



# Artificial Neural Networks

[2500WETANN]

José Oramas



# Modeling Sequences with Neural Networks

José Oramas

# Today's Lecture – Outline

- **Intro/Recap - Sequence Modeling**

→ [Algorithmically] How to approach the problem

- **Sequence Modeling with Recurrent Architectures**

→ RNNs, LSTMs, GRUs, etc.

- **Predictions from Sequences & Sequence Generation**

- **Transformers and Attention Mechanisms**

# Recap: Supervised Image Recognition Task

**Given:** an input image  $x$

**Do:** predict a label  $\hat{y}$

( out of a set of class labels )



- Training data

$$\{x, y\}_i$$

- Model

$$\hat{y} \approx f_{\theta}(x)$$

- Loss

$$L(\theta) = \sum_{i=1}^N l(f_{\theta}(x_i), y_i)$$

- Optimization

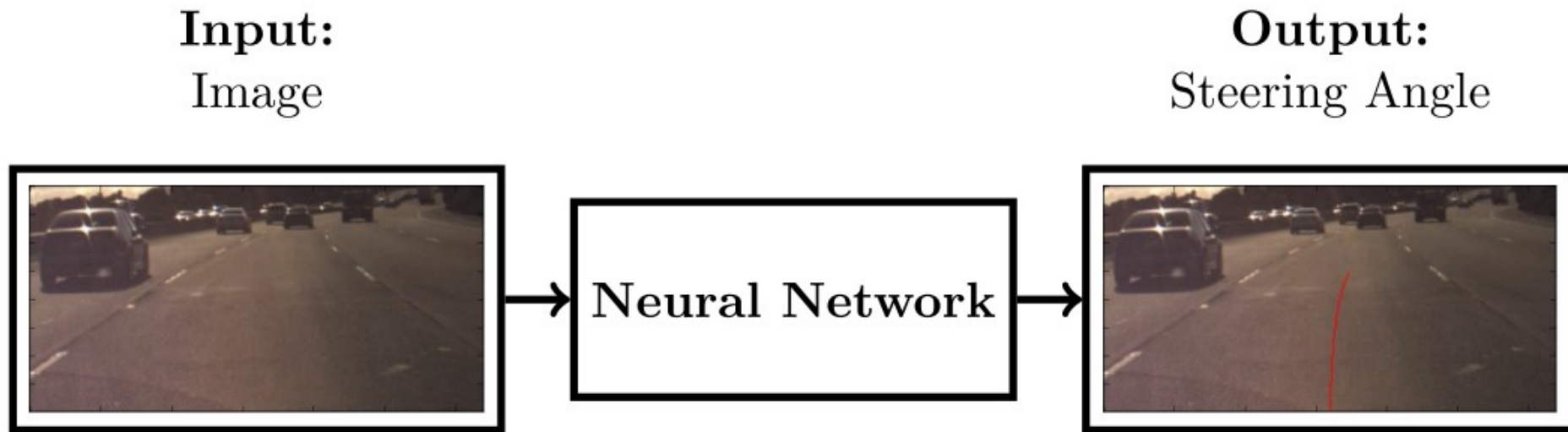
$$\theta^* = \arg \min_{\theta} L(\theta)$$



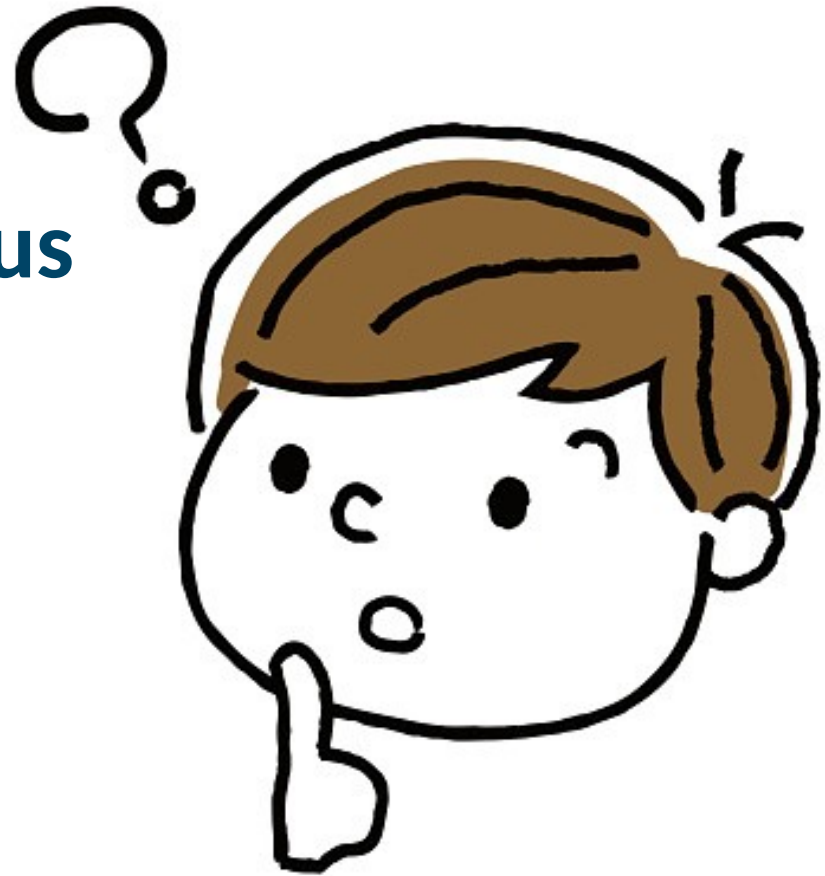
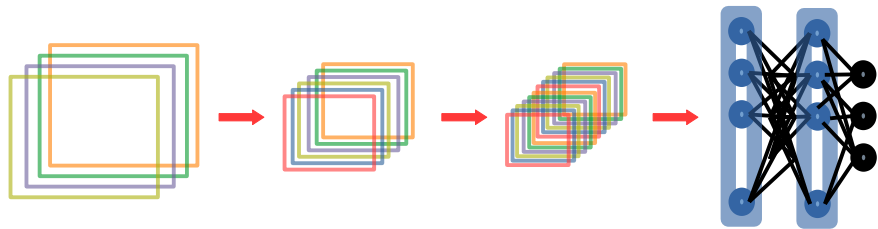
# Now: Consider the Following Problem

## Autonomous Driving

- **Given:** an input video  $x$  ( *sequence of images* )
- **Do:** predict a label  $\hat{y}$  ( *out of a set of action class labels* )



Ok, but...  
Can't we use the previous  
architectures for that ?

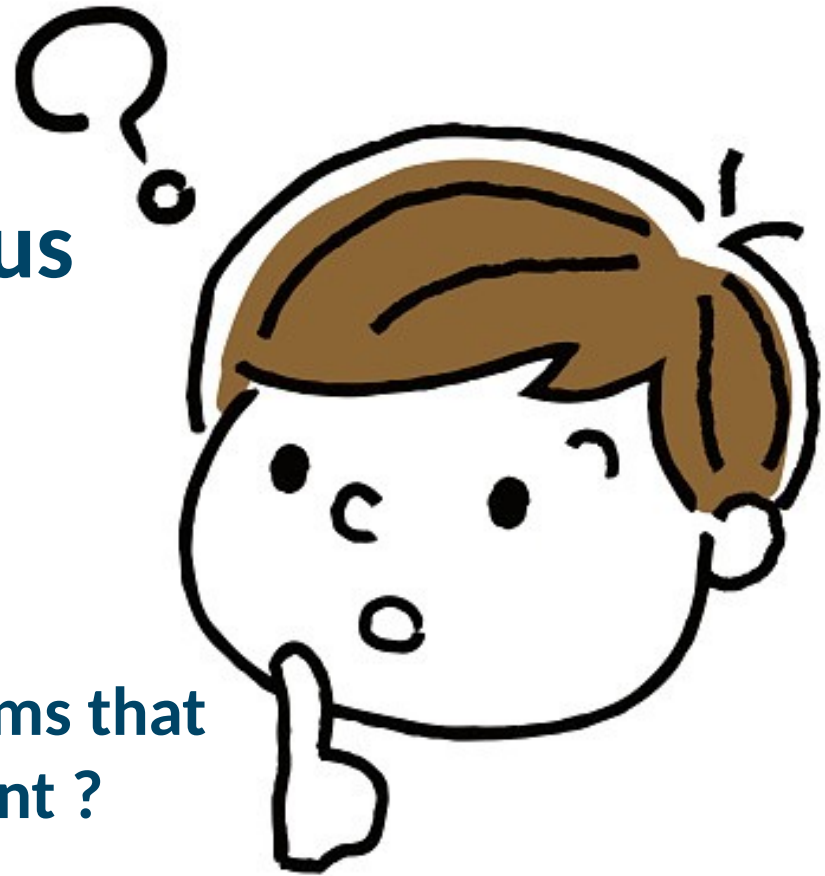


Ok, but...

**Can't we use the previous architectures for that ?**

and ...

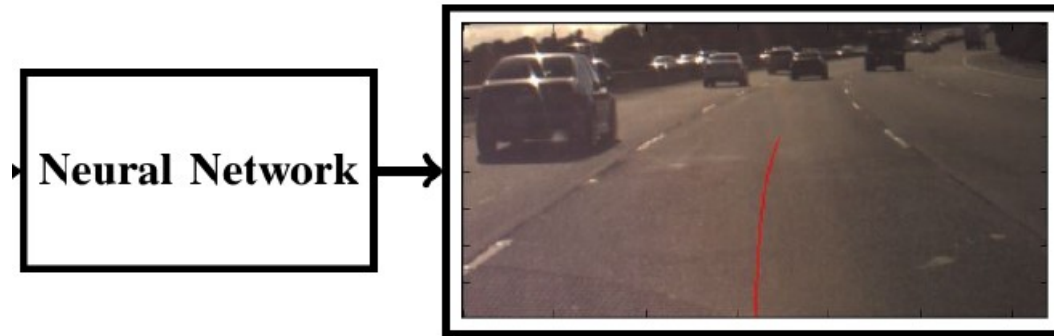
**Are there any other problems that we need to take into account ?**



# Autonomous Navigation Task

## Stacking Elements from the Sequence

**Output:**  
Steering Angle

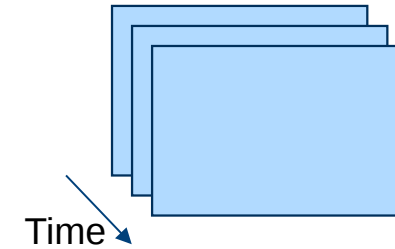
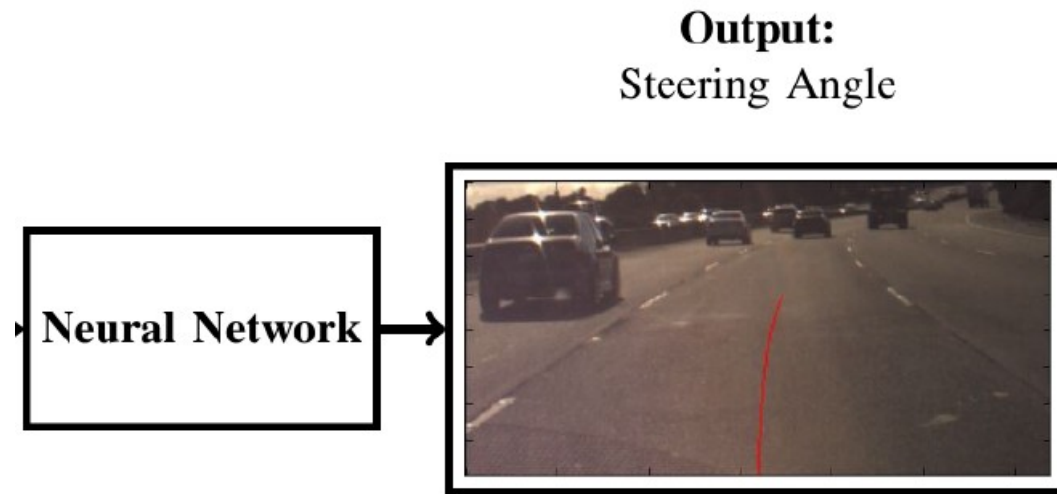


[Heylen et al., 2018]



# Autonomous Navigation Task

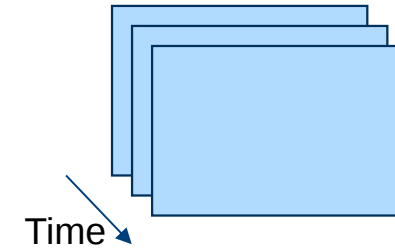
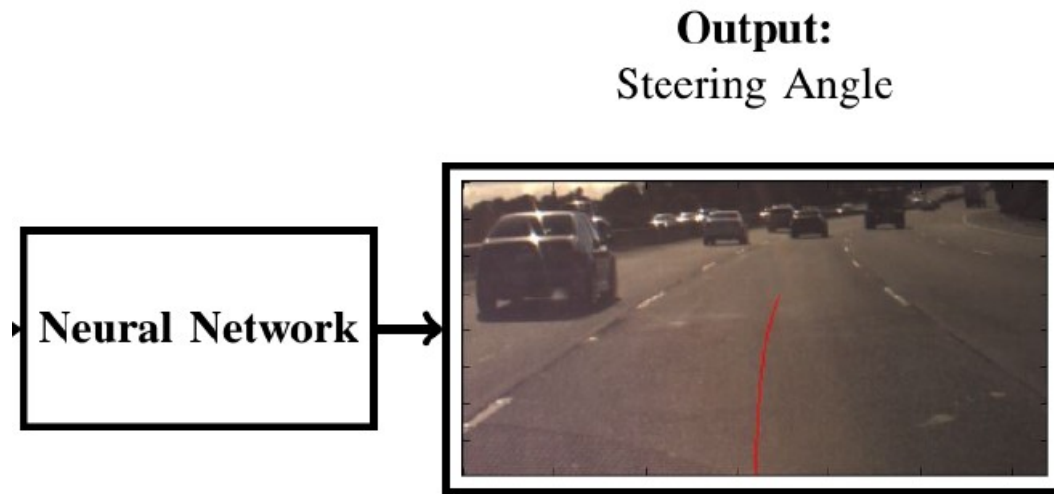
## Stacking Elements from the Sequence



[Heylen et al., 2018]

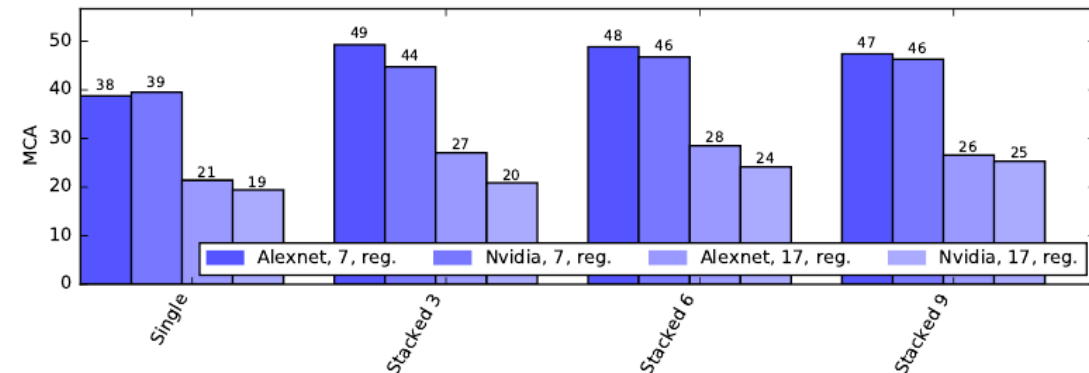
# Autonomous Navigation Task

## Stacking Elements from the Sequence



## Observations

- Considering sequence helps
- Reduced gains as we go further... why?



[Heylen et al., 2018]

# Modeling Data Sequences

[ How to do it... in theory ]

# Modeling Data Sequences [ in theory ]

## Some Foundations

### ▪ Supervised Learning

#### - Data

$$\{x, y\}_i$$

#### - Model

$$\hat{y} \approx f_{\theta}(x)$$

#### - Loss

$$L(\theta) = \sum_{i=1}^N l(f_{\theta}(x_i), y_i)$$

#### - Optimization

$$\theta^* = \arg \min_{\theta} L(\theta)$$

# Modeling Data Sequences [ in theory ]

## Some Foundations

### ▪ Supervised Learning

#### - Data

$$\{x, y\}_i$$

#### - Model

$$\hat{y} \approx f_{\theta}(x)$$

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$$L(\theta) = \sum_{i=1}^N l(f_{\theta}(x_i), y_i)$$

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### ▪ Modeling Sequences

#### - Data

$$\{x\}_i$$

#### - Model

$$p(x) \approx f_{\theta}(x)$$

#### - Loss

$$L(\theta) = \sum_{i=1}^N \log p(f_{\theta}(x_i))$$

#### - Optimization

$$\theta^* = \arg \max_{\theta} L(\theta)$$

# Modeling Data Sequences

[ How to do it... in practice ]



# Modeling Data Sequences [ in theory ]

**Lets consider the following sequence**

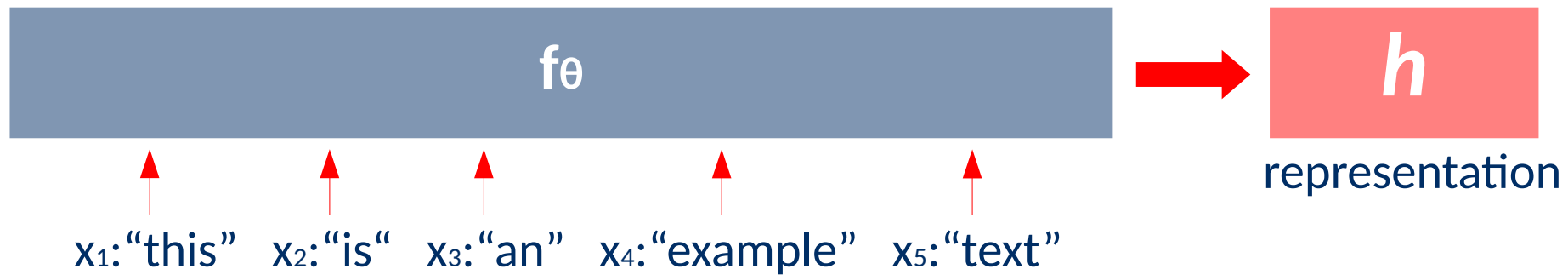
- **Idea:** Let's focus on natural language → text

[ “this” , “is” , “an” , “example” , “text” , “sequence” ]

# Modeling Data Sequences [ in practice ]

## 1. Describing/Vectorizing the Context

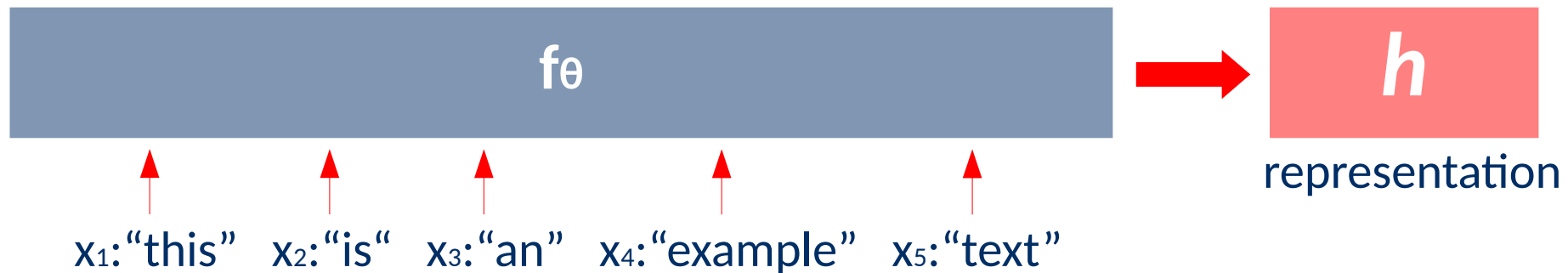
- **Idea:** Learn how to represent a sub-sequence



# Modeling Data Sequences [ in practice ]

## 1. Describing/Vectorizing the Context

- **Idea:** Learn how to represent a sub-sequence



### Desirable properties for $f_\theta$

- Ranked  $\rightarrow$  order matters
- Variable Length
- Learnable  $\rightarrow$  differentiable
- Small changes, large effects  $\rightarrow$  non-linear

# Modeling Data Sequences [ in practice ]

## 2. Modeling Conditional Probabilities

- **Idea:** Predicting the next element given the context



- **Objective:**  $p(x_t|h) \approx p(x_t|x_1, \dots, x_{t-1})$

# Modeling Data Sequences [ in practice ]

## 2. Modeling Conditional Probabilities

- **Idea:** Predicting the next element given the context



- **Objective:**  $p(x_t|h) \approx p(x_t|x_1, \dots, x_{t-1})$

### Desirable properties for $g_\theta$

- Output a distribution over vocabulary
- Small changes, large effects  $\rightarrow$  non-linear

# Recurrent Architectures

[ RNNs, LSTMs, GRUs, etc.]



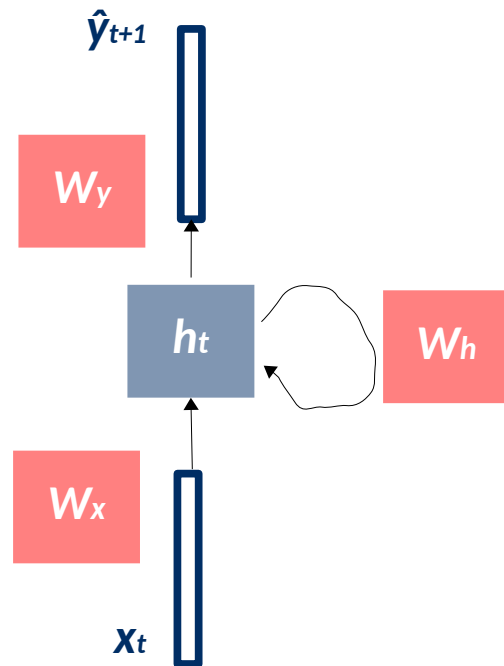
# Recurrent Neural Networks

[ The Most Popular Architecture ]

# Recurrent Neural Networks (RNNs) [ Elman, 1991 ]

## Provide Neural Networks with Memory

- Idea: Use a persistent state  $h$  that encodes past observations (context)



Defined by three equations

$$h_t = \tanh( W_h h_{t-1} + W_x x_t )$$

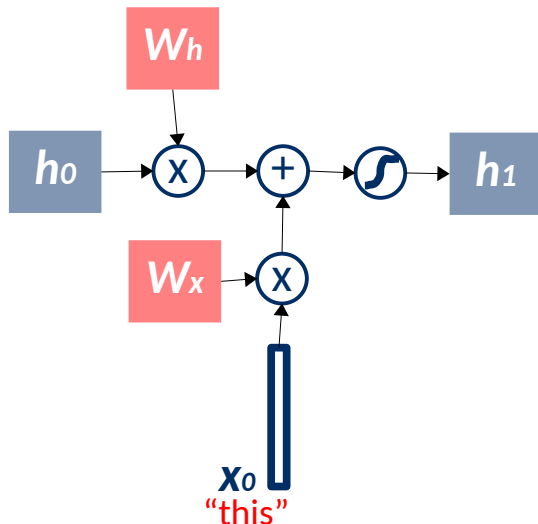
$$p(y_{t+1}) = \text{softmax}( W_y h_t )$$

$$L_{\theta}(y, \hat{y})_t = -y_t \log \hat{y}_t$$

# Recurrent Neural Networks (RNNs) [ Elman, 1991 ]

## Provide Neural Networks with Memory

- **Idea:** Use a persistent state  $h$  that encodes past observations (context)

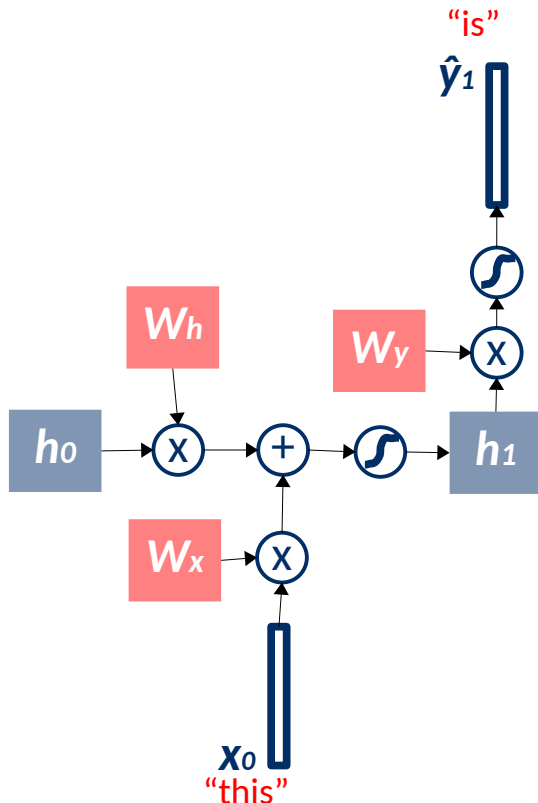


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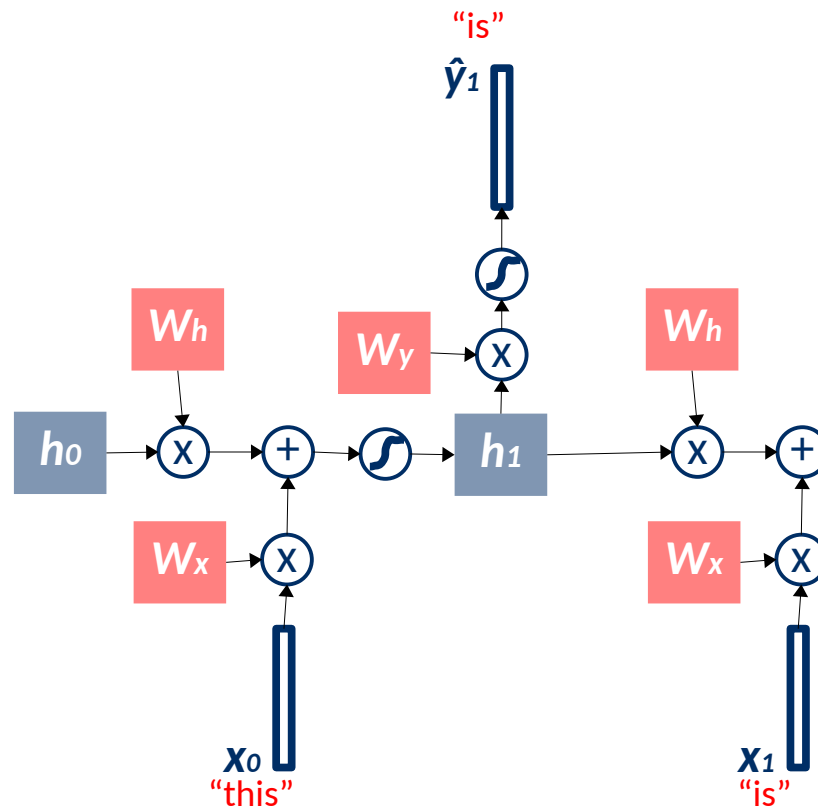
The probability of next element is obtained from the state  $h$

$$p(y_{t+1}) = \text{softmax}(W_y h_t)$$

# Recurrent Neural Networks (RNNs) [ Elman, 1991 ]

## Provide Neural Networks with Memory

- Idea: Use a persistent state  $h$  that encodes past observations (context)

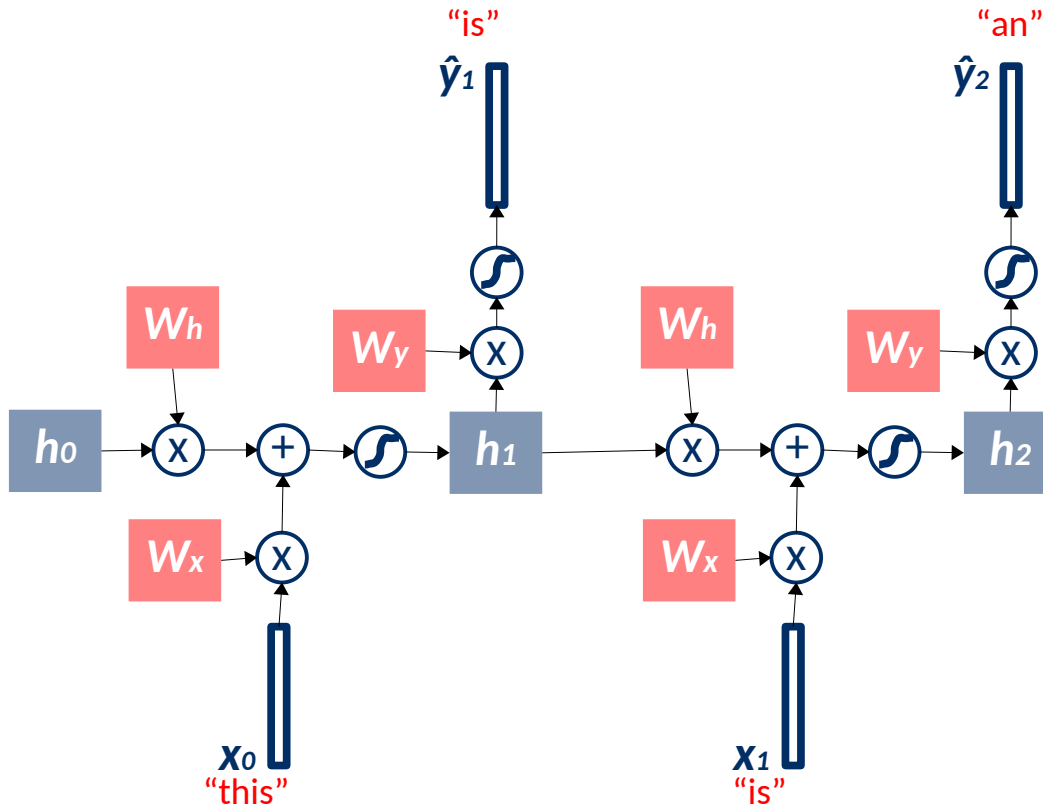


Input the next element  $x_1$  from the sequence

# Recurrent Neural Networks (RNNs) [ Elman, 1991 ]

## Provide Neural Networks with Memory

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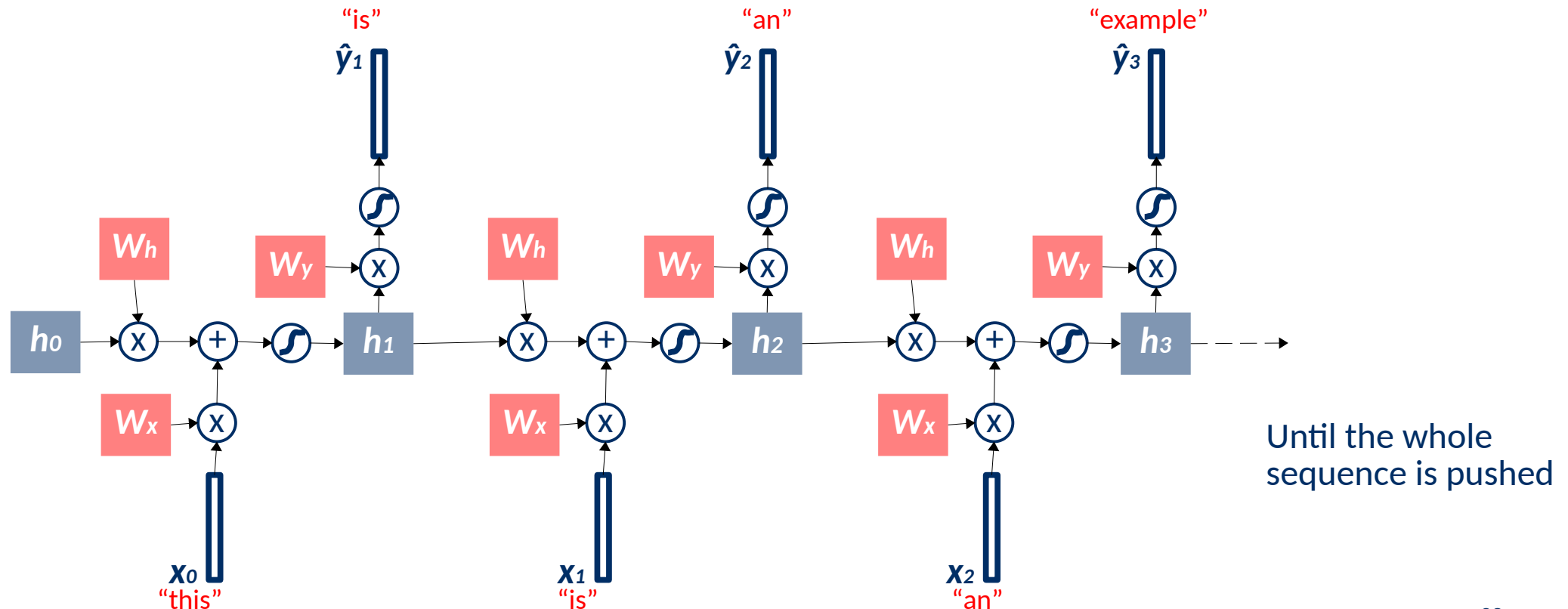
Keep going



# Recurrent Neural Networks (RNNs) [ Elman, 1991 ]

## Provide Neural Networks with Memory

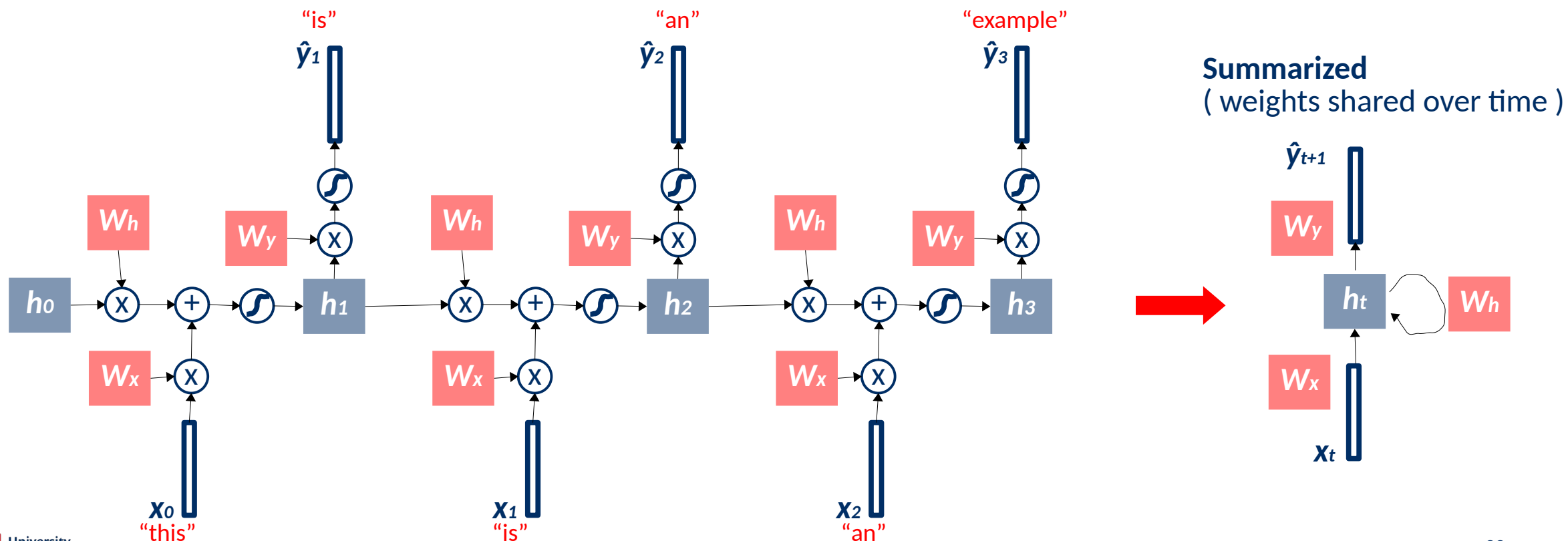
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# Recurrent Neural Networks (RNNs) [ Elman, 1991 ]

## Provide Neural Networks with Memory

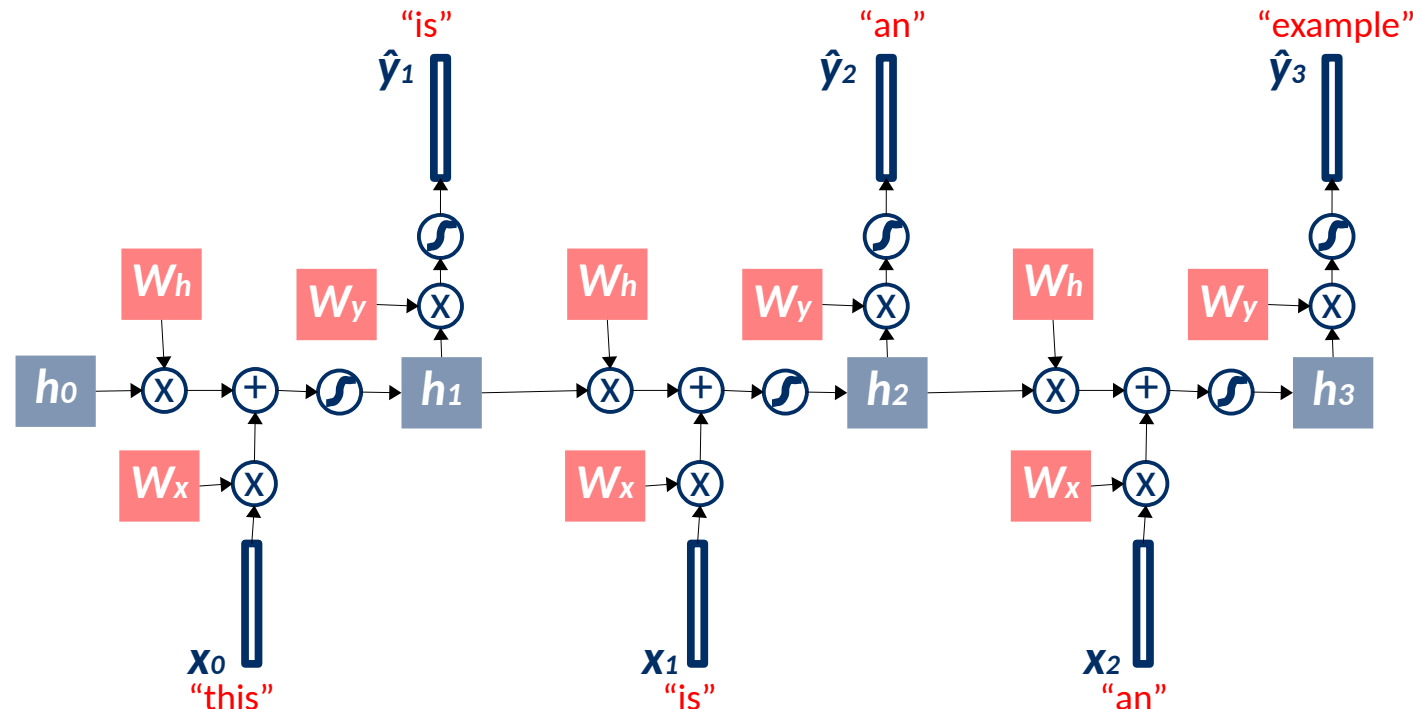
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# Recurrent Neural Networks (RNNs) [ Elman, 1991 ]

## Learning | Training

- **Idea:** Formulate the next-word prediction as a classification problem
- Number of classes = vocabulary\_size  $\rightarrow$  Use the cross-entropy loss.



# Recurrent Neural Networks (RNNs) [ Elman, 1991 ]

## Learning | Training

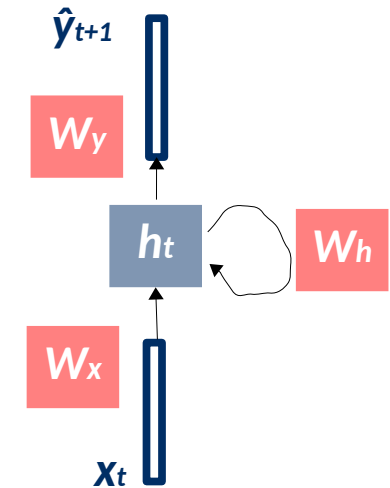
- **Idea:** Formulate the next-word prediction as a classification problem
- Number of classes = vocabulary\_size → Use the cross-entropy loss.

Given a sequence of  $T$  elements:

For one element  $t \rightarrow L_{\theta}(y, \hat{y})_t = -y_t \log \hat{y}_t$

For the sequence  $\rightarrow L_{\theta}(y, \hat{y}) = -\sum_{t=1}^T y_t \log \hat{y}_t$

Trainable parameters  $\rightarrow \theta = \{W_x, W_h, W_y\}$



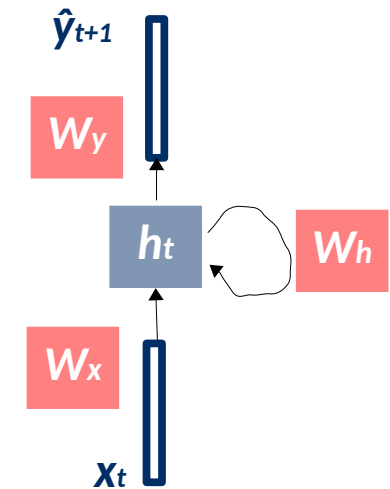
# Recurrent Neural Networks (RNNs) [ Elman, 1991 ]

**Back-Prop. - Differentiation wrt. the parameters**  $\theta = \{W_x, W_h, W_y\}$

$$\begin{aligned} h_t &= \tanh( W_h h_{t-1} + W_x x_t ) \\ p(y_{t+1}) &= \text{softmax}( W_y h_t ) \\ L_\theta(y, \hat{y})_t &= -y_t \log \hat{y}_t \end{aligned}$$

**Differentiating wrt.  $W_y$**

$$\begin{aligned} \frac{\partial L_{\theta,t}}{\partial W_y} &= \frac{\partial L_{\theta,t}}{\partial \hat{y}_t} \frac{\partial \hat{y}_t}{\partial W_y} \\ &= (y_t - \hat{y}_t) h_t \end{aligned}$$



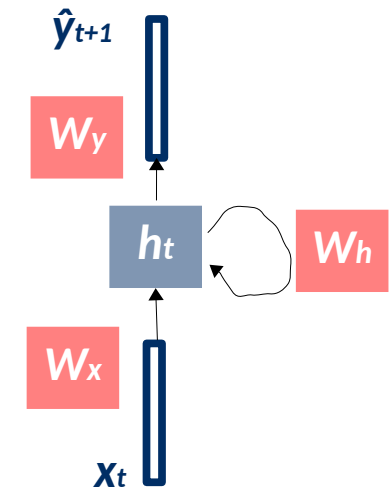
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**Differentiating wrt.  $W_h$**

$$\frac{\partial L_{\theta,t}}{\partial W_h} = \frac{\partial L_{\theta,t}}{\partial \hat{y}_t} \frac{\partial \hat{y}_t}{\partial h_t} \frac{\partial h_t}{\partial W_h}$$





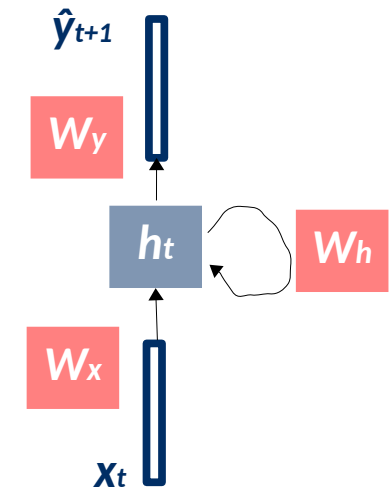
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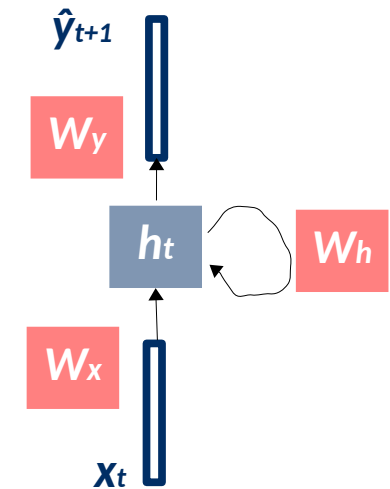
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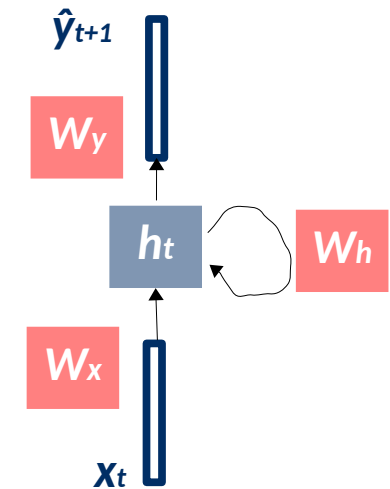
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**Differentiating wrt.  $W_h$**

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# Recurrent Neural Networks (RNNs) [ Elman, 1991 ]

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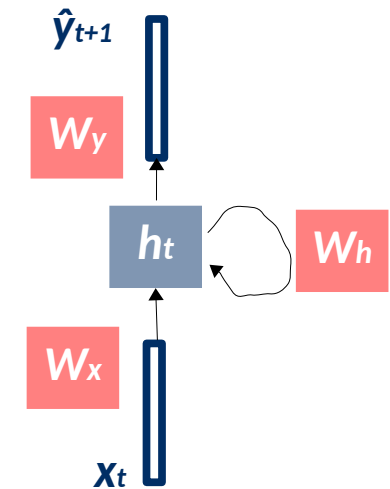
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$$\frac{\partial L_{\theta,t}}{\partial W_h} = \frac{\partial L_{\theta,t}}{\partial \hat{y}_t} \frac{\partial \hat{y}_t}{\partial h_t} \frac{\partial h_t}{\partial W_h}$$

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Back-propagation through time



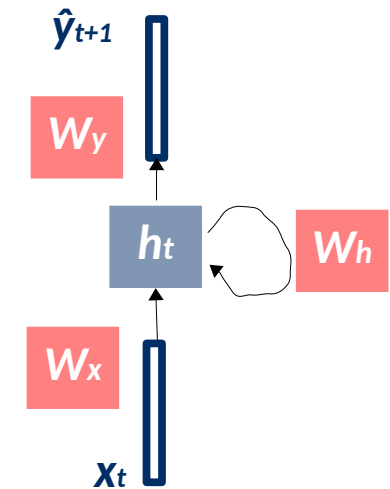
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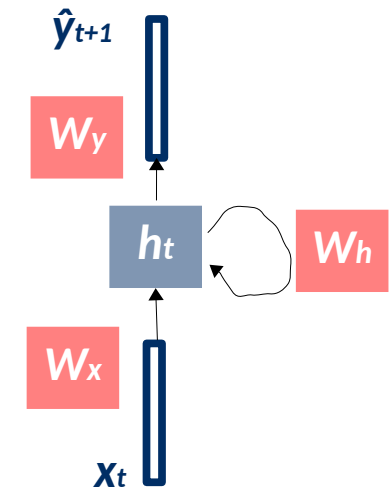
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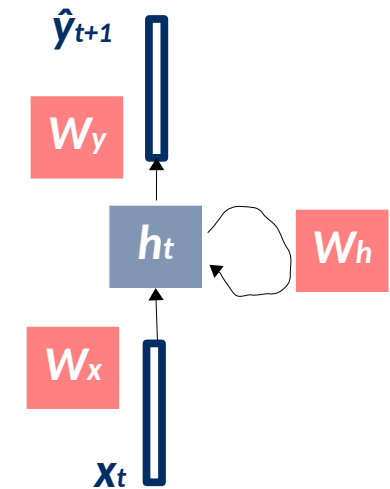
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# Recurrent Neural Networks (RNNs) [ Elman, 1991 ]

## Summarizing

- + Good at modeling sequences of variable length
- + Trainable via Back-Prop. → differentiable
- – Suffer from vanishing gradients for long sequences



# Long Short-Term Memory Networks

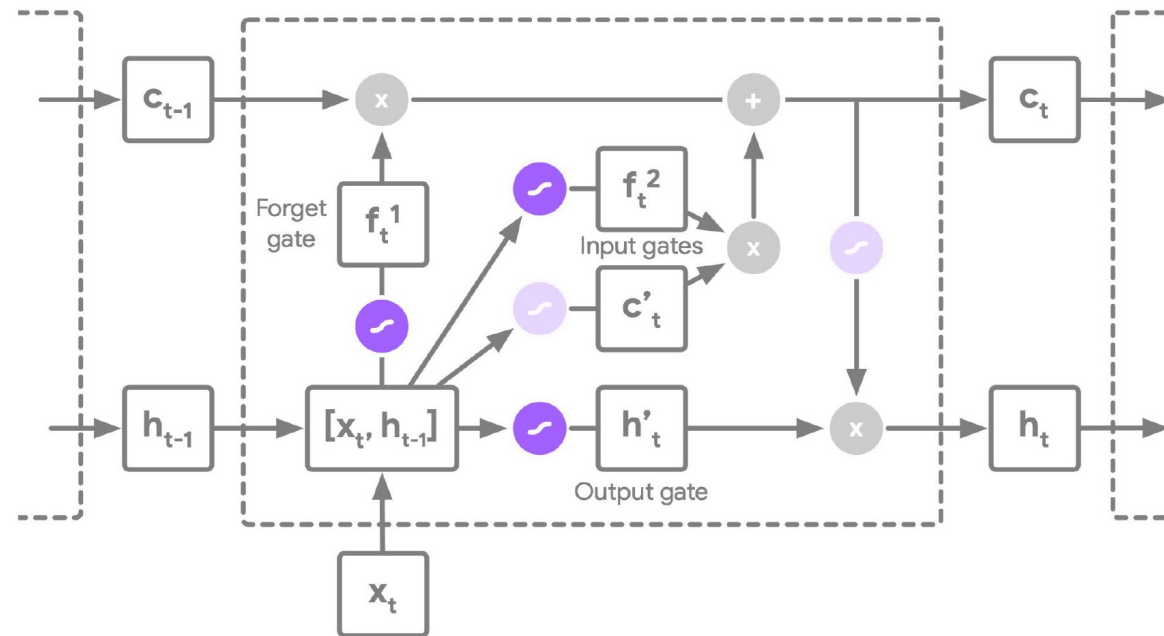
[ RNNs with Extra Memory ]

# Long Short-Term Memory Networks (LSTMs)

[ Hochreiter & Jurgens , 1997 ]

**Provide the capability of choosing what to remember/forget**

- **Idea:** Provide special gates to control the flow of “memories”

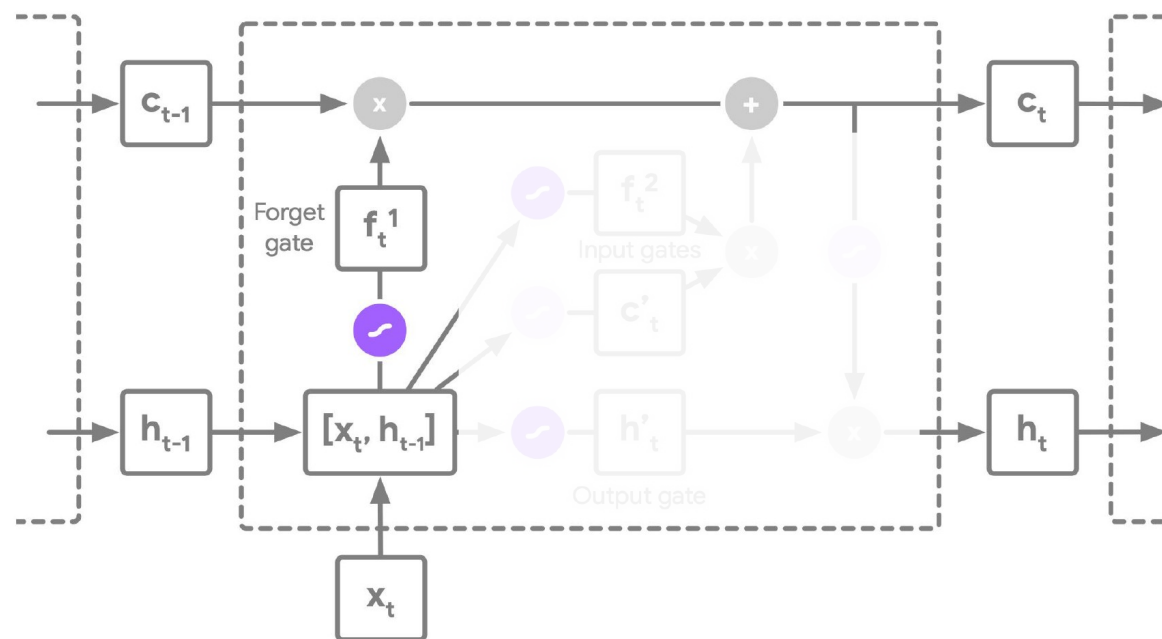


# Long Short-Term Memory Networks (LSTMs)

[ Hochreiter & Jurgens , 1997 ]

Provide the capability of choosing what to remember/forget

- $f_1$ : Forget Gate



regulate what  
information to  
keep/ignore

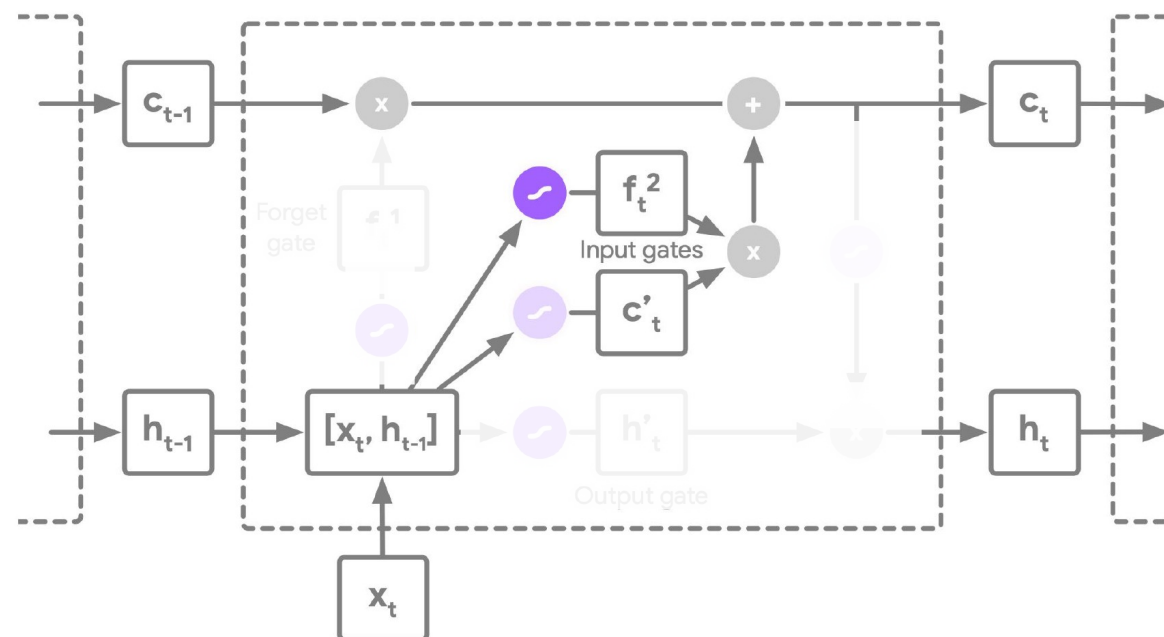
$$f_t^1 = \sigma( W_{f^1} \cdot [h_{t-1}, x_t] + b_{f^1} )$$

# Long Short-Term Memory Networks (LSTMs)

[ Hochreiter & Jurgens , 1997 ]

Provide the capability of choosing what to remember/forget

- $f_2$ : Input Gate



Decides what  
information to  
update

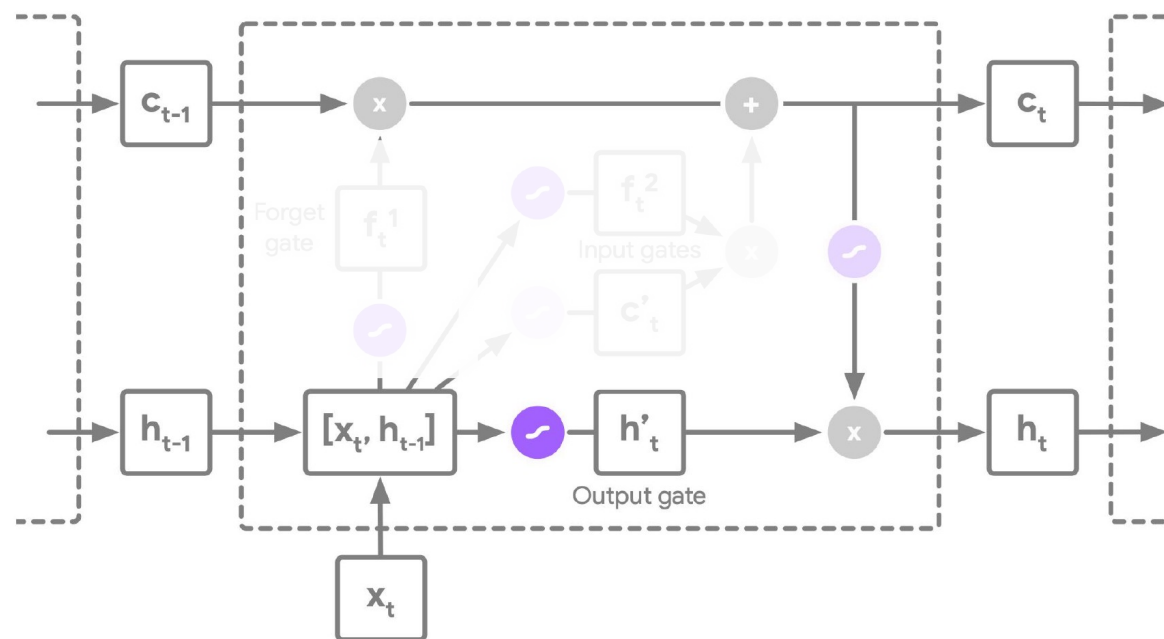
$$= \sigma( W_{f^2} \cdot [h_{t-1}, x_t] + b_{f^2} ) \odot \tanh( W_{c'} [h_{t-1}, x_t] + b_{c'} )$$

# Long Short-Term Memory Networks (LSTMs)

[ Hochreiter & Jurgens , 1997 ]

Provide the capability of choosing what to remember/forget

- $h'_t$ : Output Gate



$$= \sigma( W_{h'_t} \cdot [h_{t-1}, x_t] + b_{h'_t} ) \odot \tanh( c_t )$$

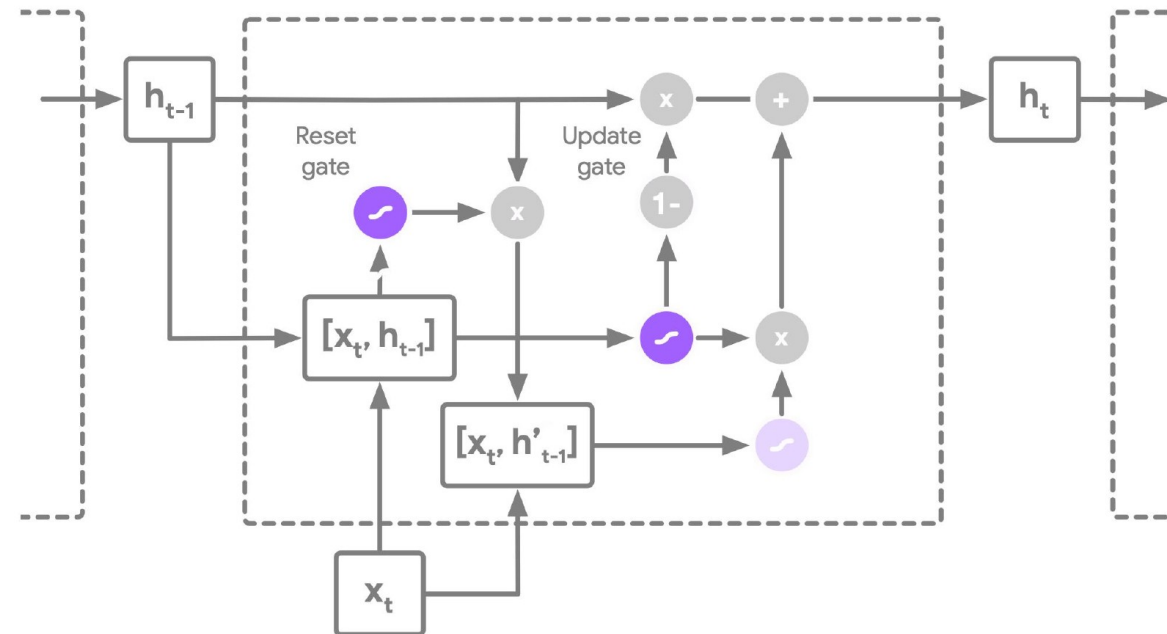
# Gated Recurrent Units

[ A Simplified LSTM ]

# Gated Recurrent Units (GRUs) [ Cho et al. , 2014 ]

## A Simplified LSTM Network

- **Idea:** Provide special gates to control the flow of “memories”



# LSTMs and GRUs

## Summarizing

- + Good at modeling sequences of variable length
- + Trainable via Back-Prop. → differentiable
- + Capable of handling long sequences  
( robust to vanishing/exploding gradients )

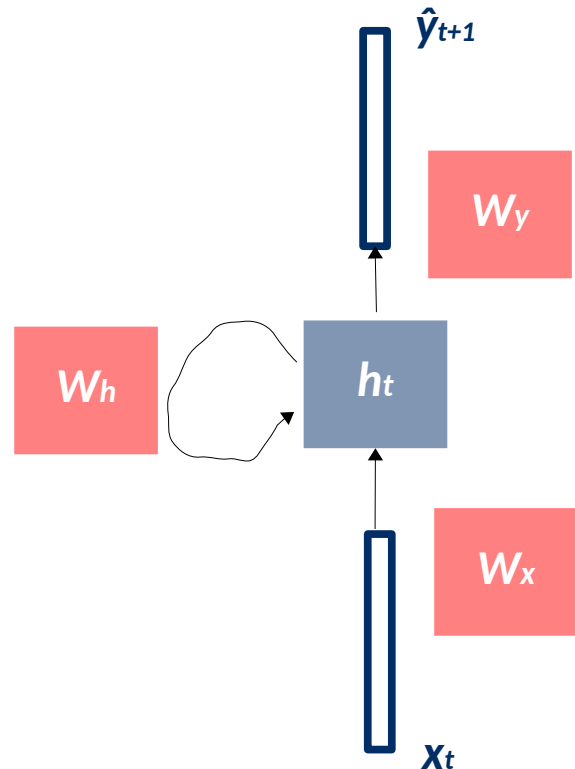


# Predictions from Sequences

# Predictions from Sequences

## Training Classifiers/Regressors from Sequences

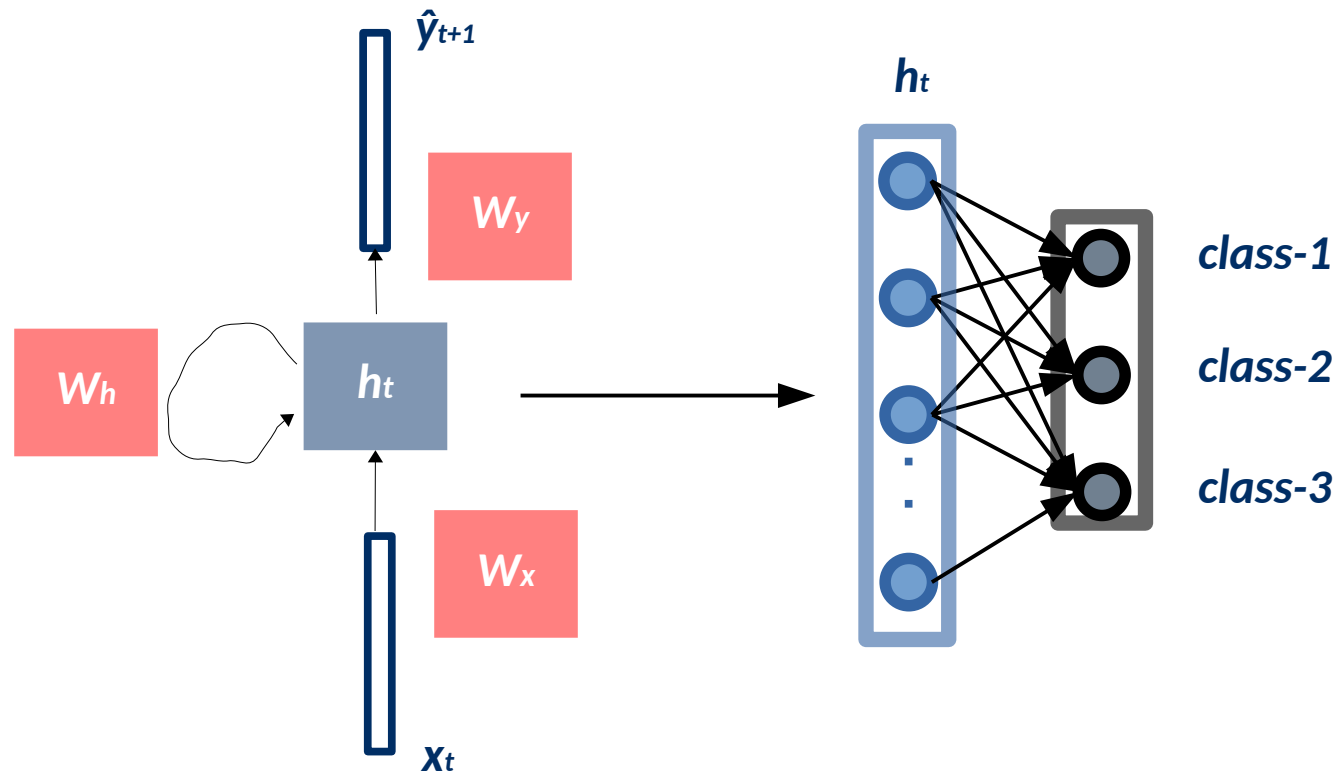
- 1) Attach a related head (classification, regression, etc.) to the *persistent* state
- 2) Measure the loss wrt. the prediction task



# Predictions from Sequences

## Training Classifiers/Regressors from Sequences

- 1) Attach a related head (classification, regression, etc.) to the *persistent* state
- 2) Measure the loss wrt. the prediction task

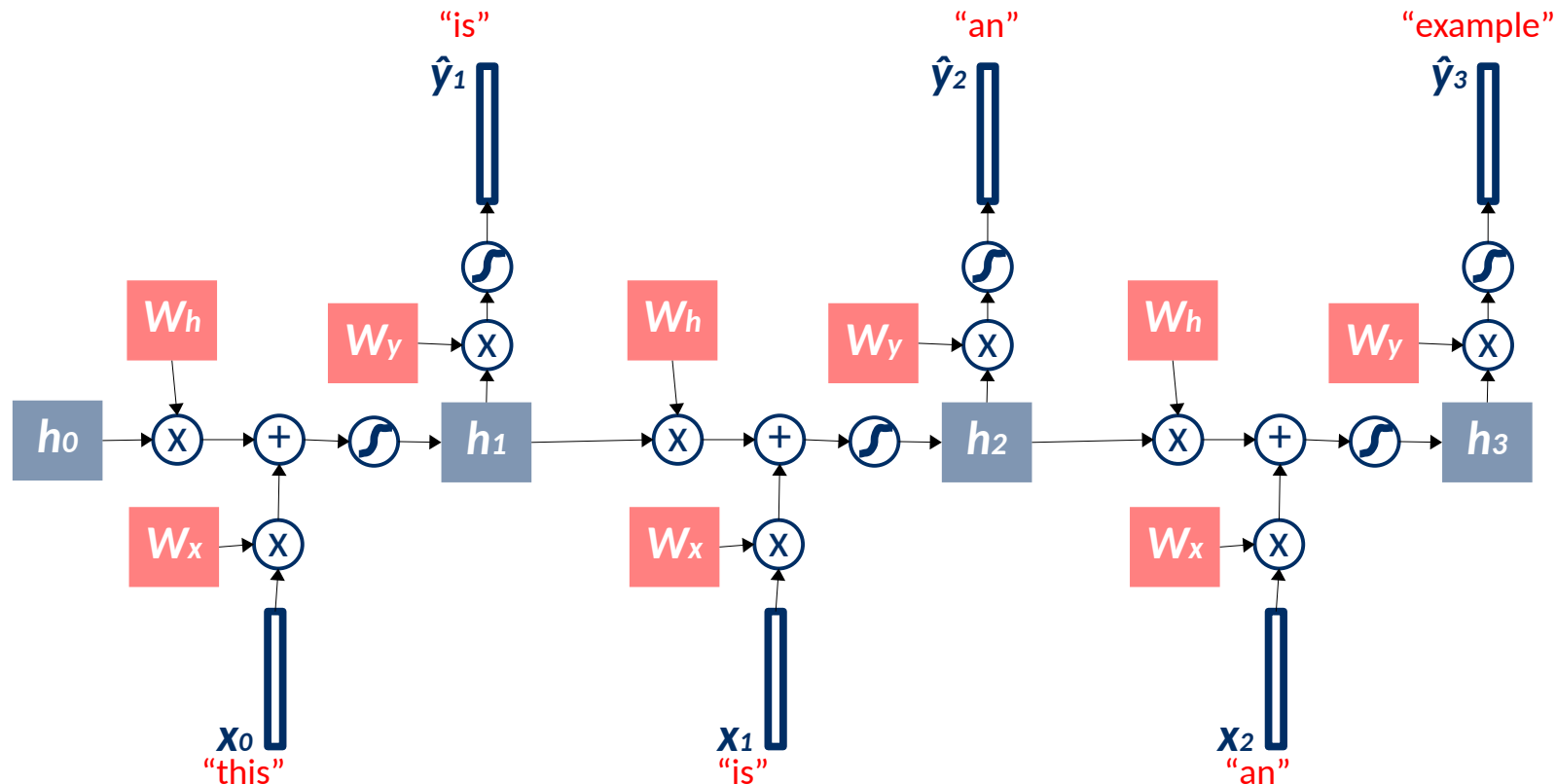


# Generating Sequences

# Generating Sequences

Sample the next best element from the predicted distribution

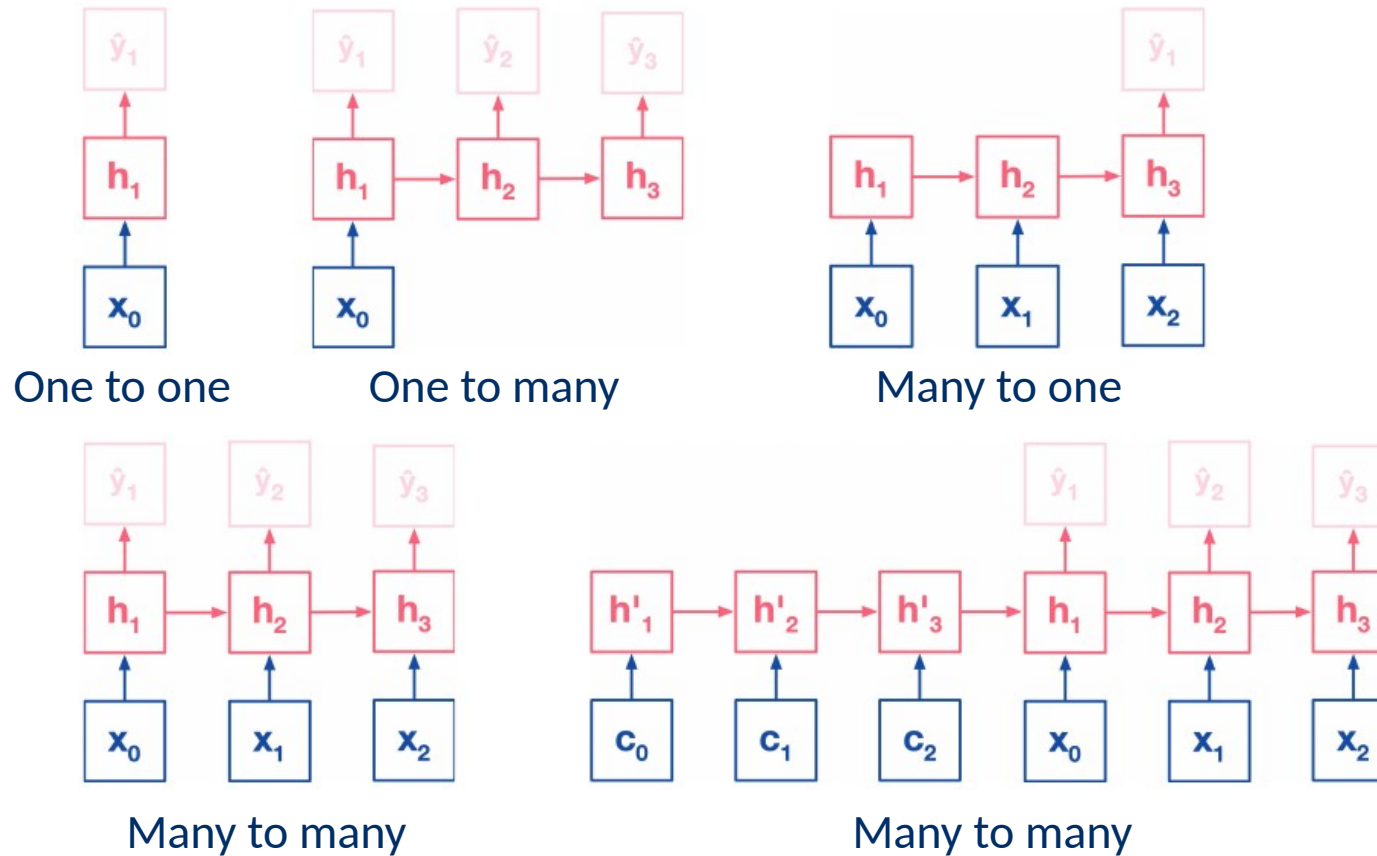
- **Idea:** Use the predicted element  $\hat{y}_t$  as input in the next iteration



# Generating Sequences

Several options are possible – beyond text sequences

- **Idea:** Different ways to define inputs, context and outputs



## Some Applications

- Language Translation
- Speech-to-Text
- Contextual Search
- Image Captioning

# Break

[ Let's meet again in 15 mins. ]

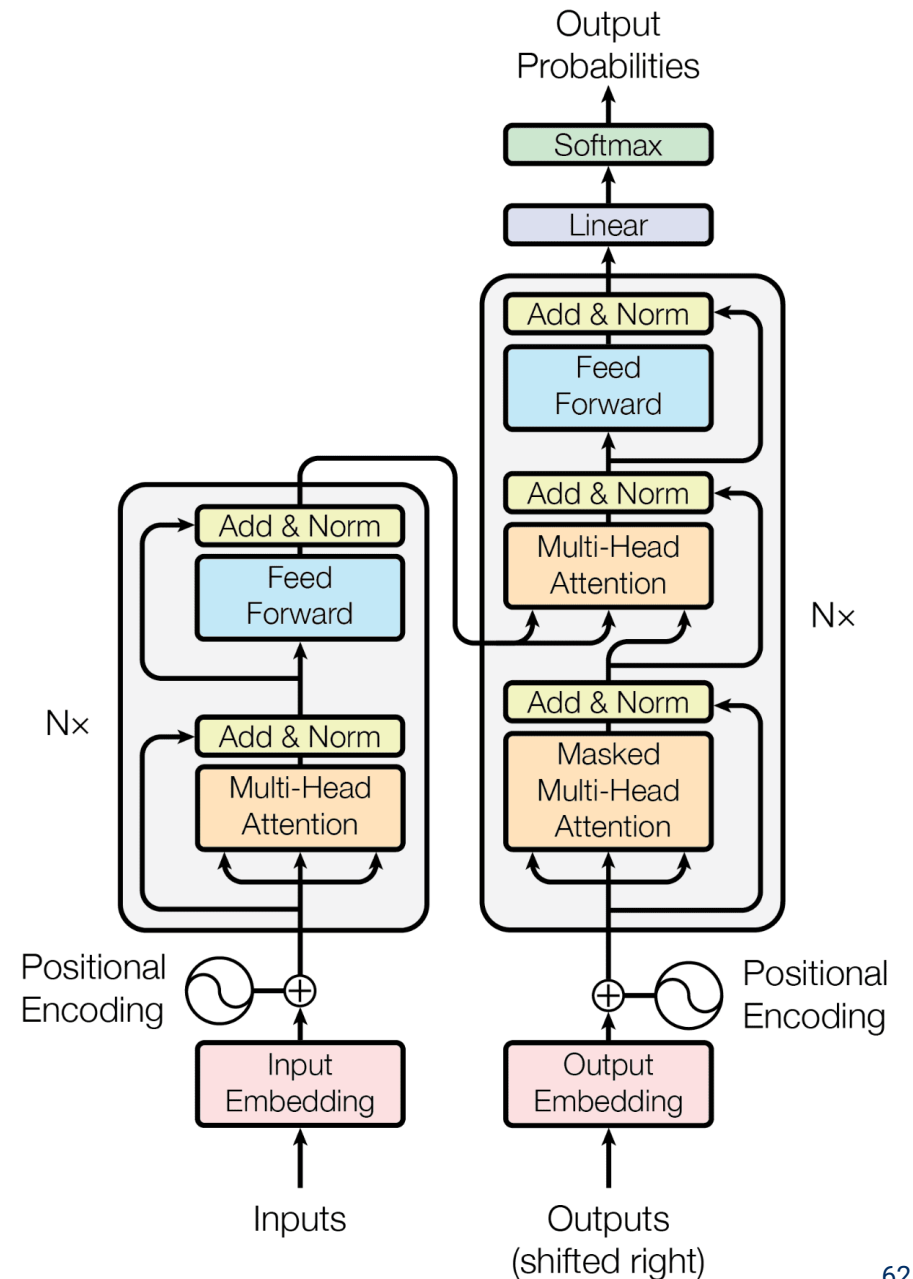
# Transformers



# Transformers [Vaswani et al., 2017]

## Some specs

- Removed Recurrence components
- Based solely on the attention mechanism
- Originally addressed translation tasks  
[English-German | English-French]



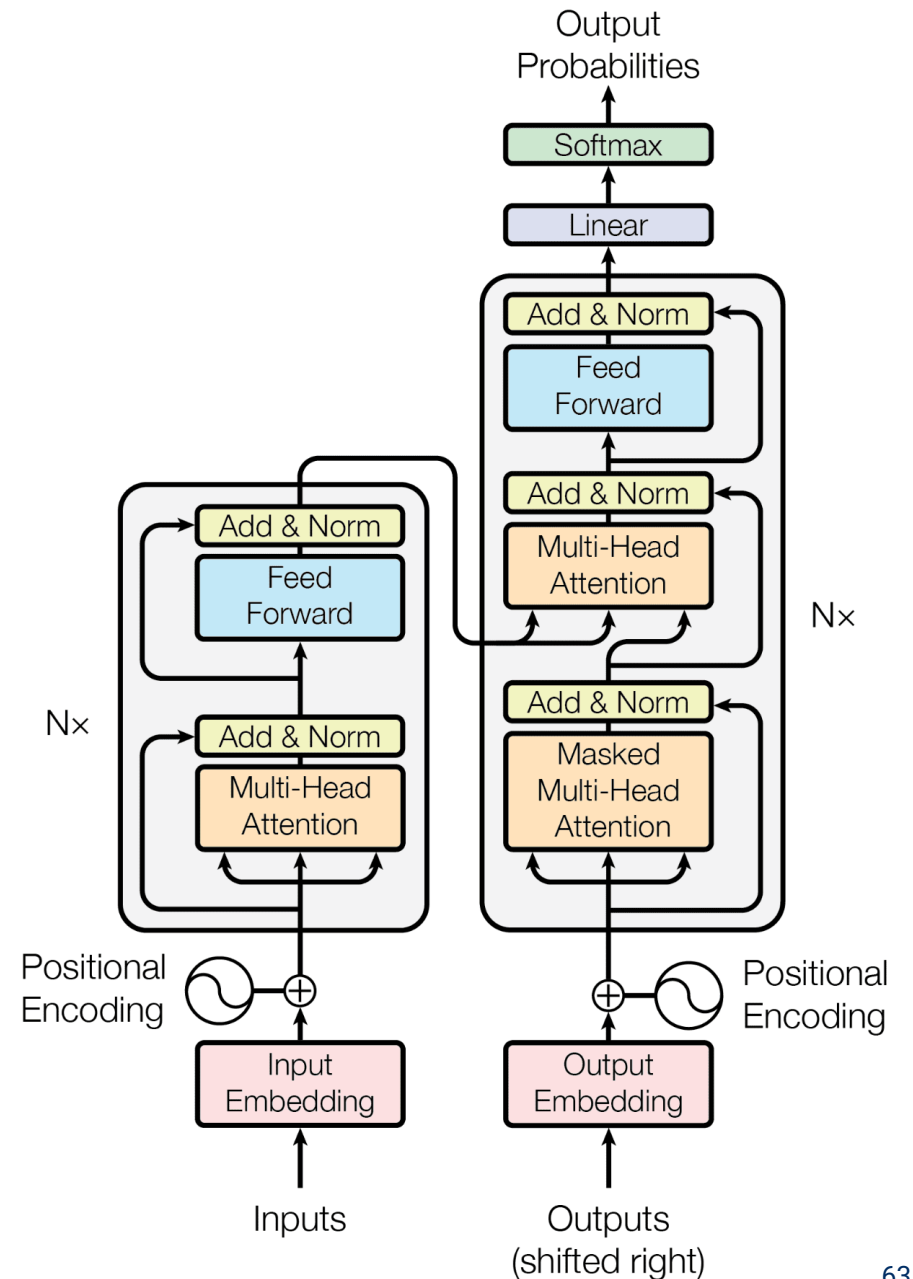
# Transformers [Vaswani et al., 2017]

## Some specs

- Removed Recurrence components
- Based solely on the attention mechanism
- Originally addressed translation tasks  
[English-German | English-French]



Scary-looking yes, difficult not  
Let's follow Thomas' presentation



# Modeling Data Sequences with Transformers

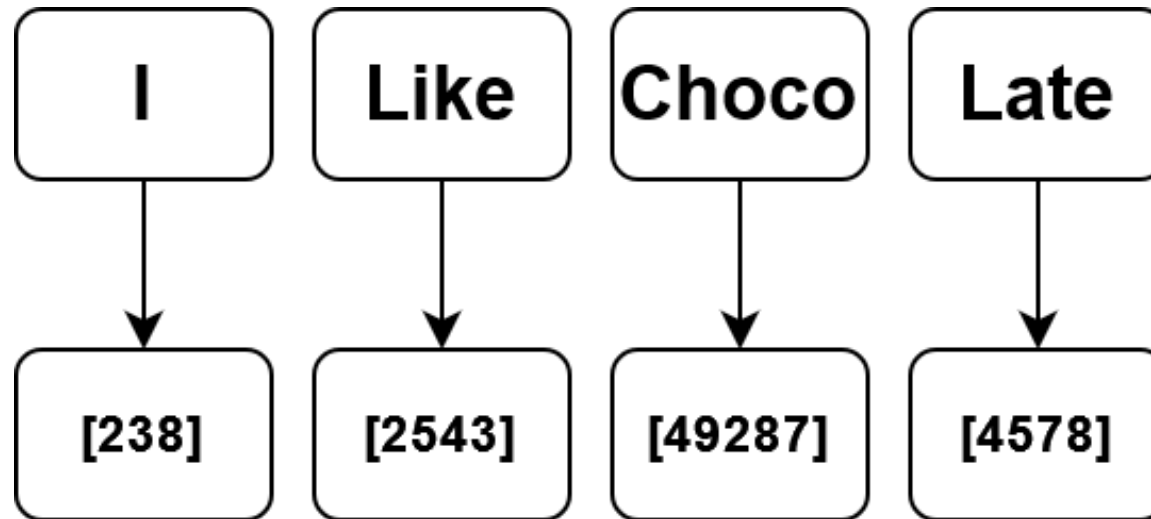
Lets consider the following sequence

“I like chocolate”

# Modeling Data Sequences with Transformers

## Tokenization: defining granular unit of processing

- Break the input into smaller units (*tokens*)
- Different levels of codification possible (character, word, etc.)

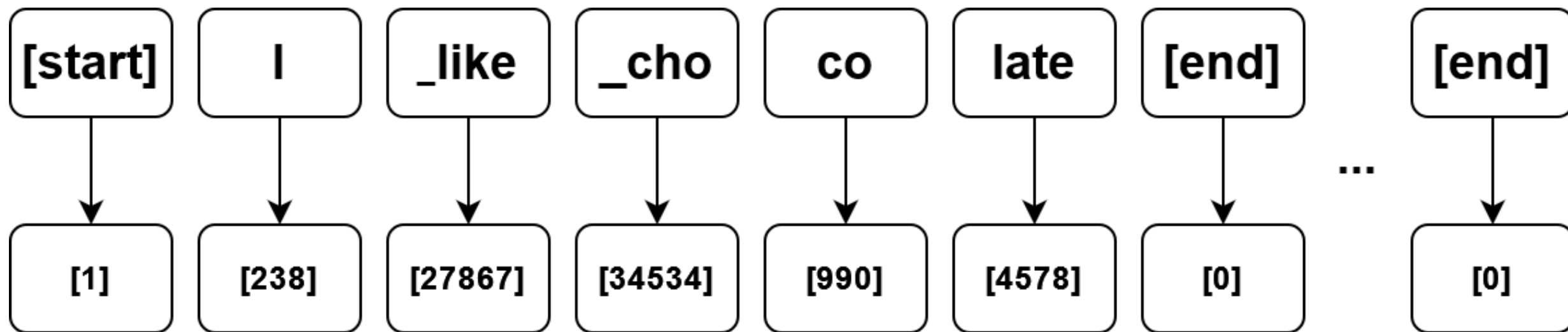


# Modeling Data Sequences with Transformers

## Tokenization: defining granular unit of processing

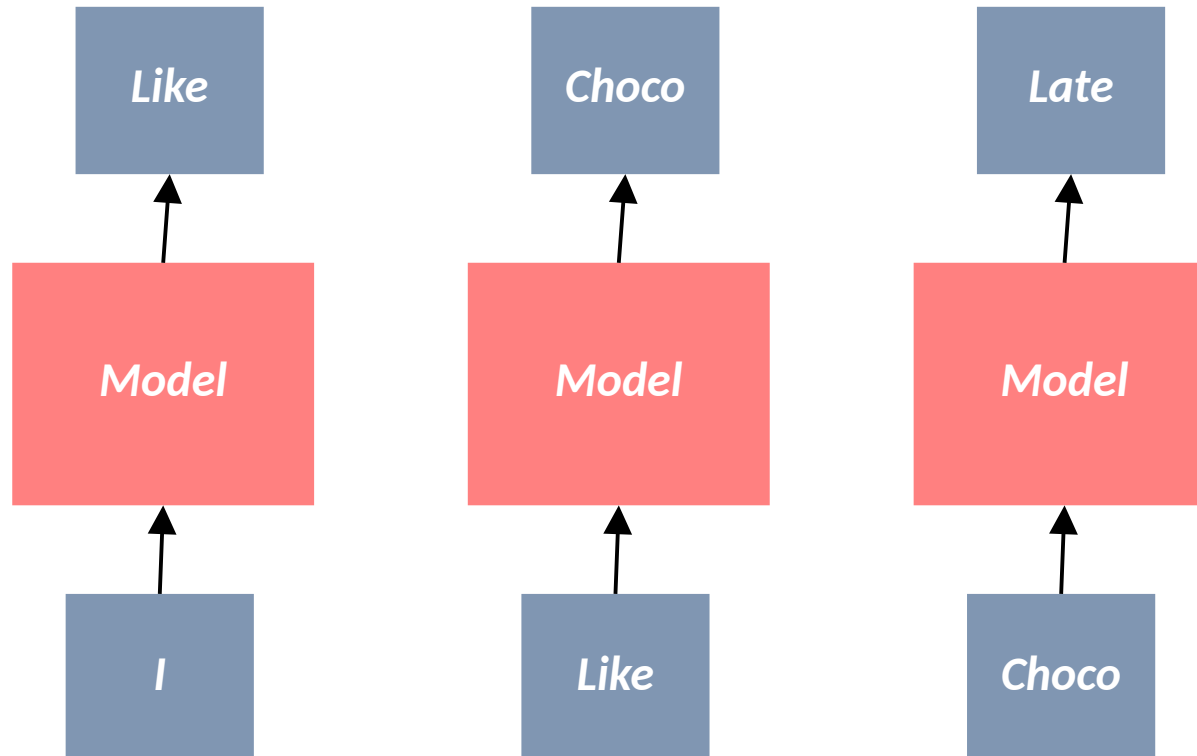
- Break the input into smaller units (*tokens*)
- Different levels of codification possible (character, word, etc.)

*\*In reality it is not that straight-forward*



# Modeling Data Sequences with Transformers

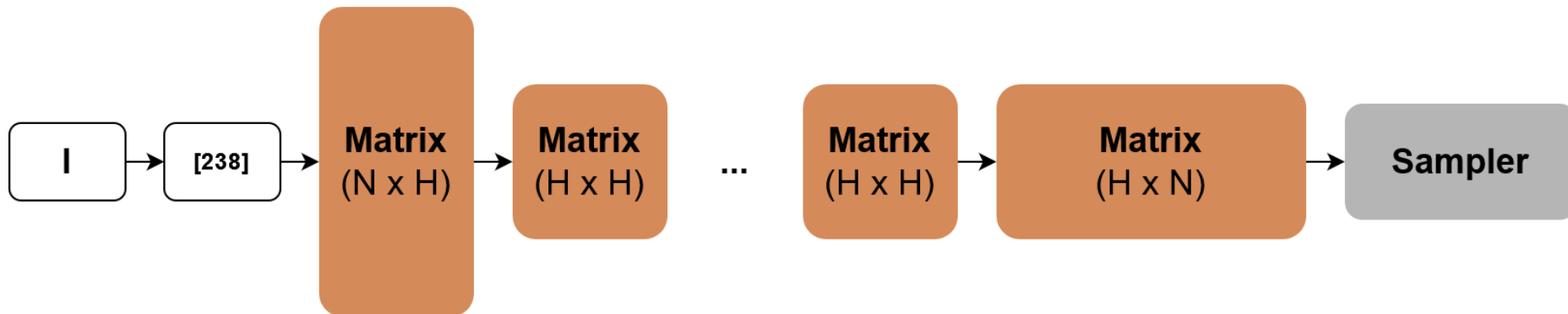
Predicting the next element (token)



# Sequence Modelling with Transformers

## A Very Popular Recipe

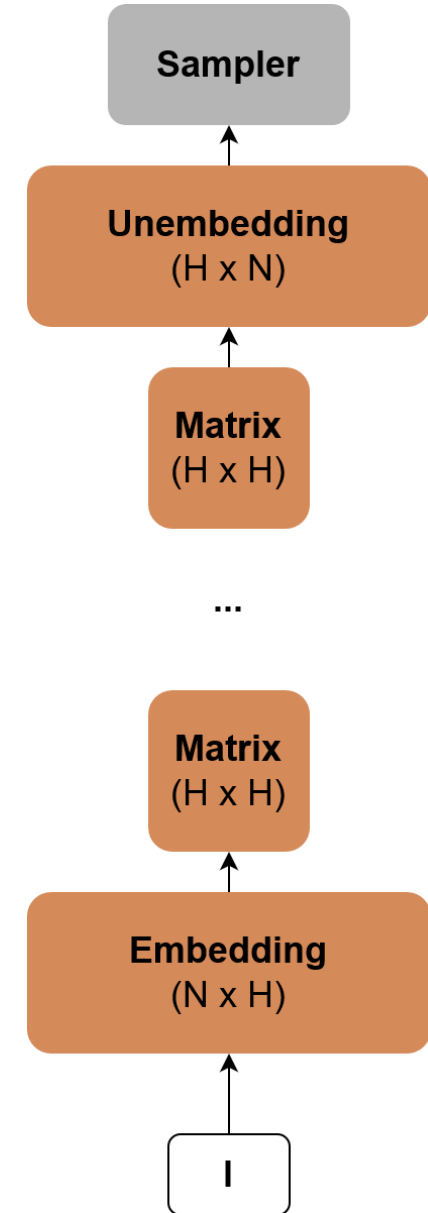
- Moving to a lower dimensional space (determined by  $H$ )



# Sequence Modelling with Transformers

## A Very Popular Recipe

- Moving to a lower dimensional space (determined by  $H$ )

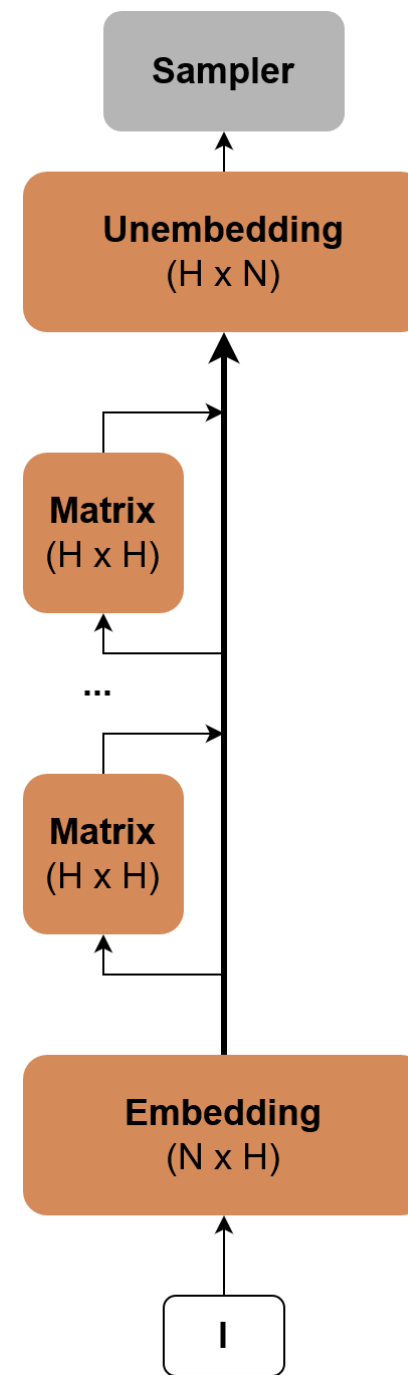




# Sequence Modelling with Transformers

## A Very Popular Recipe

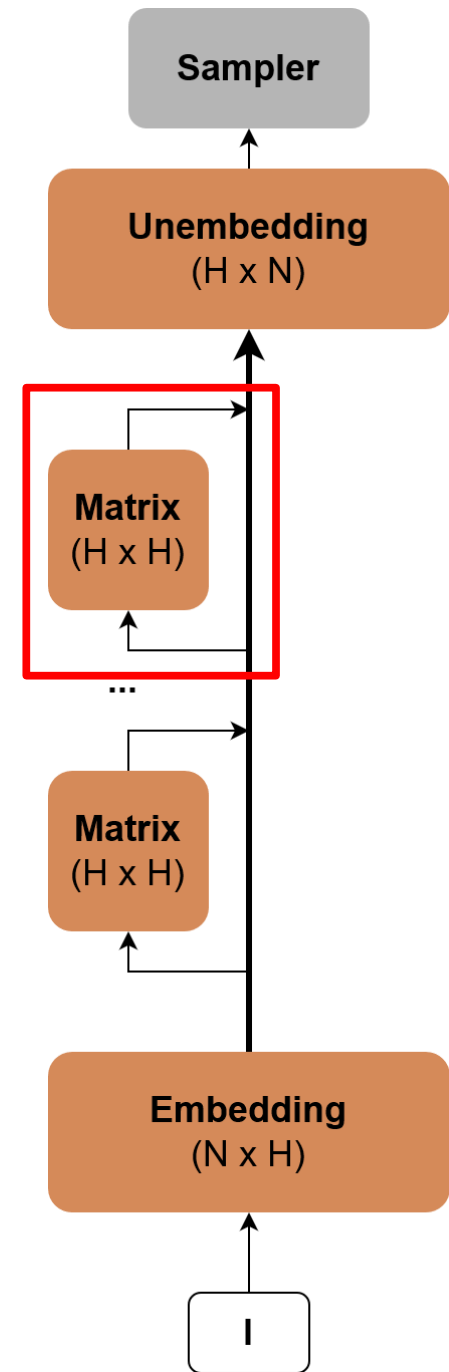
- Moving to a lower dimensional space (determined by  $H$ )
- Using residual layers (**why?**)



# Sequence Modelling with Transformers

## A Very Popular Recipe

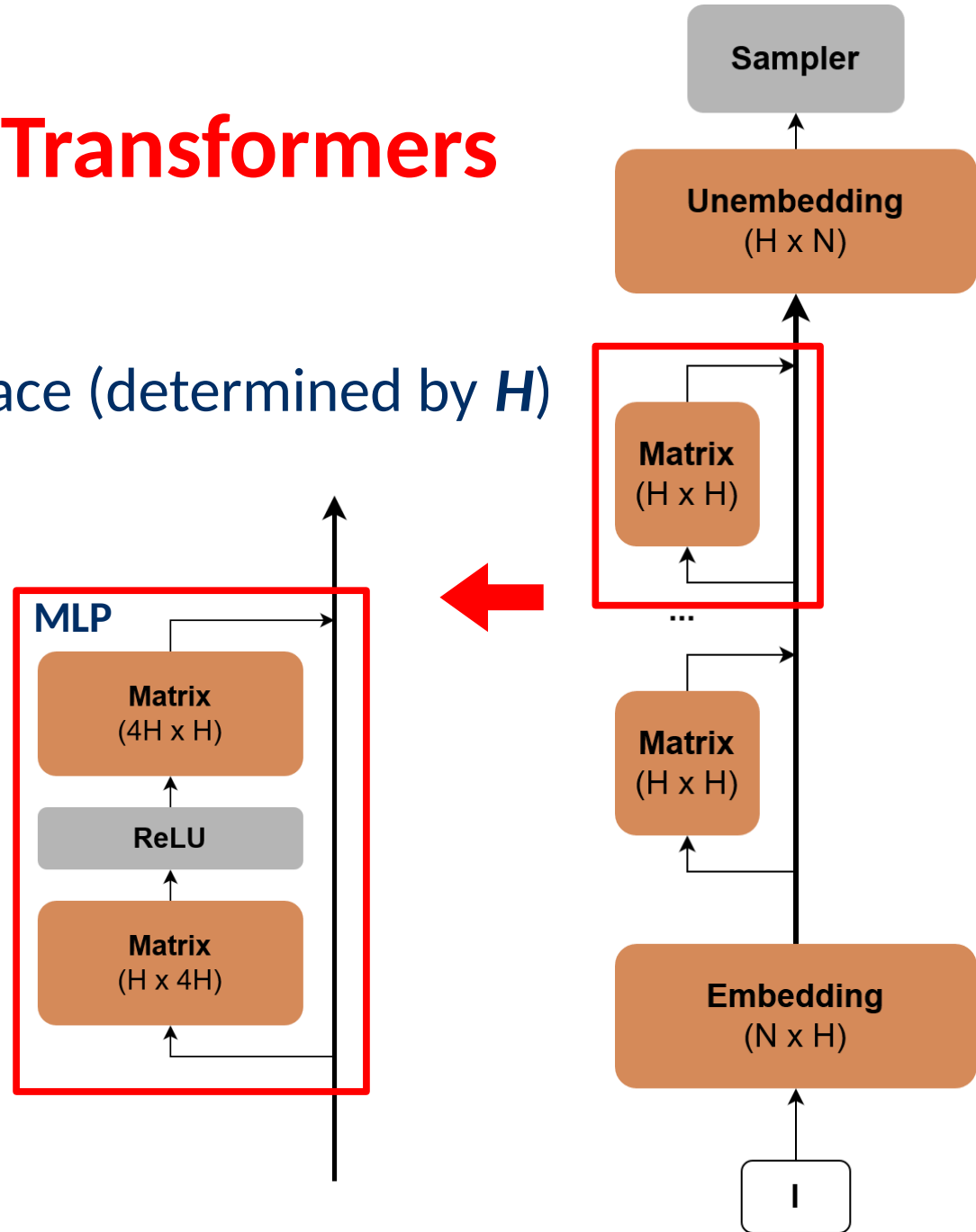
- Moving to a lower dimensional space (determined by  $H$ )
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# Sequence Modelling with Transformers

## A Very Popular Recipe

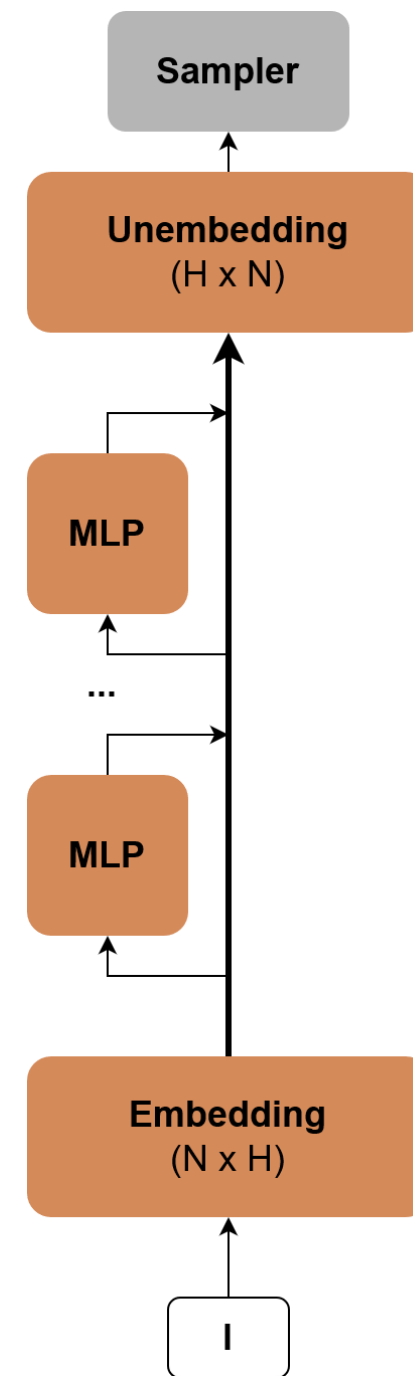
- Moving to a lower dimensional space (determined by  $H$ )
- Using residual layers - MLP



# Sequence Modelling with Transformers

## A Very Popular Recipe

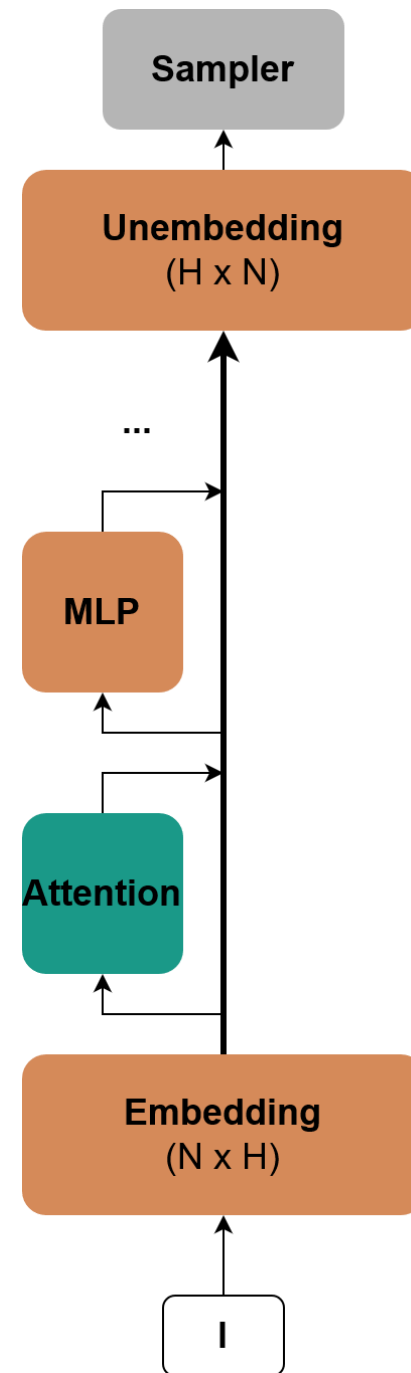
- Moving to a lower dimensional space (determined by  $H$ )
- Using residual layers - MLP



# Sequence Modelling with Transformers

## A Very Popular Recipe

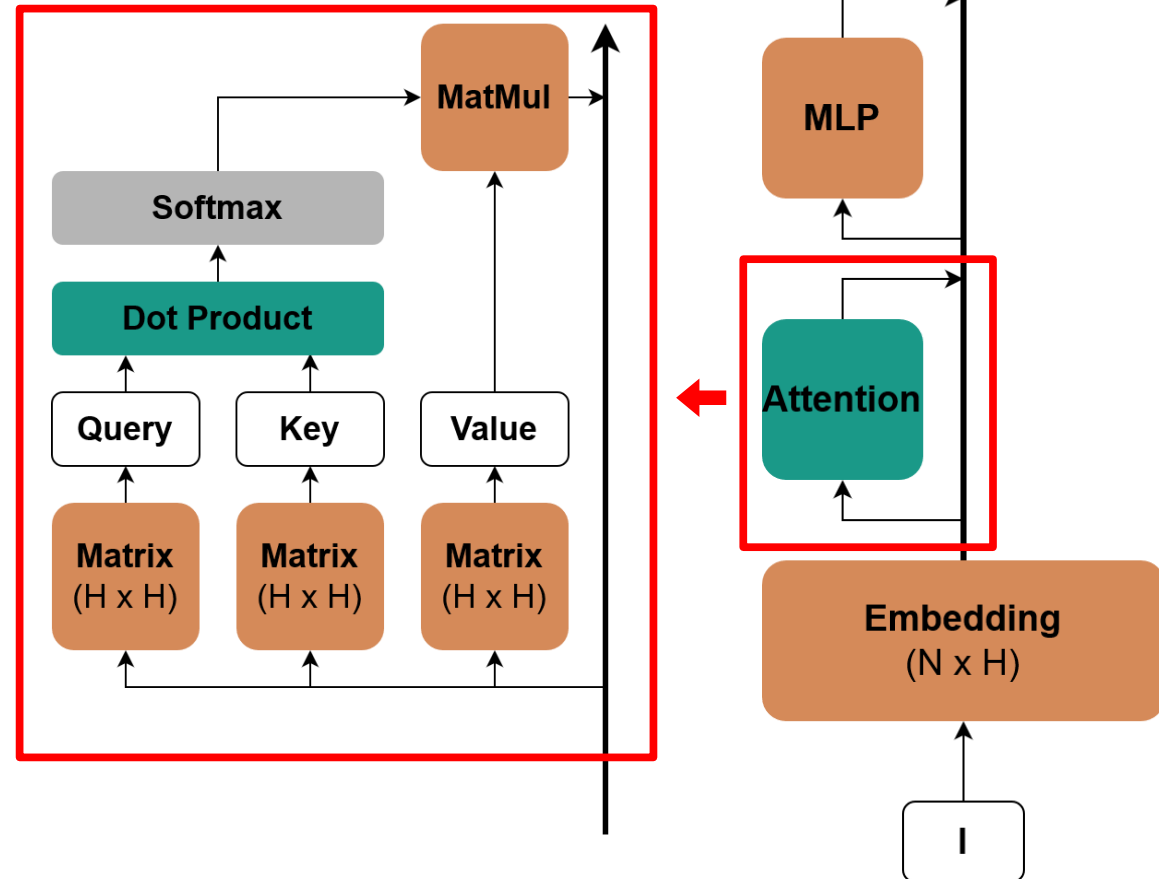
- Moving to a lower dimensional space (determined by  $H$ )
- Using residual layers - MLP
- Add an [self] attention layer



# Sequence Modelling with Transformers

## A Very Popular Recipe

- Moving to a lower dimensional space (determined by  $H$ )
- Using residual layers - MLP
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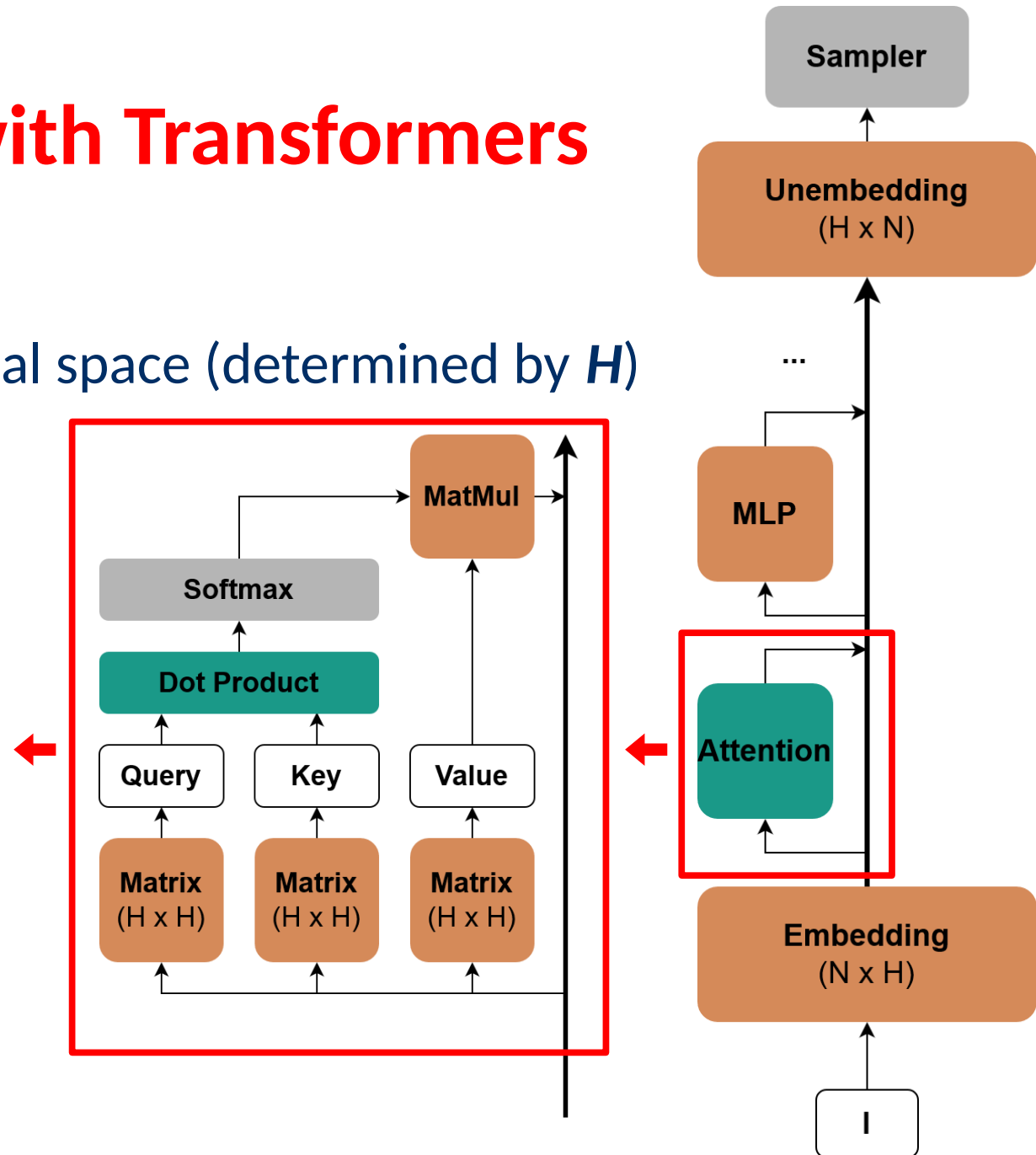


# Sequence Modelling with Transformers

## A Very Popular Recipe

- Moving to a lower dimensional space (determined by  $H$ )
- Using residual layers - MLP
- Add an [self] attention layer

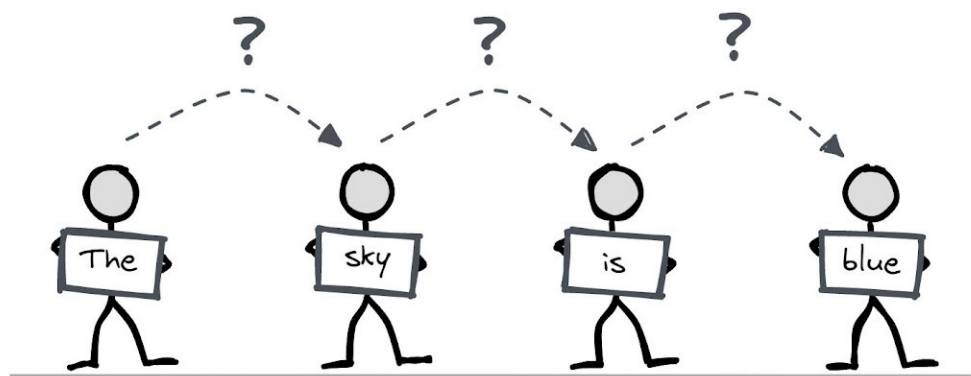
$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$



# Sequence Modelling with Transformers

## Attention Mechanism – An Intuition

Each person in the line tries to guess what word the person in front of them is holding.

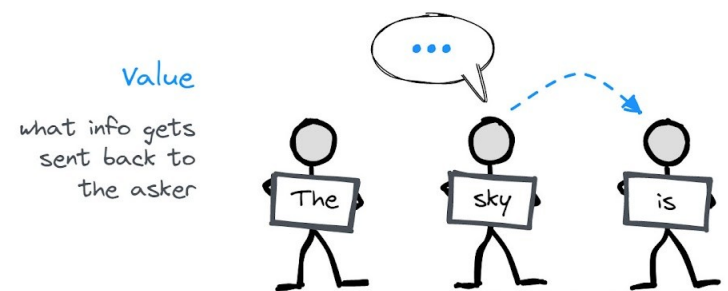
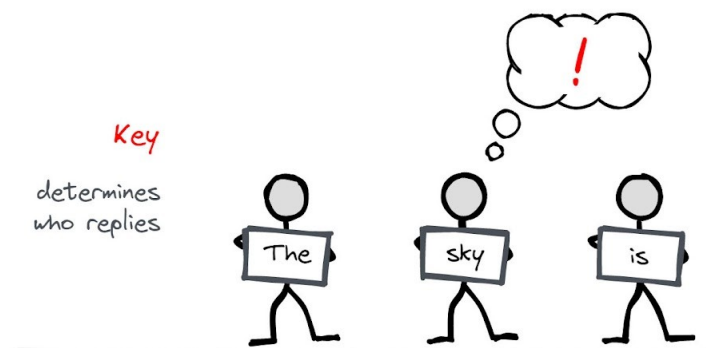
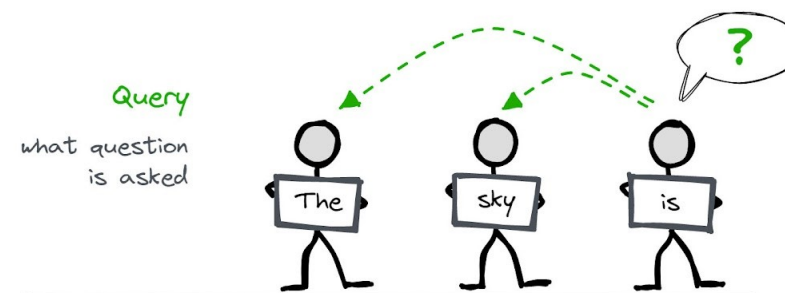
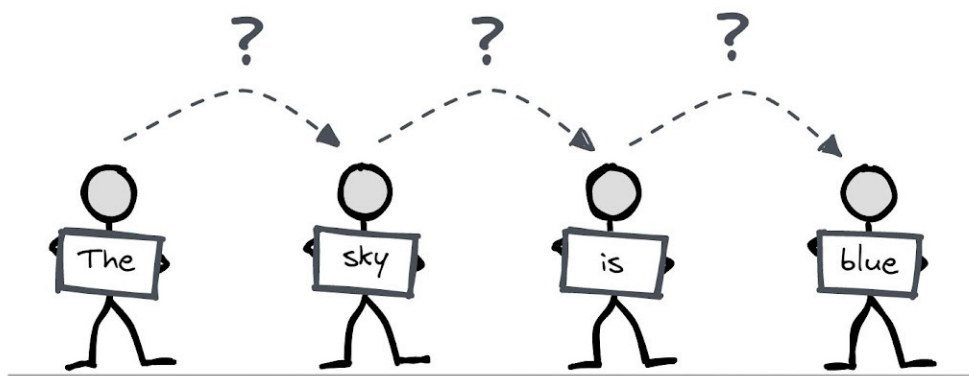




# Sequence Modelling with Transformers

## Attention Mechanism – An Intuition

Each person in the line tries to guess what word the person in front of them is holding.

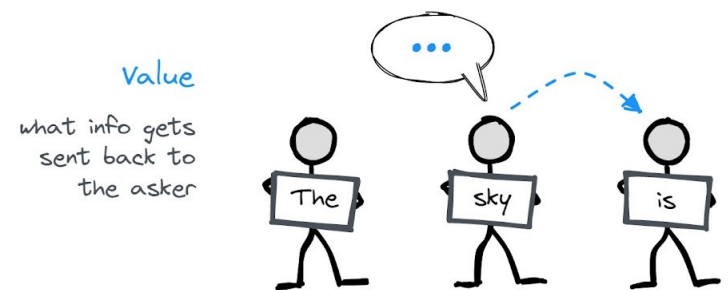
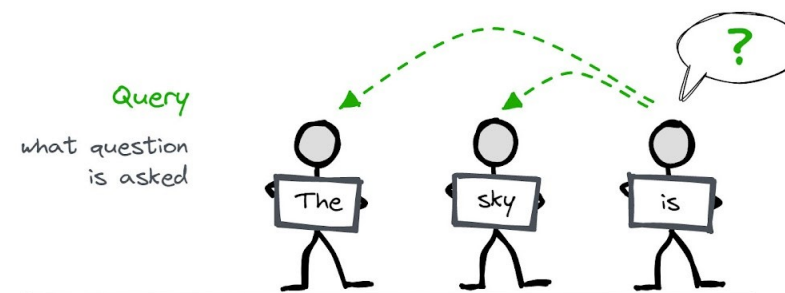
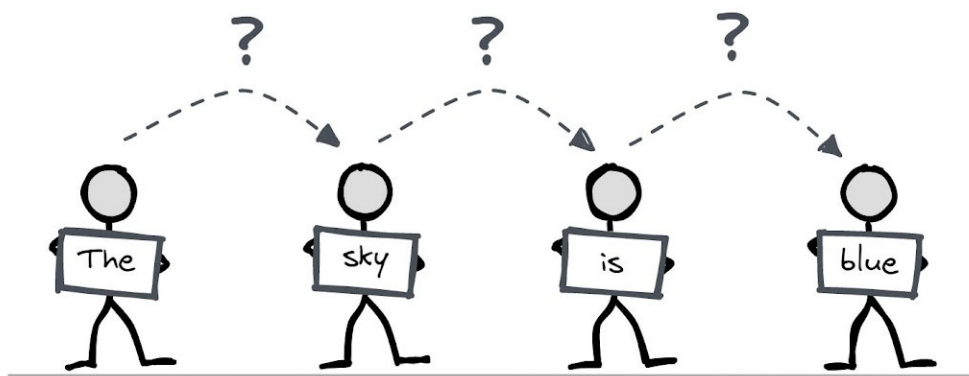


# Sequence Modelling with Transformers

## Attention Mechanism – An Intuition

- $Q \rightarrow$  the question
- $K \rightarrow$  critical element to focus on
- $V \rightarrow$  the information to be forwarded

Each person in the line tries to guess what word the person in front of them is holding.



# Sequence Modelling with Transformers

## Attention Mechanism – An Intuition

- $Q \rightarrow$  the question
- $K \rightarrow$  critical element to focus on
- $V \rightarrow$  the information to be forwarded

### A database Analogy

	Query = 5	Values	Output
Key = 1	0	1	0
Key = 5	1	2	2
Key = 3	0	3	0
Key = 4	0	4	0
Key = 5	1	5	5
			7

# Sequence Modelling with Transformers

## Attention Mechanism – An Intuition

- Q → the question
- K → critical element to focus on
- V → the information to be forwarded

### A database Analogy

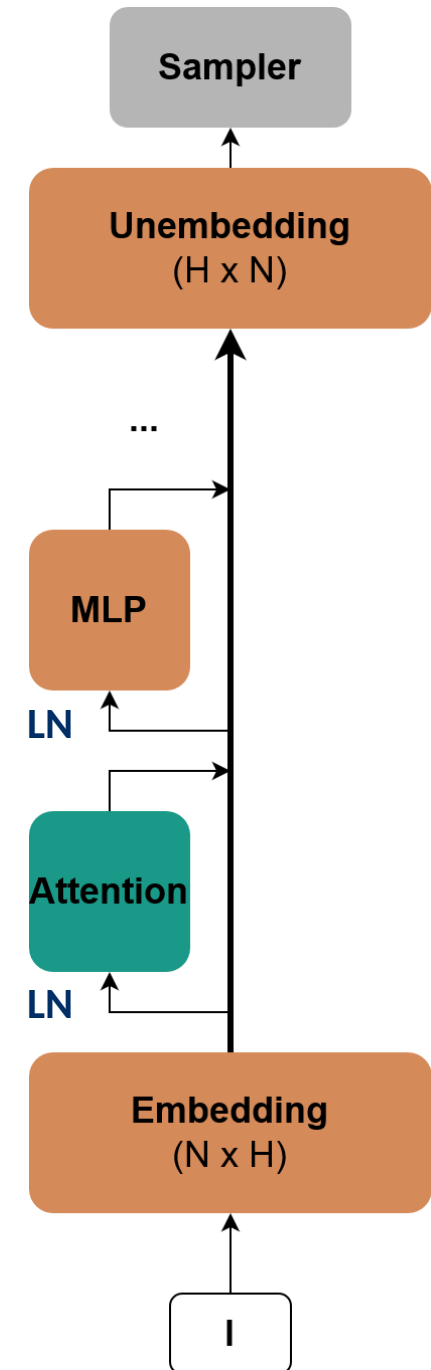
Like convolution but with dynamic weight (query-key similarity)

	Query = 5	Values	Output
Key = 1	0.125	1	0.125
Key = 5	1	2	2
Key = 3	0.25	3	0.75
Key = 4	0.5	4	2
Key = 5	1	5	5
			9.875

# Sequence Modelling with Transformers

## A Very Popular Recipe

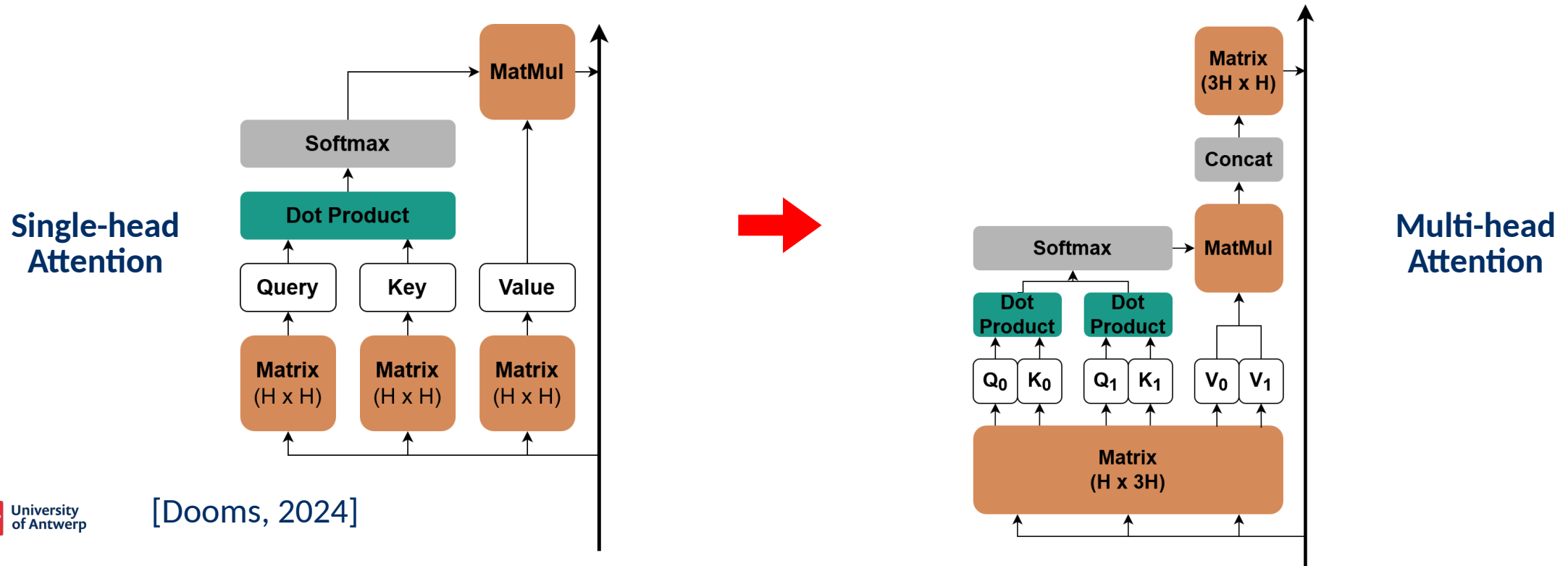
- Moving to a lower dimensional space (determined by  $H$ )
- Using residual layers - MLP
- Add an [self] attention layer
- Add some intermediate normalization



# Sequence Modelling with Transformers

## Single vs. Multi-head Attention

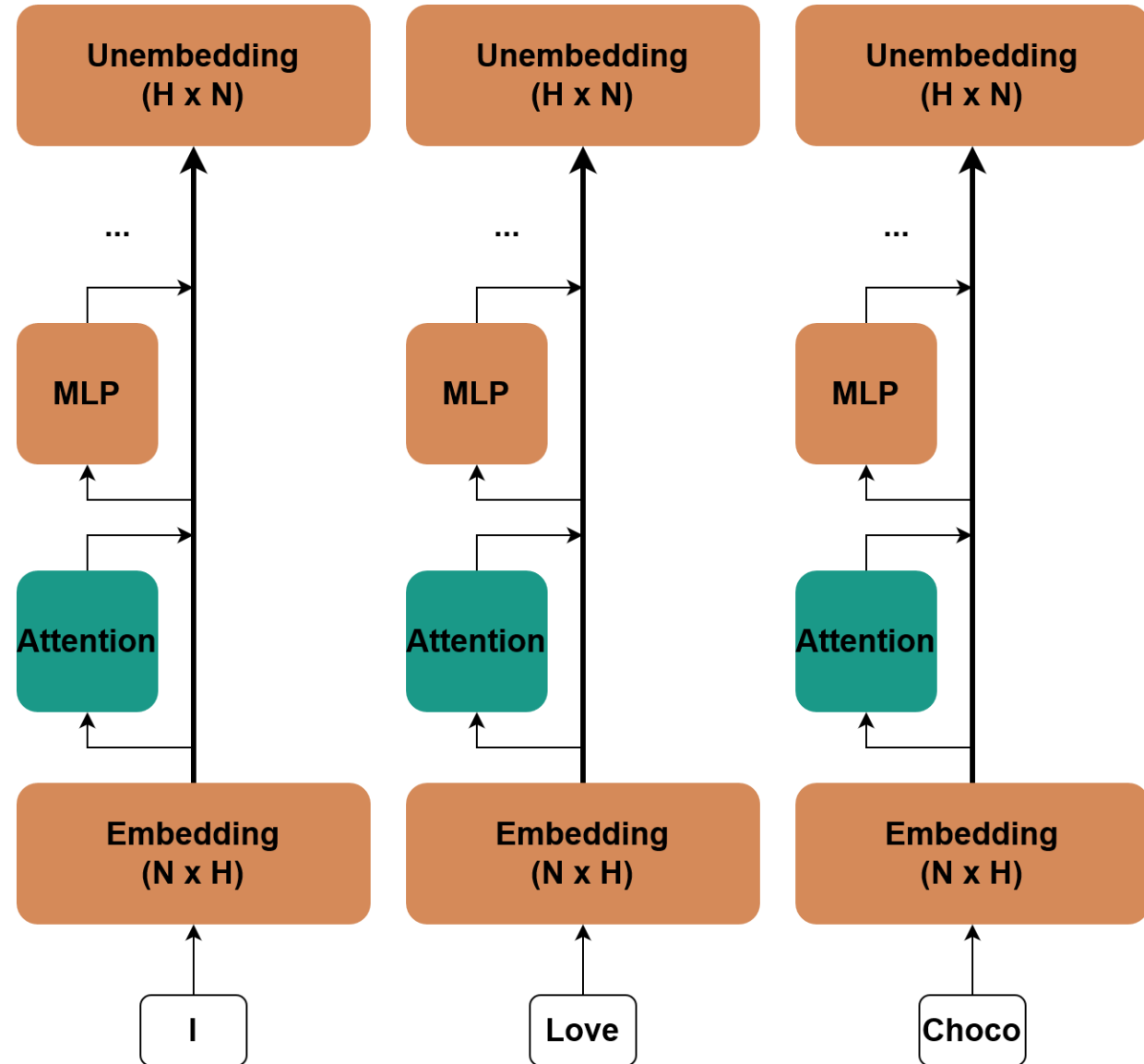
- Single: Each layer ask one question via the single QKV matrices.
- Multi: Split the QKV matrices into smaller ones → ask more/simpler questions



# Sequence Modelling with Transformers

## Strengths: Communication

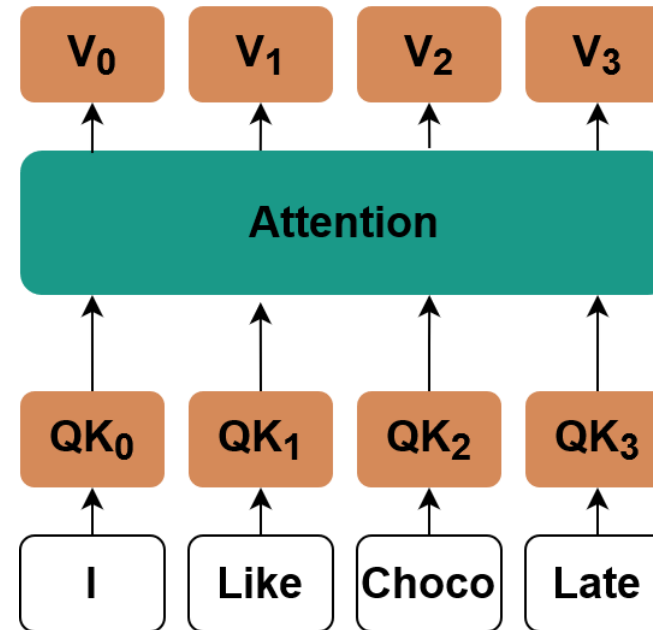
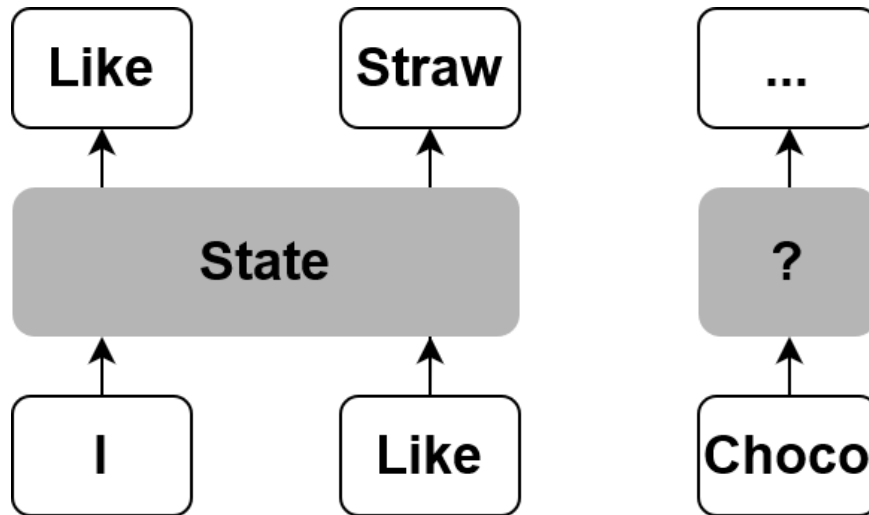
- Depth: more specialized and structured
- Through attention: across tokens



# RNNs VS Transformers

## Context Sources

- Information from memory vs. tokens (error propagation)  
→ Sentence vs. Word -based

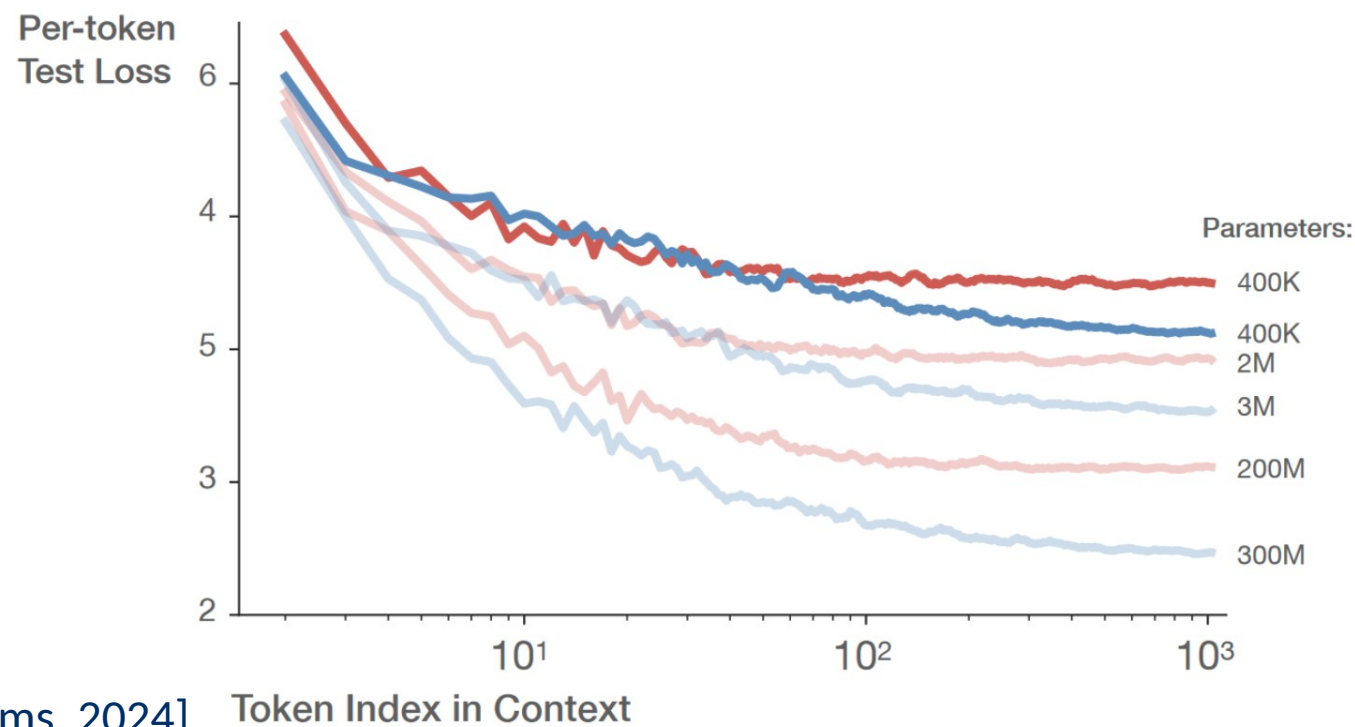




# RNNs VS Transformers

## Performance / size trade-off

- Higher performance as # of considered tokens increases
- Better use of parameters



[Kaplan, 2020]

# Summarizing

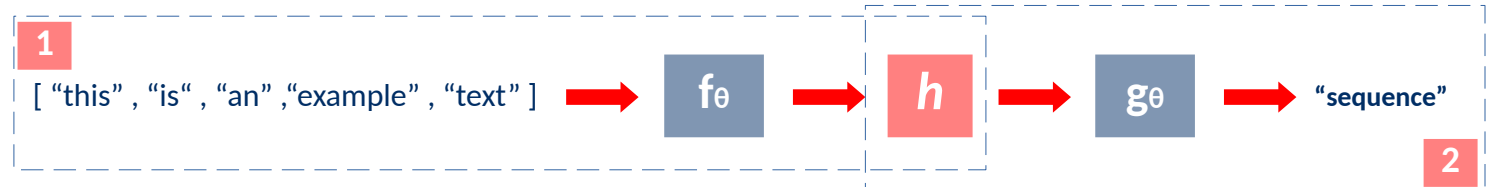
[ Finally :D ]

# Summarizing

## ■ Two Step-Approach

1. Model Context

2. Predict Next Element given Context

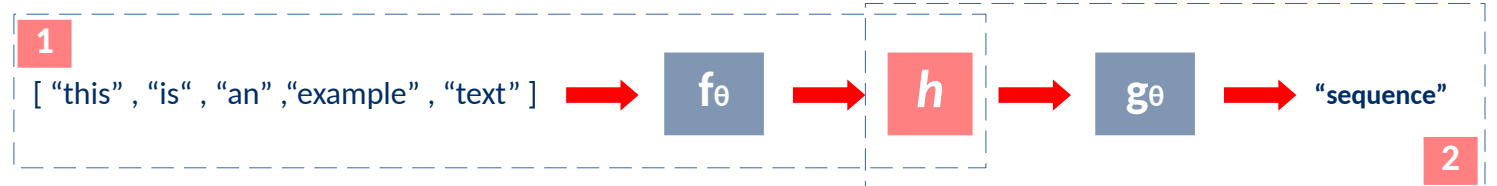


# Summarizing

## Two Step-Approach

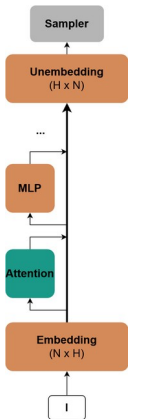
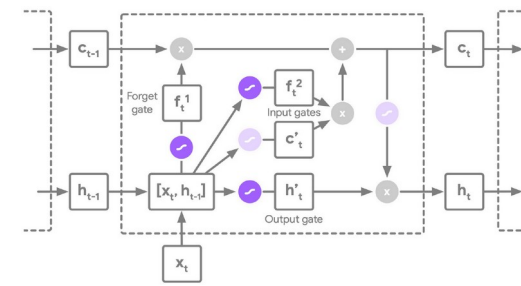
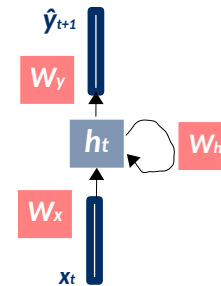
1. Model Context

2. Predict Next Element given Context



## Several architectures with different capabilities

RNNs | LSTMs | GRUs | Transformers

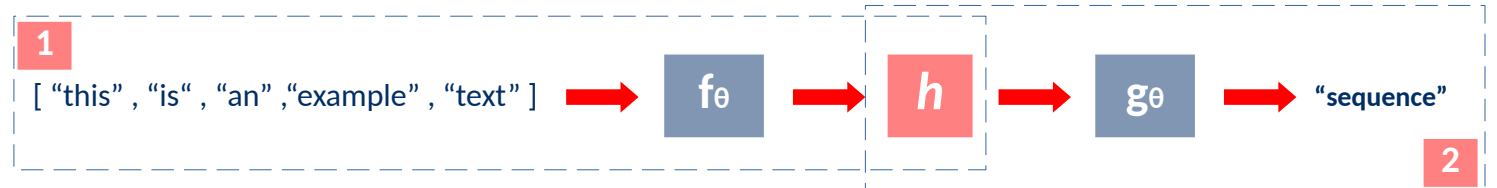


# Summarizing

- Two Step-Approach

  - 1. Model Context

  - 2. Predict Next Element given Context

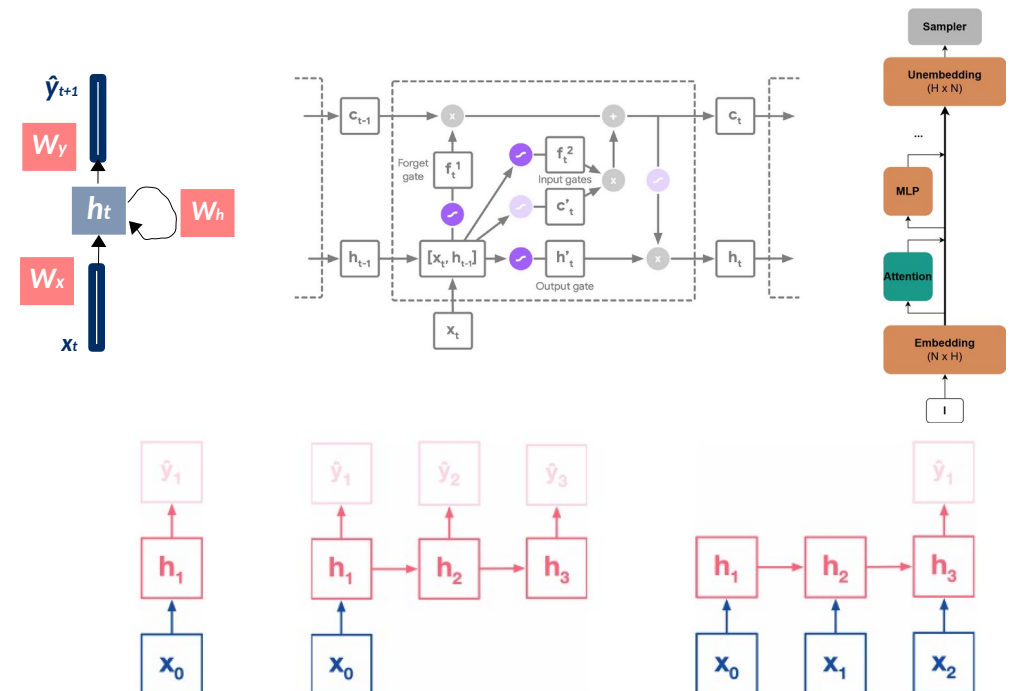


- Several architectures with different capabilities

  - RNNs | LSTMs | GRUs | Transformers

- High Flexibility towards different problems

  - one-to-one | many-to-one | many-to-many ...



# References

- K. Cho, B. van Merriënboer, Gulcehre, Caglar, D. Bahdanau; F. Bougares, H. Schwenk; Y. Bengio (2014). "**Learning Phrase Representations using RNN Encoder-Decoder for Statistical Machine Translation**". arXiv:1406.1078.
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- S. Hochreiter and J. Schmidhuber. 1997. **Long Short-Term Memory**. *Neural Comput.* 9, 8 (November 15, 1997), 1735–1780. DOI:<https://doi.org/10.1162/neco.1997.9.8.1735>
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<https://pabloinsente.github.io/the-recurrent-net>
- **Understanding LSTM Networks** - COLAH's Blog  
<http://colah.github.io/posts/2015-08-Understanding-LSTMs/>

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- **The Recurrent Neural Network - Theory and Implementation of the Elman Network and LSTM**  
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# Modeling Sequences with Neural Networks

José Oramas