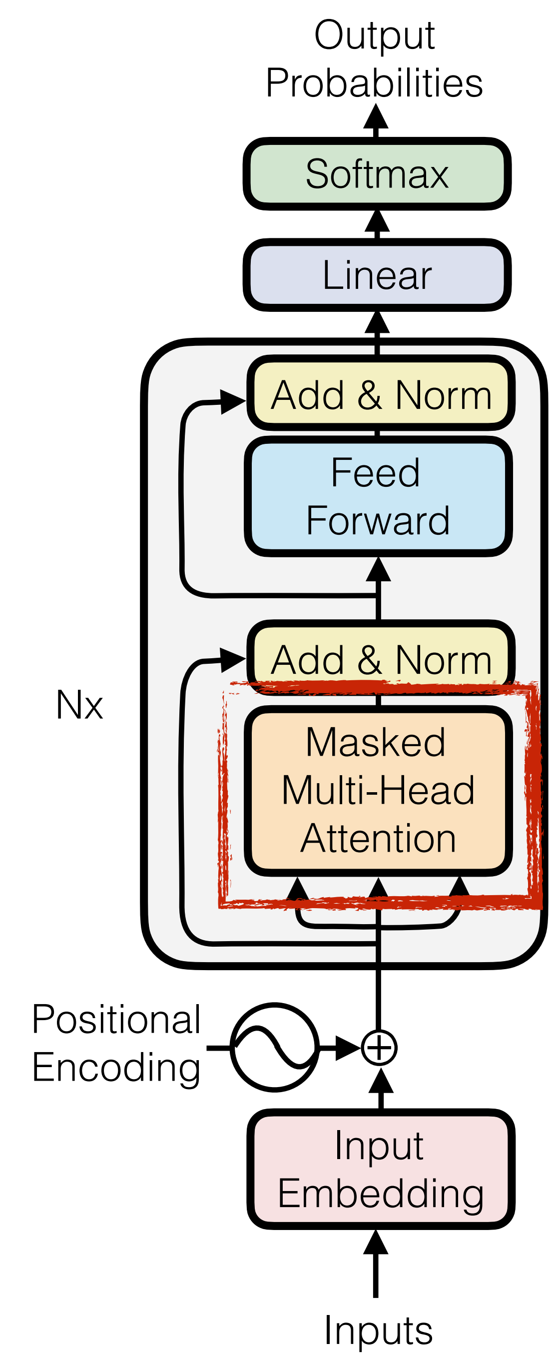
I **run** a mile in 10 minutes

The robber made a **run** for it

The stocking had a **run**

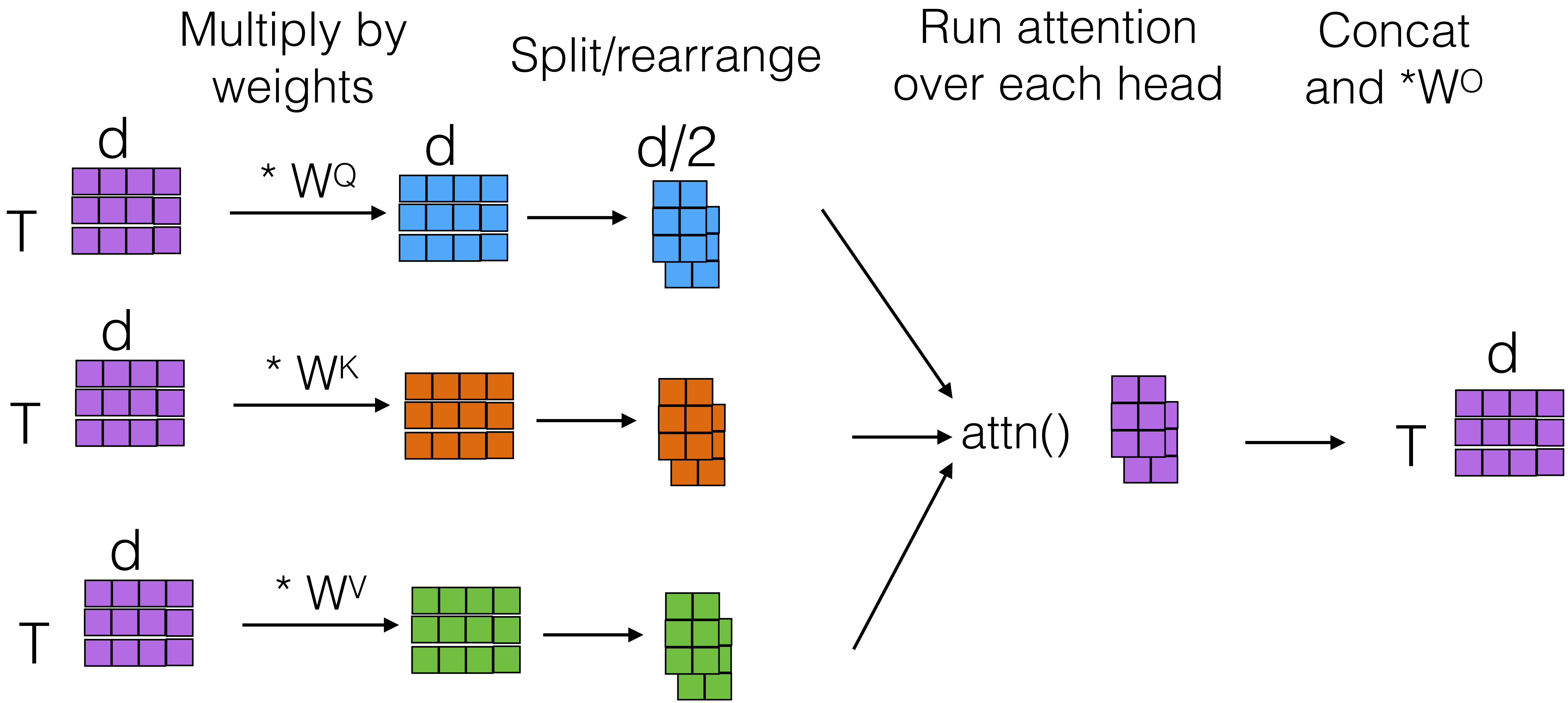
syntax
(nearby context)

semantics
(farther context)



Multi-head Attention Concept

$$\text{MultiHead}(Q, K, V) = \text{Concat}(\text{head}_1, ..., \text{head}_h)W^O$$
$$\text{where head}_i = \text{Attention}(QW_i^Q, KW_i^K, VW_i^V)$$



Typically $d_k = d_v = d/$numheads

Code Example

```python
def forward(self, x):
    B, T, C = x.size() # batch size, sequence length, embedding dimensionality (n_embd)

    # calculate query, key, values for all heads in batch and move head forward to be the batch dim
    q, k ,v  = self.c_attn(x).split(self.n_embd, dim=2)
    k = k.view(B, T, self.n_head, C // self.n_head).transpose(1, 2) # (B, nh, T, hs)
    q = q.view(B, T, self.n_head, C // self.n_head).transpose(1, 2) # (B, nh, T, hs)
    v = v.view(B, T, self.n_head, C // self.n_head).transpose(1, 2) # (B, nh, T, hs)

    # causal self-attention; Self-attend: (B, nh, T, hs) x (B, nh, hs, T) -> (B, nh, T, T)
    att = (q @ k.transpose(-2, -1)) * (1.0 / math.sqrt(k.size(-1)))
    att = att.masked_fill(self.bias[:,:,:T,:T] == 0, float('-inf'))
    att = F.softmax(att, dim=-1)
    att = self.attn_dropout(att)
    y = att @ v # (B, nh, T, T) x (B, nh, T, hs) -> (B, nh, T, hs)
    y = y.transpose(1, 2).contiguous().view(B, T, C) # re-assemble all head outputs side by side

    # output projection
    y = self.resid_dropout(self.c_proj(y))
    return y
```

https://github.com/karpathy/minGPT/blob/master/mingpt/model.py

What Happens w/ Multi-heads?

- Example from Vaswani et al.

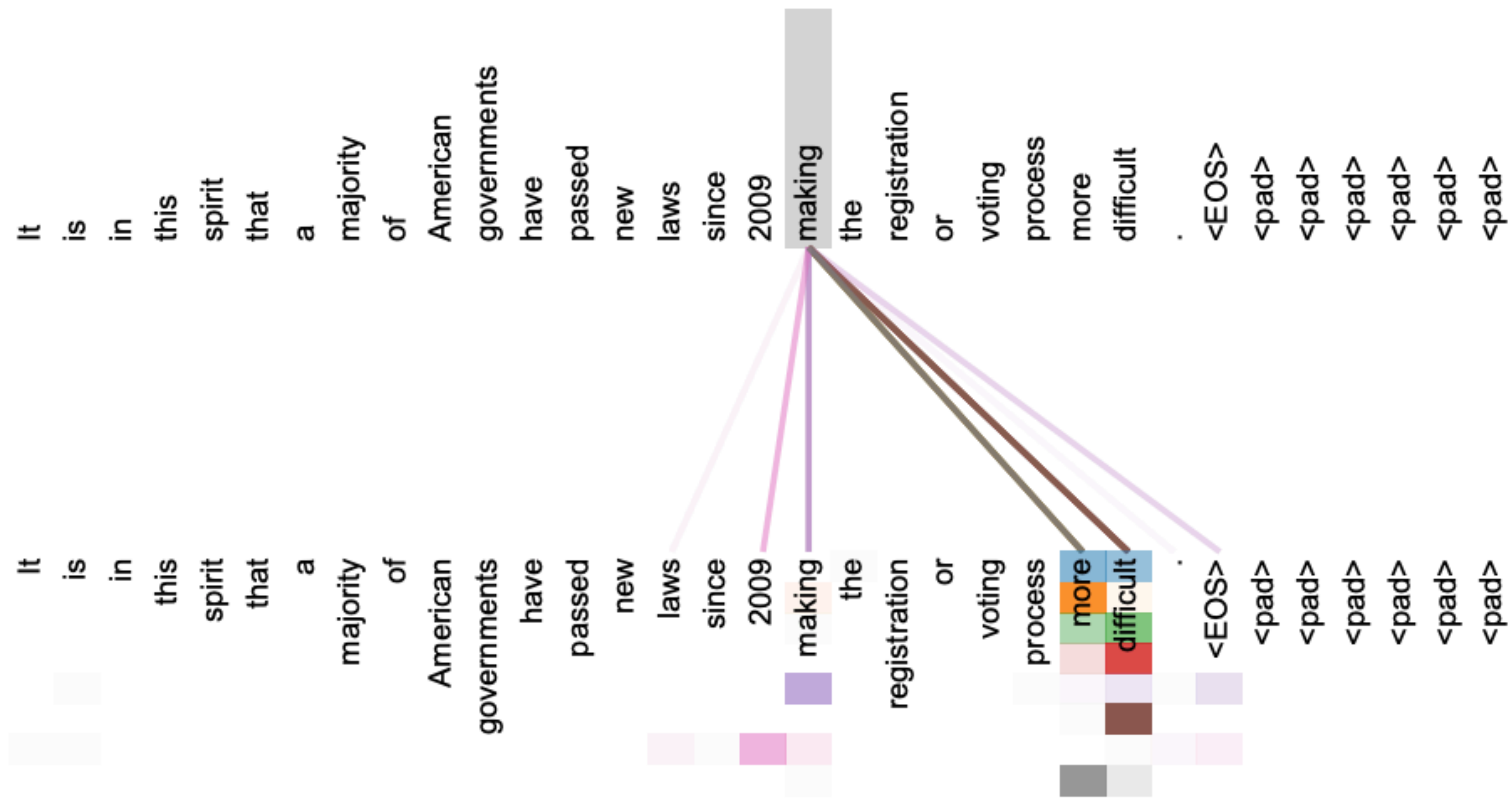
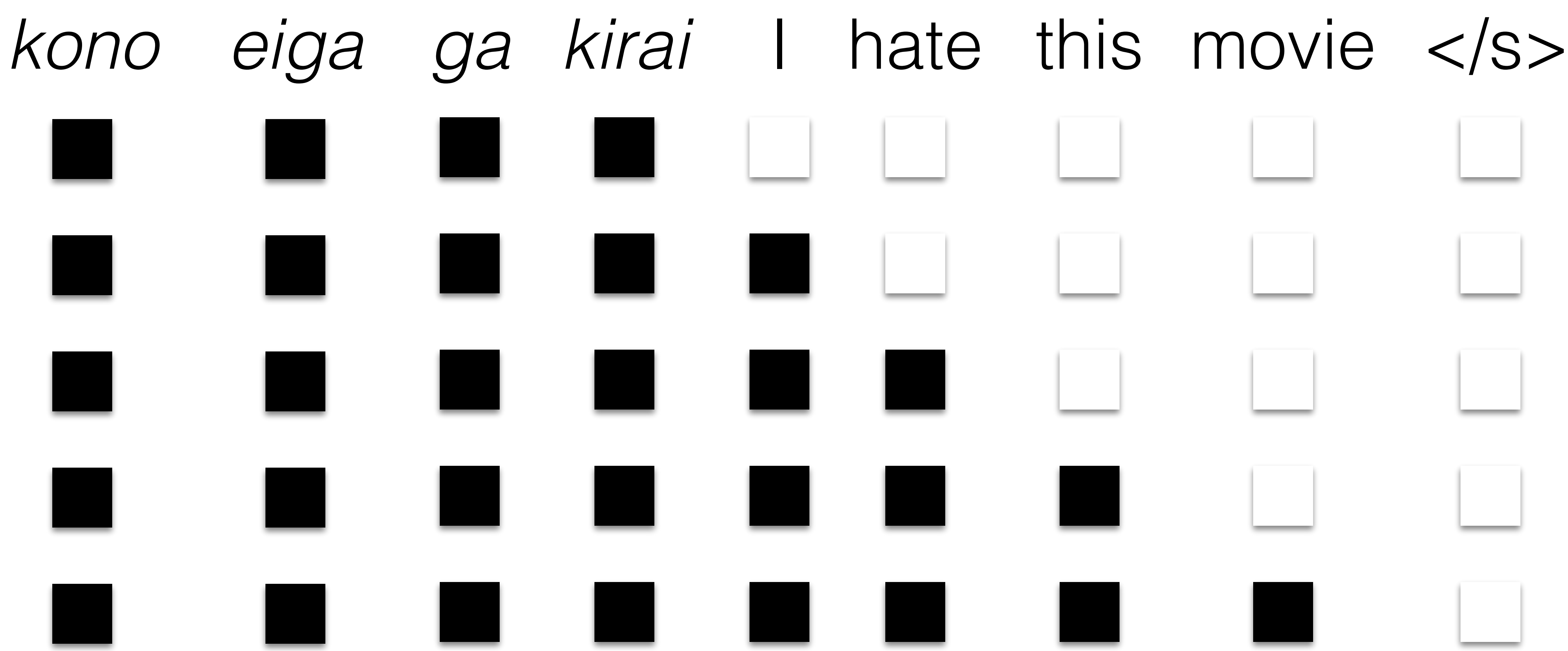


Figure 3: An example of the attention mechanism following long-distance dependencies in the encoder self-attention in layer 5 of 6. Many of the attention heads attend to a distant dependency of the verb 'making', completing the phrase 'making...more difficult'. Attentions here shown only for the word 'making'. Different colors represent different heads. Best viewed in color.

- See also BertVis: https://github.com/jessevig/bertviz

Masking for Language Model Training

- Mask the attention from future timesteps
  - Prevents the model from cheating when predicting the next token



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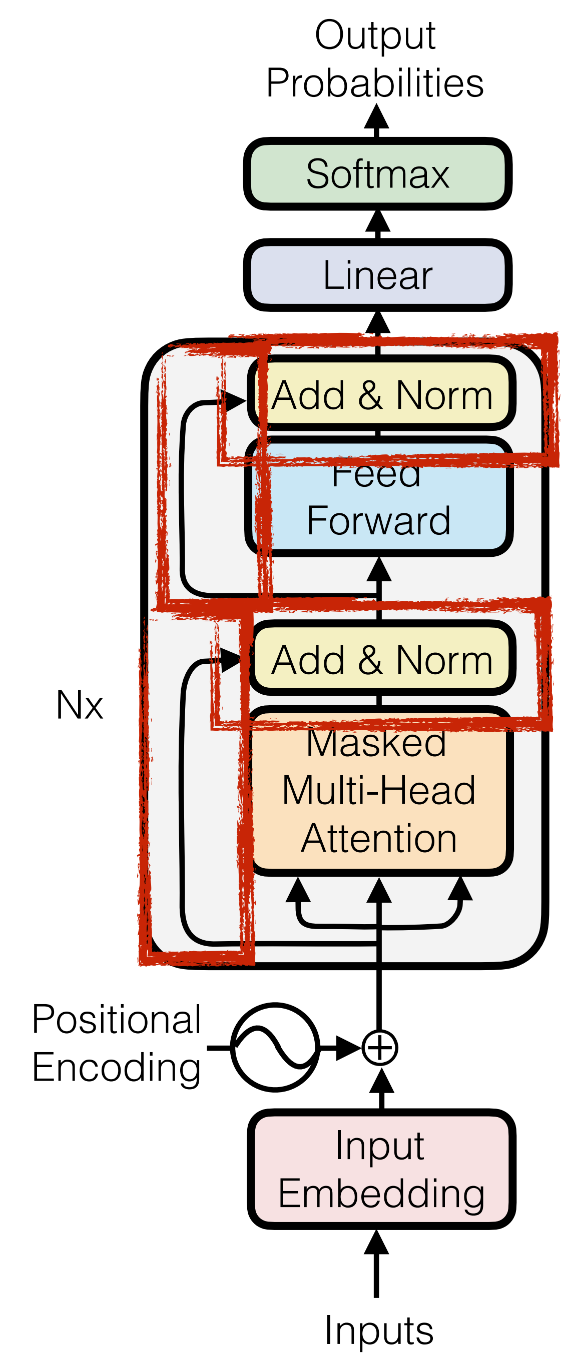
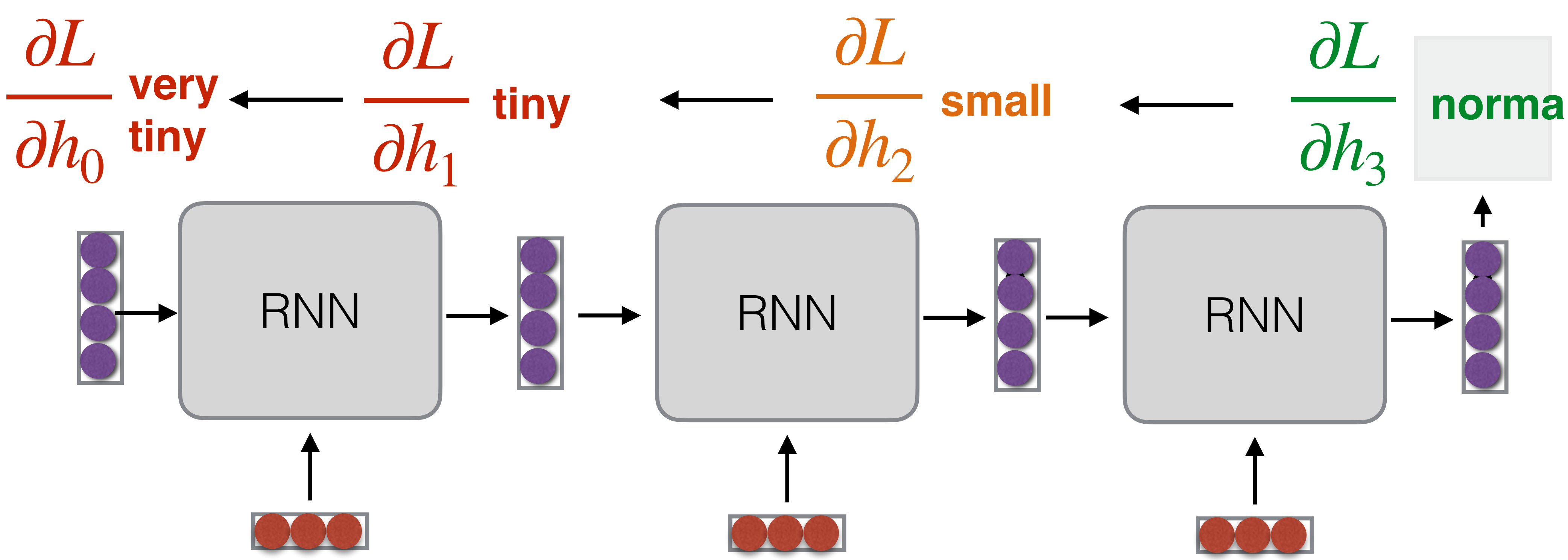
- **Residual + layer normalization**
- Feed-forward layer



Layer Normalization and Residual Connections

Reminder: Gradients and Training Instability

- RNNs: backpropagation can make gradients vanish or explode



- The same issue occurs in multi-layer transformers!

Layer Normalization
(Ba et al. 2016)

- Normalizes the outputs to be within a consistent range, preventing too much variance in scale of outputs

gain

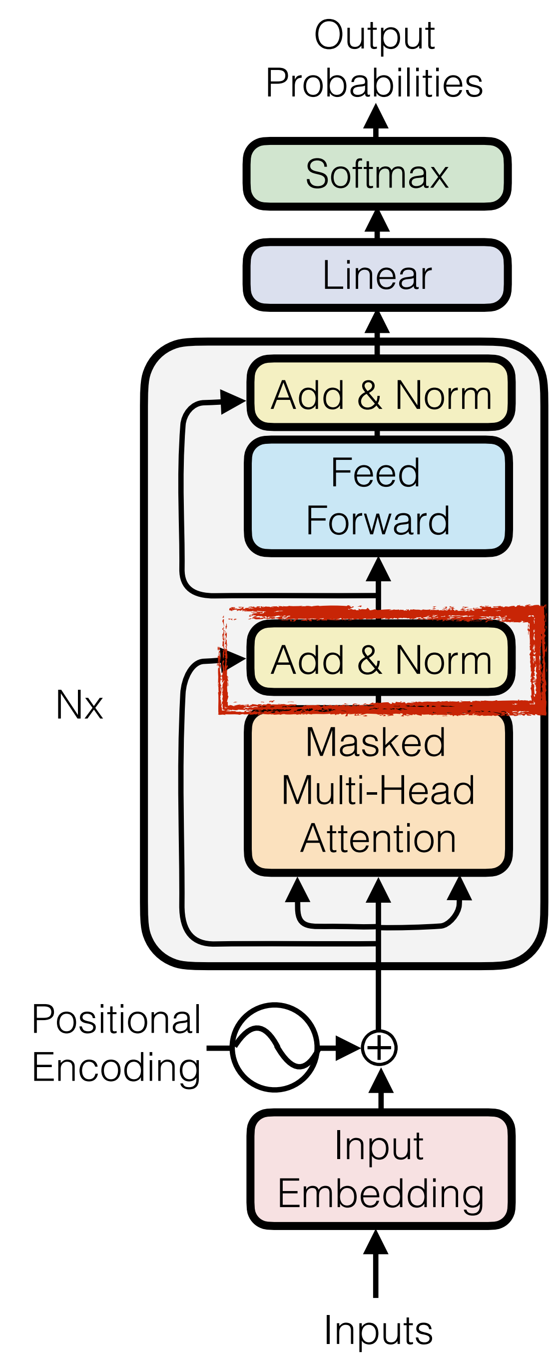
bias

$$\text{LayerNorm}(\mathbf{x}; \mathbf{g}, \mathbf{b}) = \frac{\mathbf{g}}{\sigma(\mathbf{x})} \odot (\mathbf{x} - \mu(\mathbf{x})) + \mathbf{b}$$

vector stddev

vector mean

$$\mu(\mathbf{x}) = \frac{1}{n}\sum_{i=1}^{n} x_i \qquad \sigma(\mathbf{x}) = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_i - \mu)^2}$$

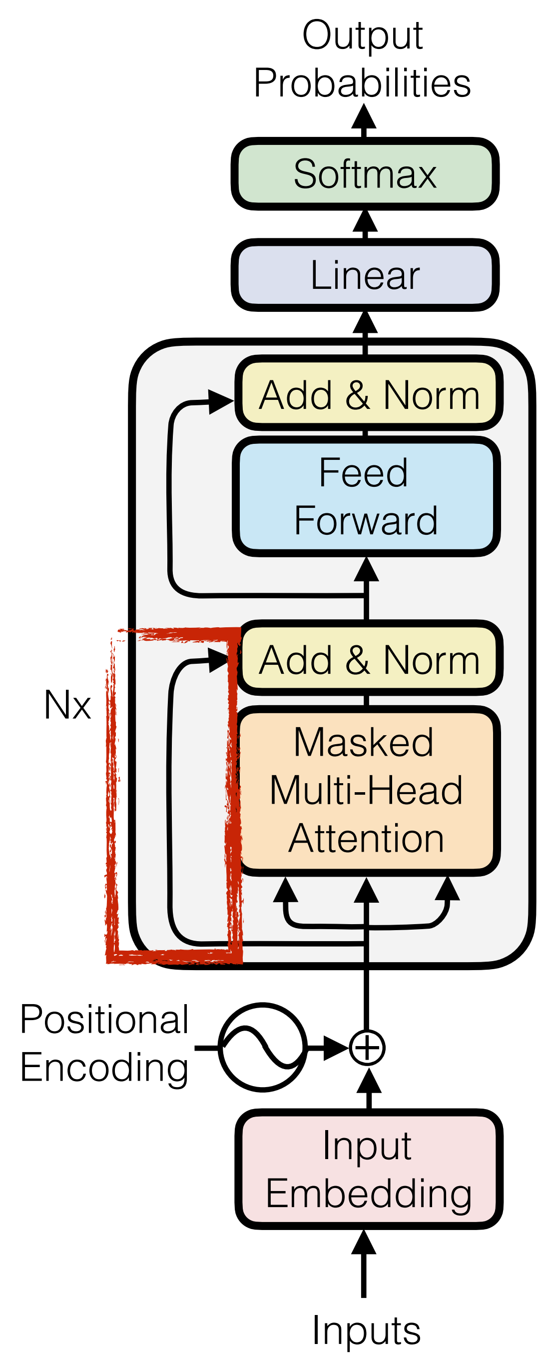


Residual Connections

- Add an additive connection between the input and output

$$\text{Residual}(\mathbf{x}, f) = f(\mathbf{x}) + \mathbf{x}$$

- Prevents vanishing gradients and allows f to learn the *difference* from the input



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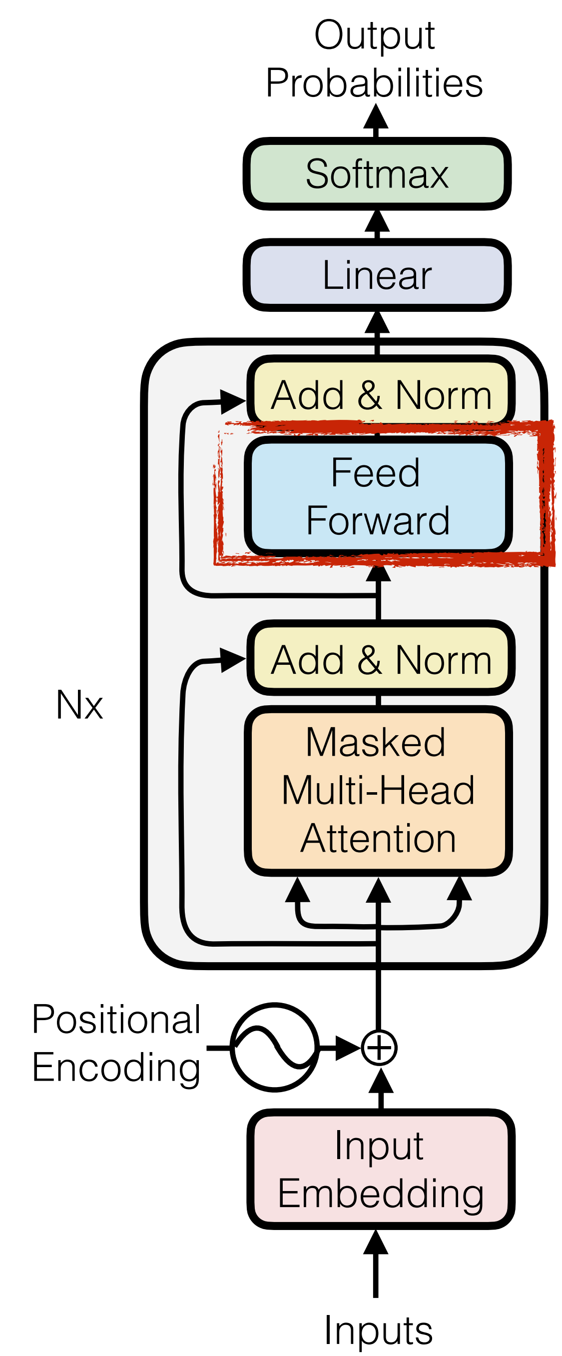
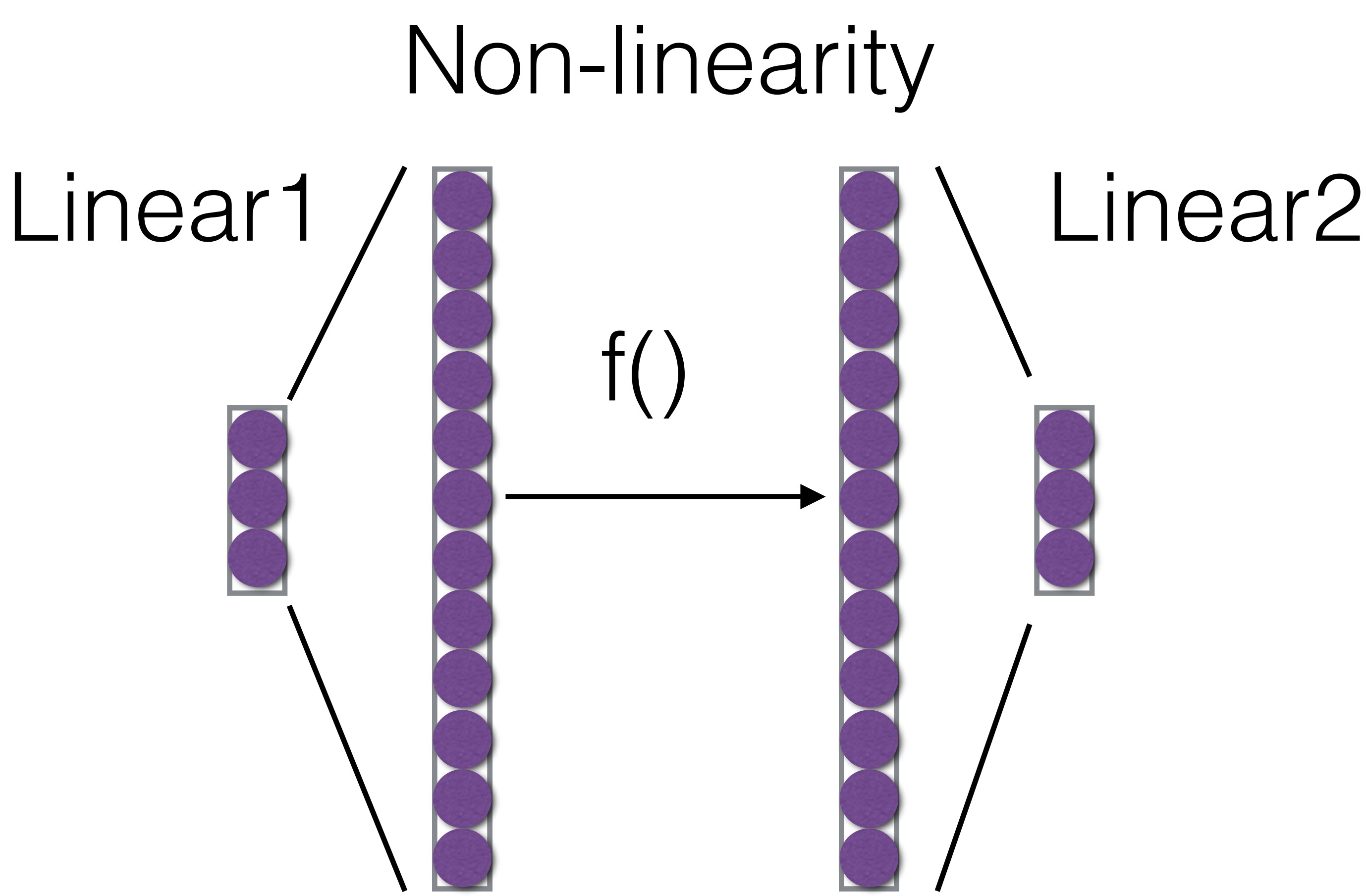


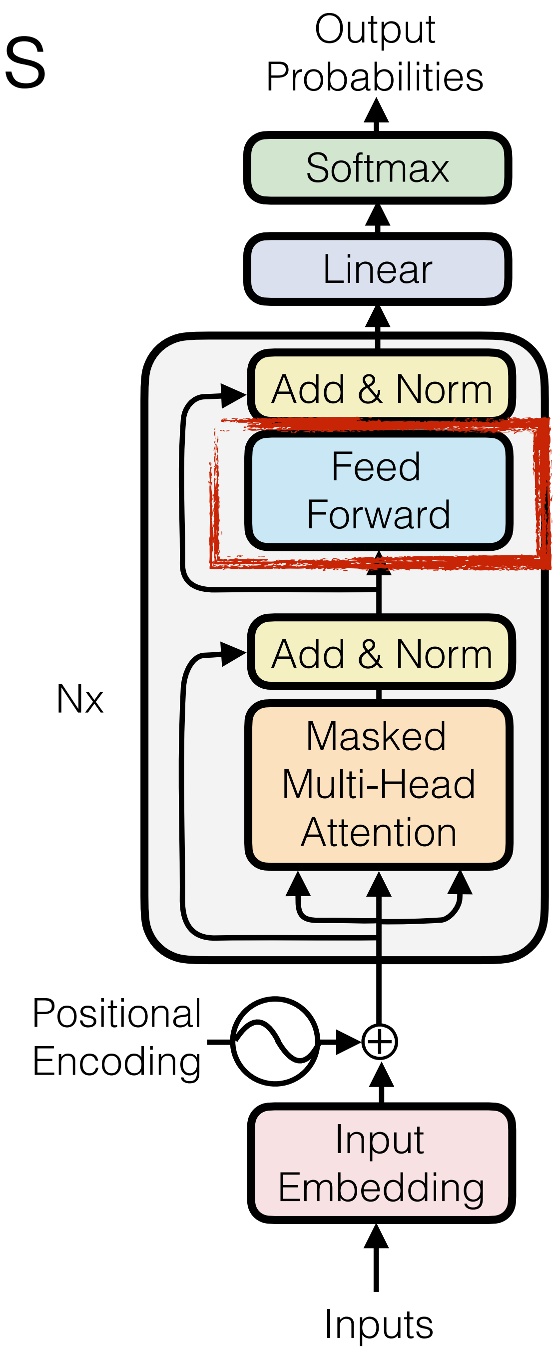
Feed Forward Layers

Feed Forward Layers

- Extract features from the attended outputs

$$\mathrm{FFN}(x; W_1, \mathbf{b}_1, W_2, \mathbf{b}_2) = f(\mathbf{x}W_1 + \mathbf{b}_1)W_2 + \mathbf{b}_2$$





In code

https://github.com/cmu-l3/anlp-fall2025-code/blob/main/05_transformers/transformer.ipynb

In code

```
import torch.nn as nn

class Block(nn.Module):
    def __init__(self, d_model, nhead, dim_ff=64, max_len=128):
        super(Block, self).__init__()
        self.attn = nn.MultiheadAttention(d_model, nhead, dropout=0.0, batch_first=True)
        self.ff1 = nn.Linear(d_model, dim_ff)
        self.ff2 = nn.Linear(dim_ff, d_model)
        self.ln1 = nn.LayerNorm(d_model)
        self.ln2 = nn.LayerNorm(d_model)
        self.act = nn.ReLU()
        self.register_buffer('mask', torch.triu(torch.ones(max_len, max_len), diagonal=1).bool())

    def forward(self, x):
        B, T, D = x.size()

        # Self-attention block
        residual = x
        x = self.ln1(x) # Pre-normalization
        x = self.attn(x, x, x, is_causal=True, attn_mask=self.mask[:T,:T])[0]
        x = residual + x

        # Feed-forward block
        residual = x
        x = self.ln2(x)
        x = self.ff2(self.act(self.ff1(x)))
        x = residual + x
        return x
```

In code

```python
class TransformerLM(nn.Module):
    def __init__(self, vocab_size, d_model, nhead, num_layers, dim_ff, max_len=128):
        super(TransformerLM, self).__init__()
        self.embedding = nn.Embedding(vocab_size, d_model)
        self.pos_encoder = nn.Embedding(max_len, d_model)
        self.blocks = nn.ModuleList([
            Block(d_model, nhead, dim_ff) for _ in range(num_layers)
        ])
        self.fc = nn.Linear(d_model, vocab_size)
        self.d_model = d_model

    def forward(self, x):
        pos = torch.arange(x.size(1), device=x.device).unsqueeze(0)
        x = self.embedding(x) + self.pos_encoder(pos)
        for block in self.blocks:
            x = block(x)
        logits = self.fc(x)
        return logits
```

Today's lecture

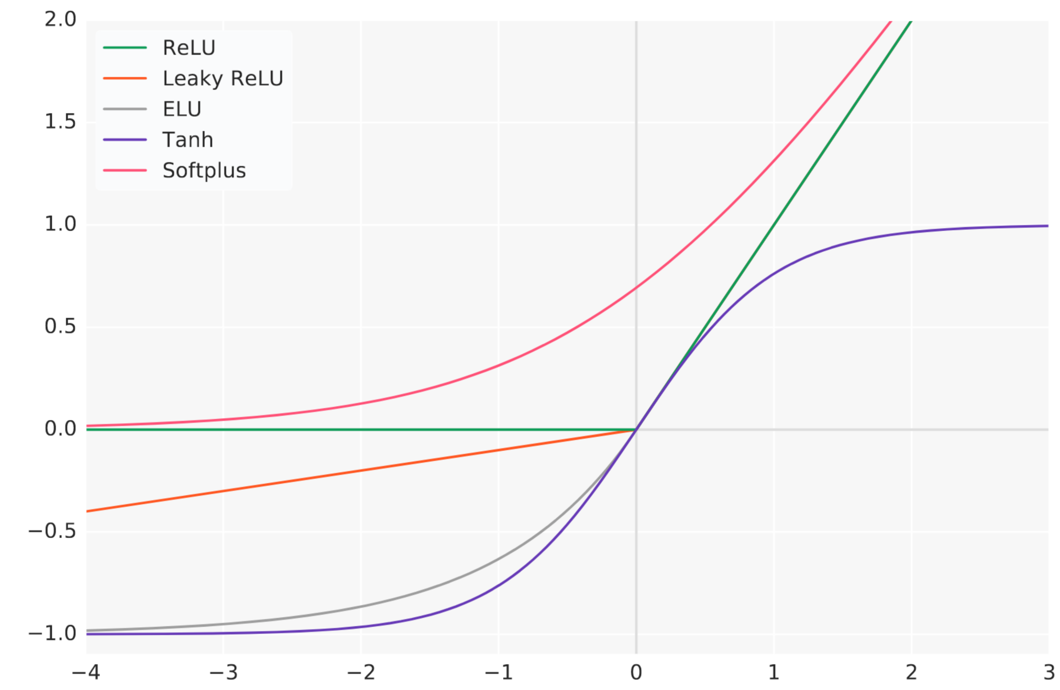
- Roadmap:
  - Attention
  - Transformer architecture
  - **Improved transformer architecture**

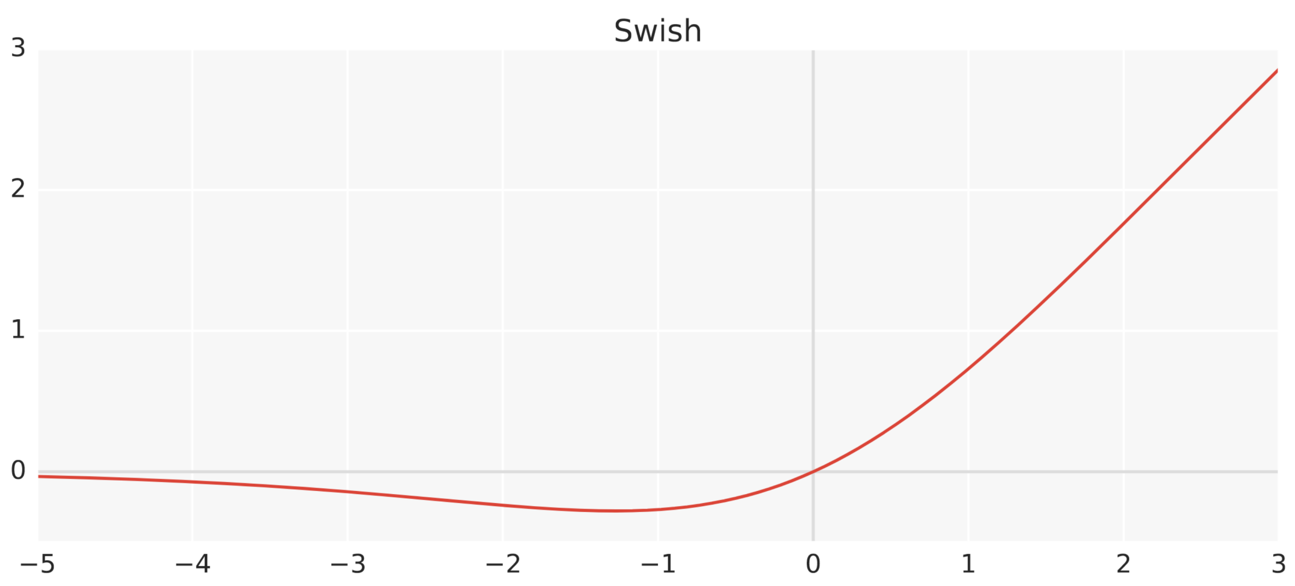
Transformer improvements

SiLU/Swish Activation

[Hendricks & Gimpel 2016, Ramachandran et al 2017]

- Sigmoid: $\sigma(x) = \dfrac{1}{1 + \exp(-x)}$
- ReLU: $f(x) = \max(0, x)$
- SiLU/Swish: $f(x) = x\sigma(x)$
    - Unbounded above
    - Bounded below
    - Non-monotonic
    - Smooth





SwiGLU Feed-Forward Layer [Shazeer 2020]

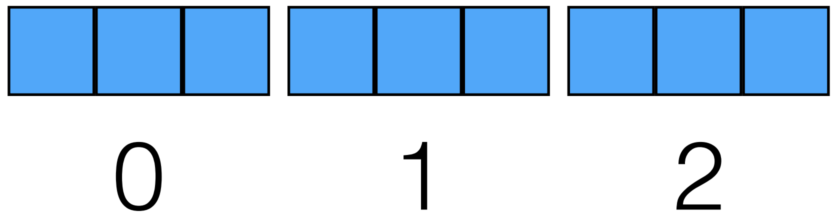
- $\text{FFN}_{\text{relu}} = \max(0, xW_1)W_2$
- $\text{FFN}_{\text{swish}} = \text{swish}(xW_1)W_2$
- $\text{FFN}_{\text{swiglu}} = (\text{swish}(xW_1) \cdot xW_3)W_2$

"gate"

We have extended the GLU family of layers and proposed their use in Transformer. In a transfer-learning setup, the new variants seem to produce better perplexities for the de-noising objective used in pre-training, as well as better results on many downstream language-understanding tasks. These architectures are simple to implement, and have no apparent computational drawbacks. We offer no explanation as to why these architectures seem to work; we attribute their success, as all else, to divine benevolence.

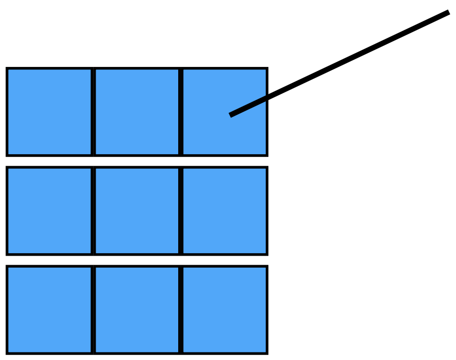
Relative Positional Encodings (Shaw+ 2018)

- **Absolute** positional encodings



- **Relative** positional encodings *explicitly* encode relative position
  - Example: inside attention layer:
    - $e_{ij} = \frac{q_i^\top k_j}{\sqrt{d_h}} + \frac{q_i^\top r_{i-j}}{\sqrt{d_h}}$
    - $\alpha_{ij} = \text{softmax}_j(e_{ij})$
    - $R \in \mathbb{R}^{(2K+1)\times d}$, rows r_Δ with $\Delta \in [-K, K]$

"Token 0 and token 2 are 2 - 0 = 2 tokens apart"



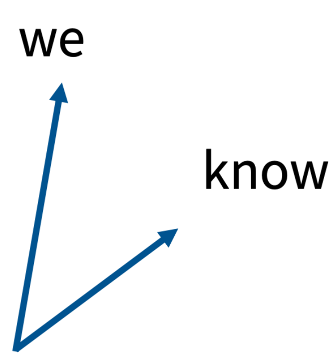
Rotary Positional Encodings (RoPE)

(Su+ 2021)

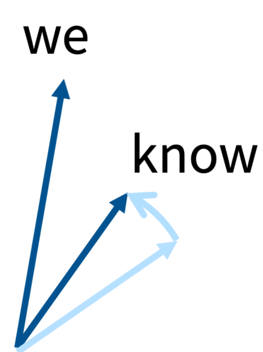
- Goal: we want the dot product of embeddings to result in a function of relative position

$$\langle f(q,t), f(k,t') \rangle = g(q,k,t'-t)$$

- Idea: leverage nice properties of rotations

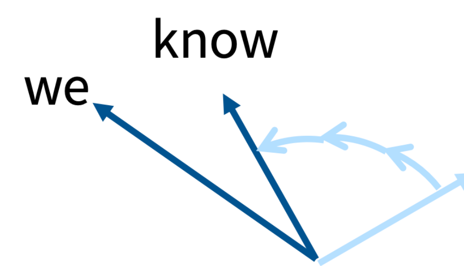


Position independent embedding



Embedding
"we know that"

Rotate we by '0 positions'
know by '1 positions'



Embedding
"of course we know"

Rotate we by '2 positions'
Rotate know by '3 positions'

Credit: Tatsu Hashimoto, cs336

Rotary Positional Encodings (RoPE)

- Recall a rotation matrix, e.g. in 2D: $R_\theta = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$
- We have:
$$(R_{\theta_1} q)^\top (R_{\theta_2} k) = q^\top R_{\theta_1}^\top R_{\theta_2} k$$
$$= q^\top R_{\theta_2 - \theta_1} k$$
- Dot product only depends on the difference between θ_2 and θ_1!
- RoPE key idea: encode positions t based on rotation matrices $R_{t\theta}$:
  - $R_{t\theta}^\top R_{t'\theta} = R_{(t'-t)\theta}$

Rotary Positional Encodings (RoPE)

- Example:
  - $f(q, t) = R_t W_q q$ where R_t is

$$R_t = \begin{pmatrix} \cos t\theta_1 & -\sin t\theta_1 & 0 & 0 & \cdots & 0 & 0 \\ \sin t\theta_1 & \cos t\theta_1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cos t\theta_2 & -\sin t\theta_2 & \cdots & 0 & 0 \\ 0 & 0 & \sin t\theta_2 & \cos t\theta_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & \cos t\theta_{d/2} & -\sin t\theta_{d/2} \\ 0 & 0 & 0 & 0 & \cdots & \sin t\theta_{d/2} & \cos t\theta_{d/2} \end{pmatrix}$$

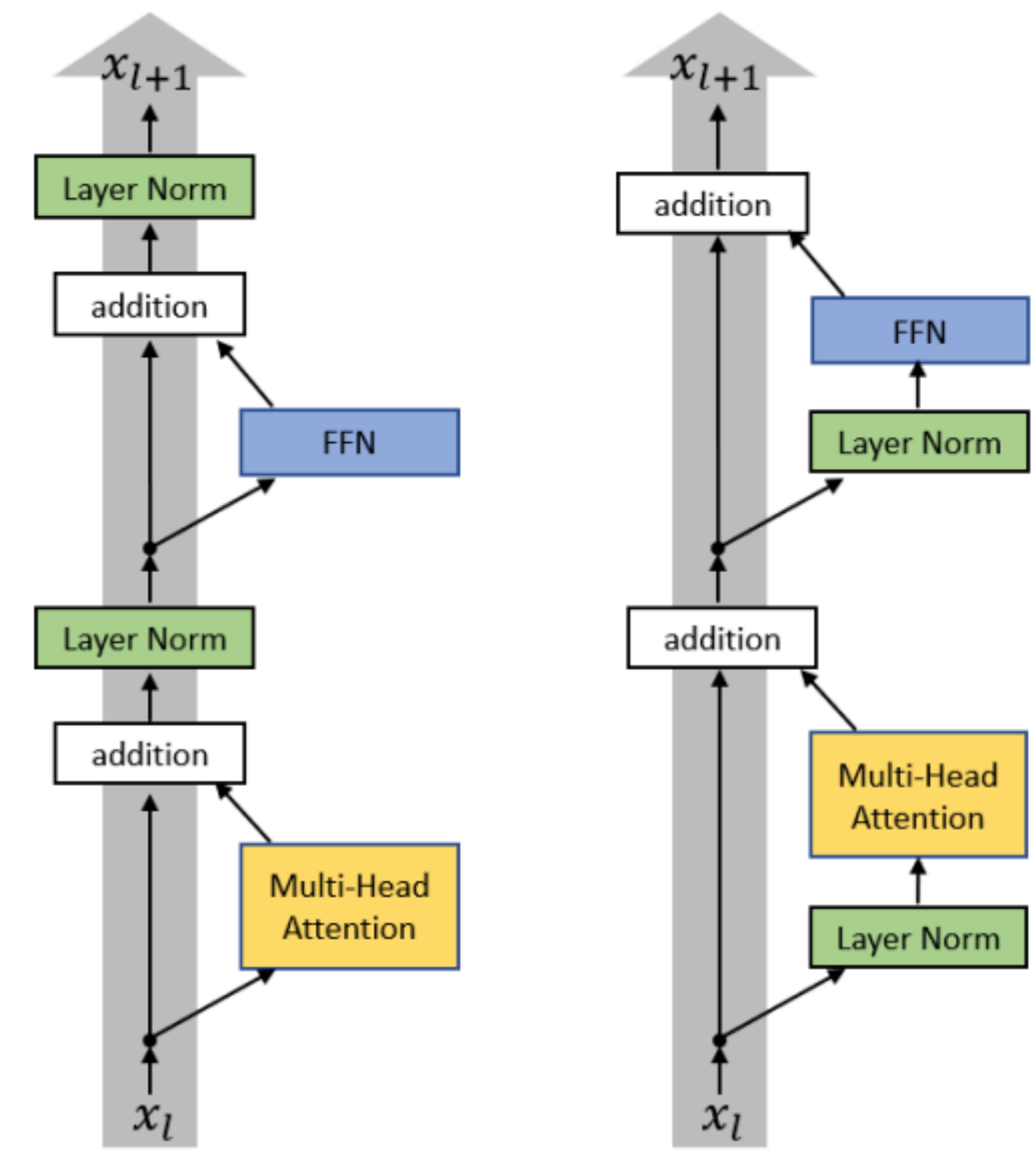
- t :Position in sequence

$$\theta_i = 10000^{-2i/d}$$

- Small i: high frequency
- Large i: low frequency

Pre- Layer Norm
(e.g. Xiong et al. 2020)

- Where should LayerNorm be applied? Before or after?
- Pre-layer-norm is better for gradient propagation



post-LayerNorm pre-LayerNorm

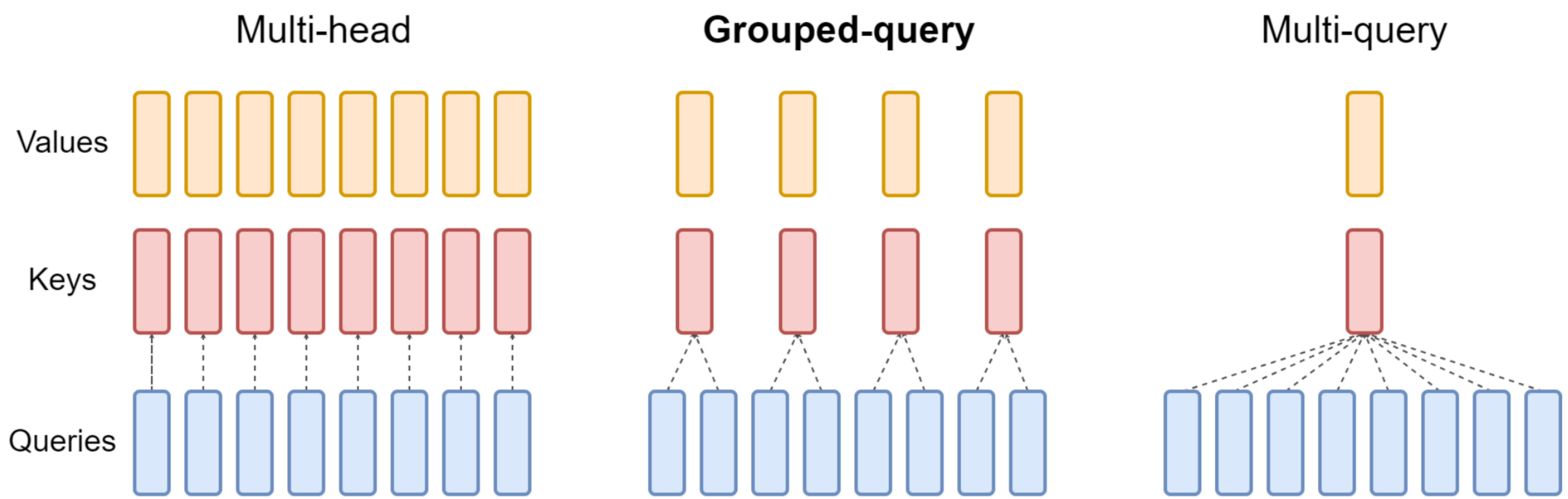
RMSNorm
(Zhang and Sennrich 2019)

- Simplifies LayerNorm by removing the mean and bias terms

$$\mathrm{RMS}(\mathbf{x}) = \sqrt{\frac{1}{n}\sum_{i=1}^{n} x_i^2}$$

$$\mathrm{RMSNorm}(\mathbf{x}) = \frac{\mathbf{x}}{\mathrm{RMS}(\mathbf{x})} \cdot \mathbf{g}$$

Grouped-query attention



- Shares key and value heads for each *group* of query heads
- Saves on memory, which leads to faster inference

In code

```
bsz, seqlen, _ = x.shape
xq, xk, xv = self.wq(x), self.wk(x), self.wv(x)

xq = xq.view(bsz, seqlen, self.n_local_heads, self.head_dim)
xk = xk.view(bsz, seqlen, self.n_local_kv_heads, self.head_dim)
xv = xv.view(bsz, seqlen, self.n_local_kv_heads, self.head_dim)
```

```
# repeat k/v heads if n_kv_heads < n_heads
keys = repeat_kv(keys, self.n_rep)  # (bs,
values = repeat_kv(values, self.n_rep)  #
```

https://github.com/meta-llama/llama/blob/main/llama/model.py

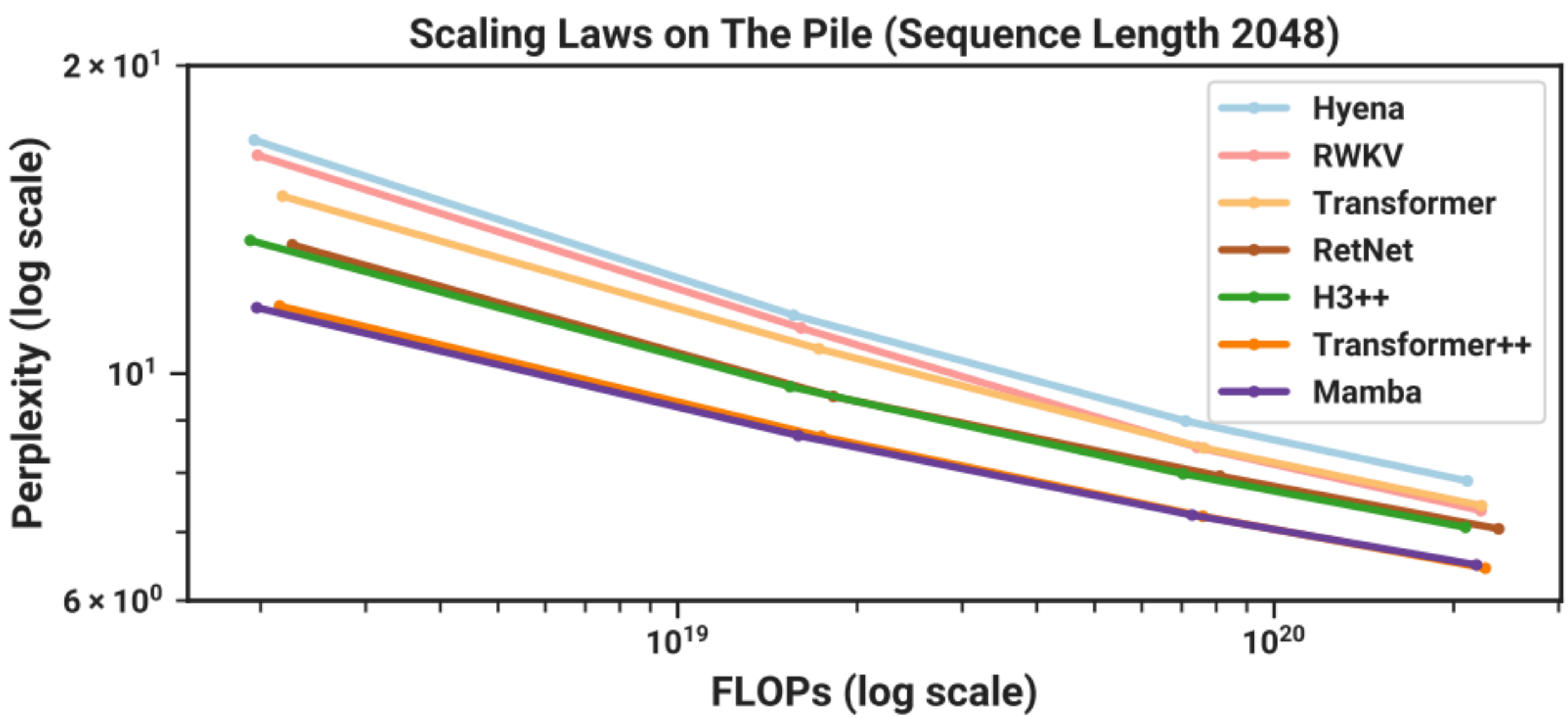
Original Transformer vs. LLama

	Vaswani et al.	LLama	Llama 2
Norm Position	Post	**Pre**	**Pre**
Norm Type	LayerNorm	**RMSNorm**	**RMSNorm**
FFN/ Activation	ReLU	**SwiGLU**	**SwiGLU**
Positional Encoding	Sinusoidal	**RoPE**	**RoPE**
Attention	Multi-head	Multi-head	**Grouped-query**

S: Gemma 2

How Important is It?

- “Transformer” is Vaswani et al., “Transformer++” is (basically) LLaMA2



- Stronger architecture is ≈10x more efficient!

Image: Gu and Dao (2023)

Recap

- **Transformer**: a sequence model based on attention
- We saw:
  - Attention
  - Transformer architecture
  - Improved transformer architecture

Additional topics

- Adam optimizer
- Transformer vs. RNN

Optimizer: Adam

- Most standard optimization option in NLP and beyond
  - Each parameter has an adaptive learning rate
  - Incorporates 2 key ideas: momentum and RMSProp

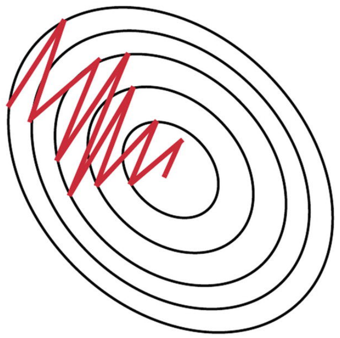
Optimizer: Adam

- Momentum

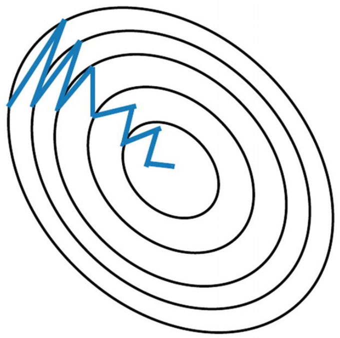
$$\theta_{t+1} = \theta_t - \alpha m_t$$

$$m_t = \beta_1 m_{t-1} + (1 - \beta_1) \nabla_\theta$$

Intuition: reduces oscillations



Stochastic Gradient Descent **withhout** Momentum



Stochastic Gradient Descent **with** Momentum

source

- $m_t \in \mathbb{R}^{|\theta|}$, i.e. per-parameter adjustment
- Running estimate of $\mathbb{E}[\nabla_\theta]$

Optimizer: Adam

- RMSProp

$$\theta_{t+1} = \theta_t - \frac{\alpha_t}{\sqrt{v_t + \epsilon}} \nabla_\theta$$

$$v_t = \beta_2 v_{t-1} + (1 - \beta_2)(\nabla_\theta)^2$$

- v is per-parameter
- Normalizes the update magnitude
  - $(\nabla_\theta[i, j])^2$ large: update gets smaller
  - $(\nabla_\theta[i, j])^2$ small: update gets larger
- Running estimate of $\mathbb{E}[(\nabla_\theta)^2]$

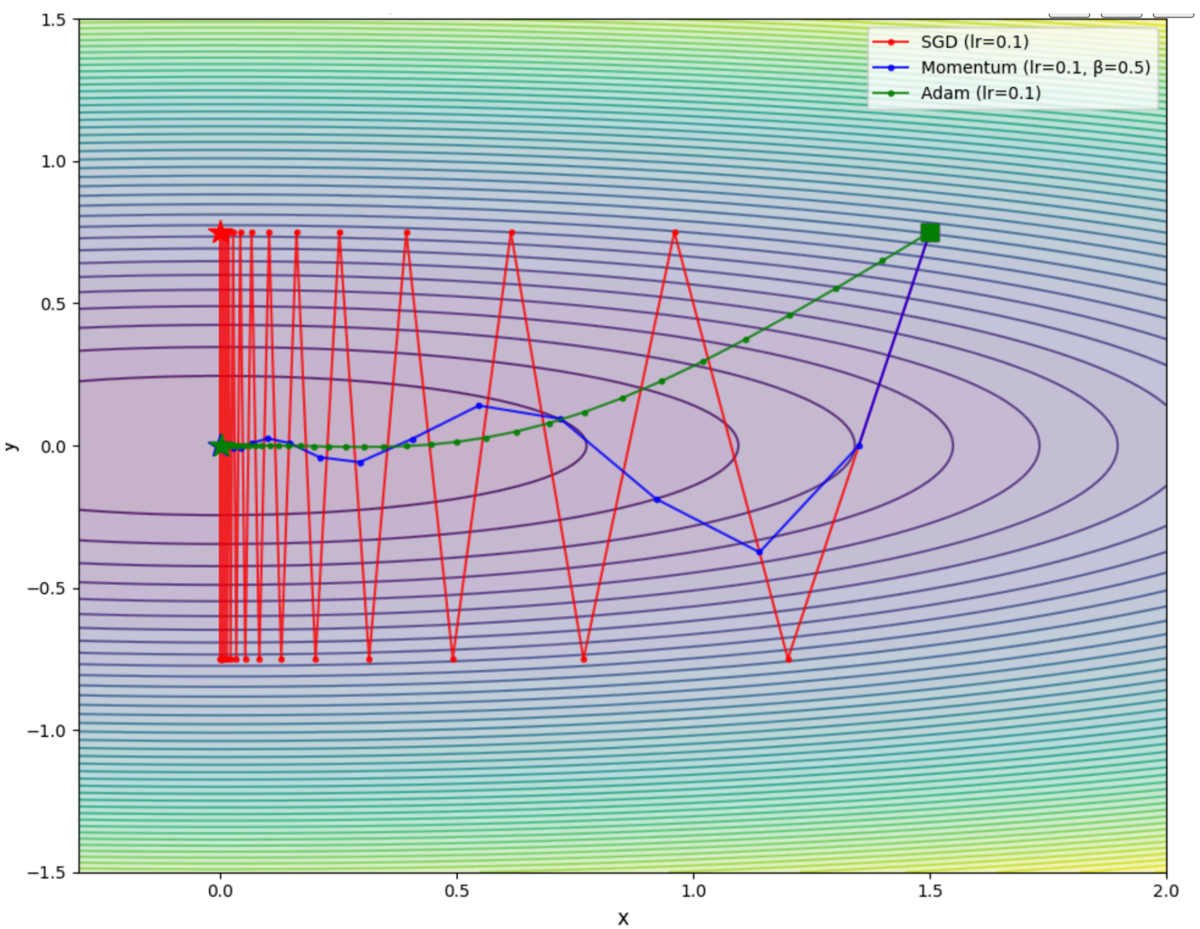
Optimizer: Adam

- Running estimate of $\mathbb{E}[\nabla_\theta]$
  $m_t = \beta_1 m_{t-1} + (1-\beta_1)\nabla_\theta$
- Running estimate of $\mathbb{E}[(\nabla_\theta)^2]$
  $v_t = \beta_2 v_{t-1} + (1-\beta_2)(\nabla_\theta)^2$
- Correction of early bias

$$\hat{m}_t = \frac{m_t}{1-(\beta_1)^t} \quad \hat{v}_t = \frac{v_t}{1-(\beta_2)^t}$$

- Final update

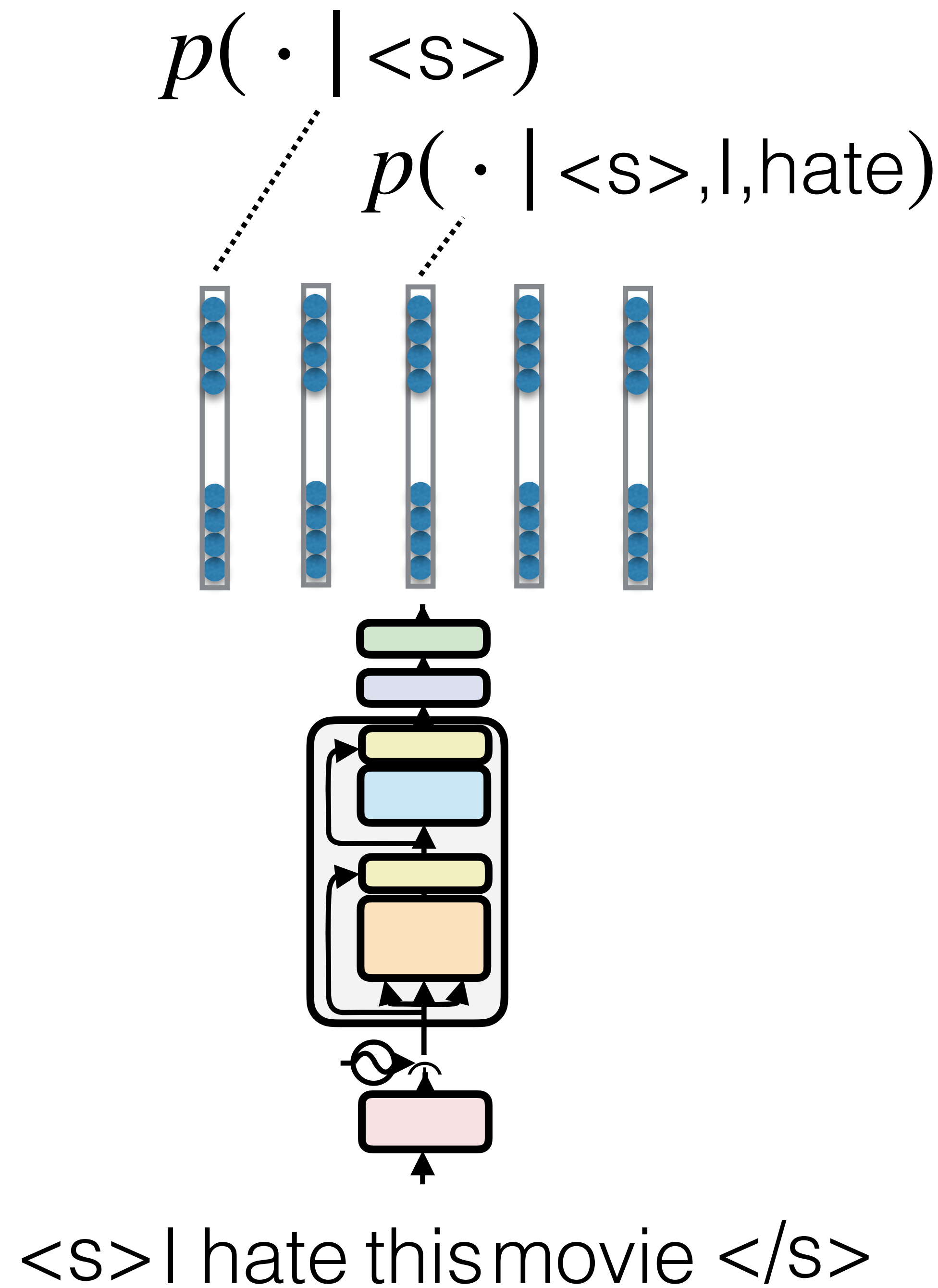
$$\theta_t = \theta_{t-1} - \frac{\eta}{\sqrt{\hat{v}_t}+\epsilon}\hat{m}_t$$



Transformer vs RNN

Transformer Training

- We can compute next-token probabilities for *all* positions at once using matrix multiplications
- No sequential hidden state (as in RNNs)
- Modern hardware (e.g. GPU) is optimized for parallel operations like the matrix multiplications in self-attention
- ∴ easy-to-parallelize training



RNNs vs. Transformers

- RNN: $O(Td^2)$
  - At each step $1, \ldots, T$, a $O(d^2)$ operation, e.g. Wh
- Transformer attention: $O(T^2 d)$
  - E.g., QK^{T}
    - $Q \in \mathbb{R}^{T \times d}$
    - $K \in \mathbb{R}^{T \times d}$ => $O(T^2 d)$

Key difference:
T (RNNs)
T^2 (Transformers)

RNNs vs. Transformers

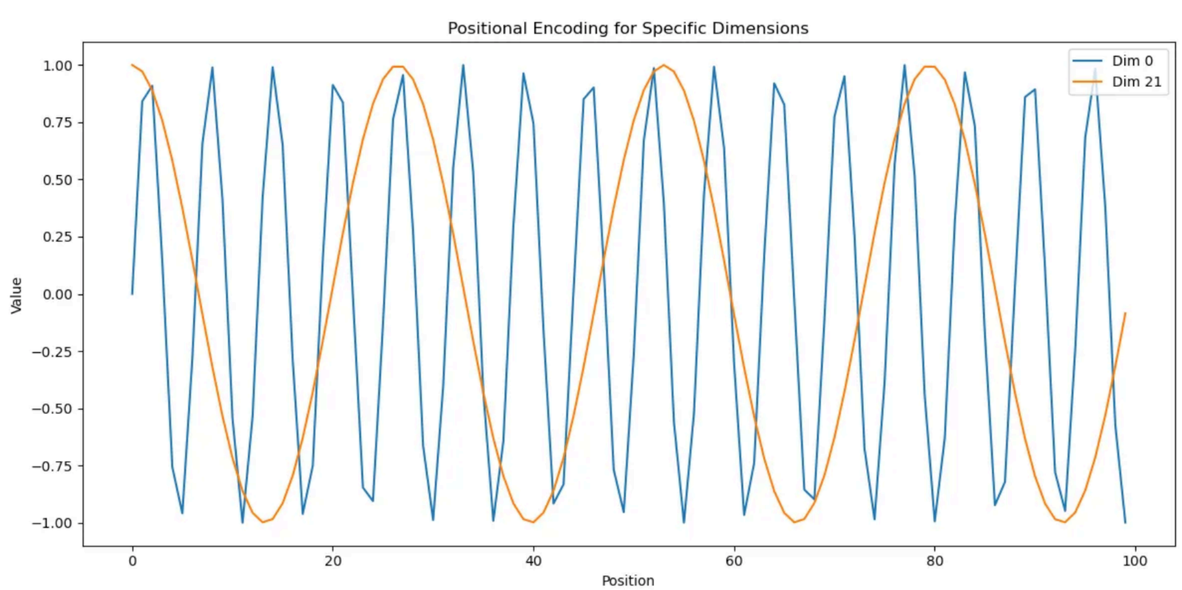
- Transformers: $O(T^2 d)$
  - Quadratic in sequence length T
    - Need to store a large $T \times T$ matrix in memory
    - Need to perform $O(T^2 d)$ computations
  - Easy to parallelize the training
  - Long-range dependency: handled by attention

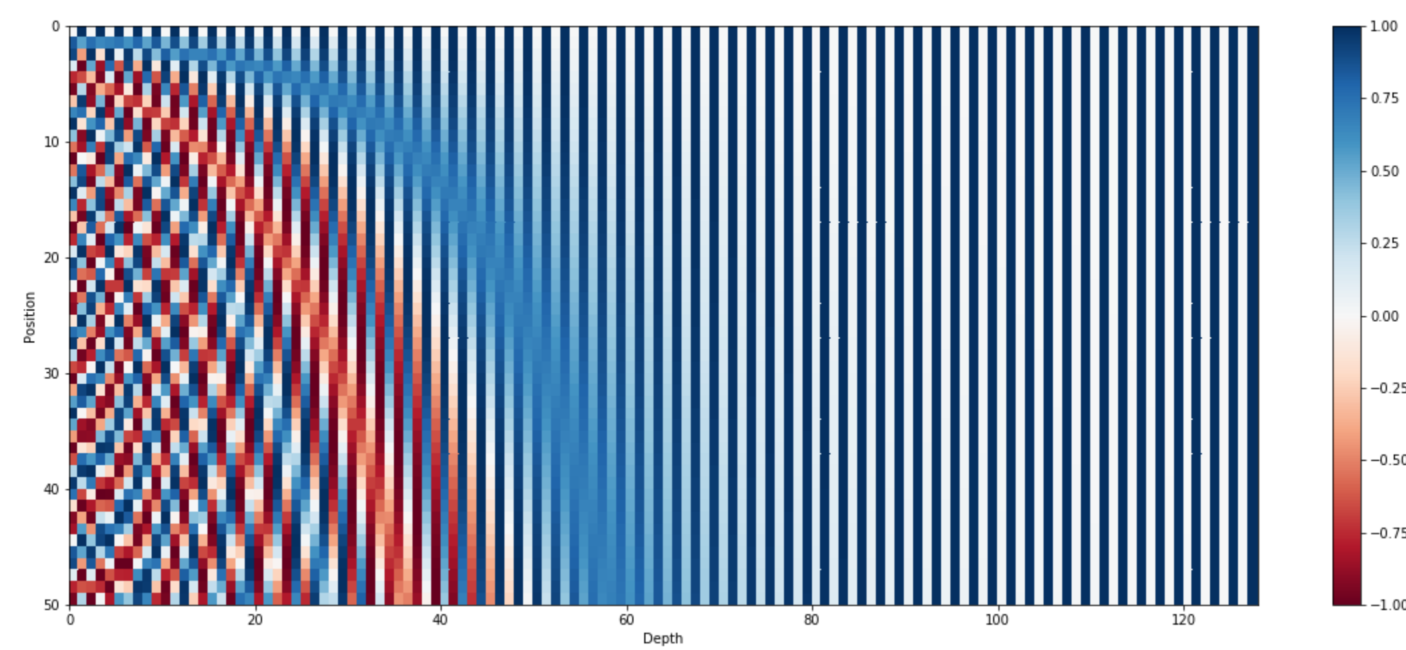
Thank you

Sinusoidal Encoding
(Vaswani+ 2017, Kazemnejad 2019)

- Calculate each dimension with a sinusoidal function

$$p_t^{(i)} = f(t)^{(i)} := \begin{cases} \sin(\omega_k \cdot t), & \text{if } i = 2k \\ \cos(\omega_k \cdot t), & \text{if } i = 2k+1 \end{cases} \quad \text{where} \quad \omega_k = \frac{1}{10000^{2k/d}}$$





- Motivation: may be easy to learn relative positions, since PE_{pos+k} is a linear function of PE_{pos}