Deep Sequence Modeling

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MIT Introduction to Deep Learning

January 9, 2023

Given an image of a ball,
can you predict where it will go next?

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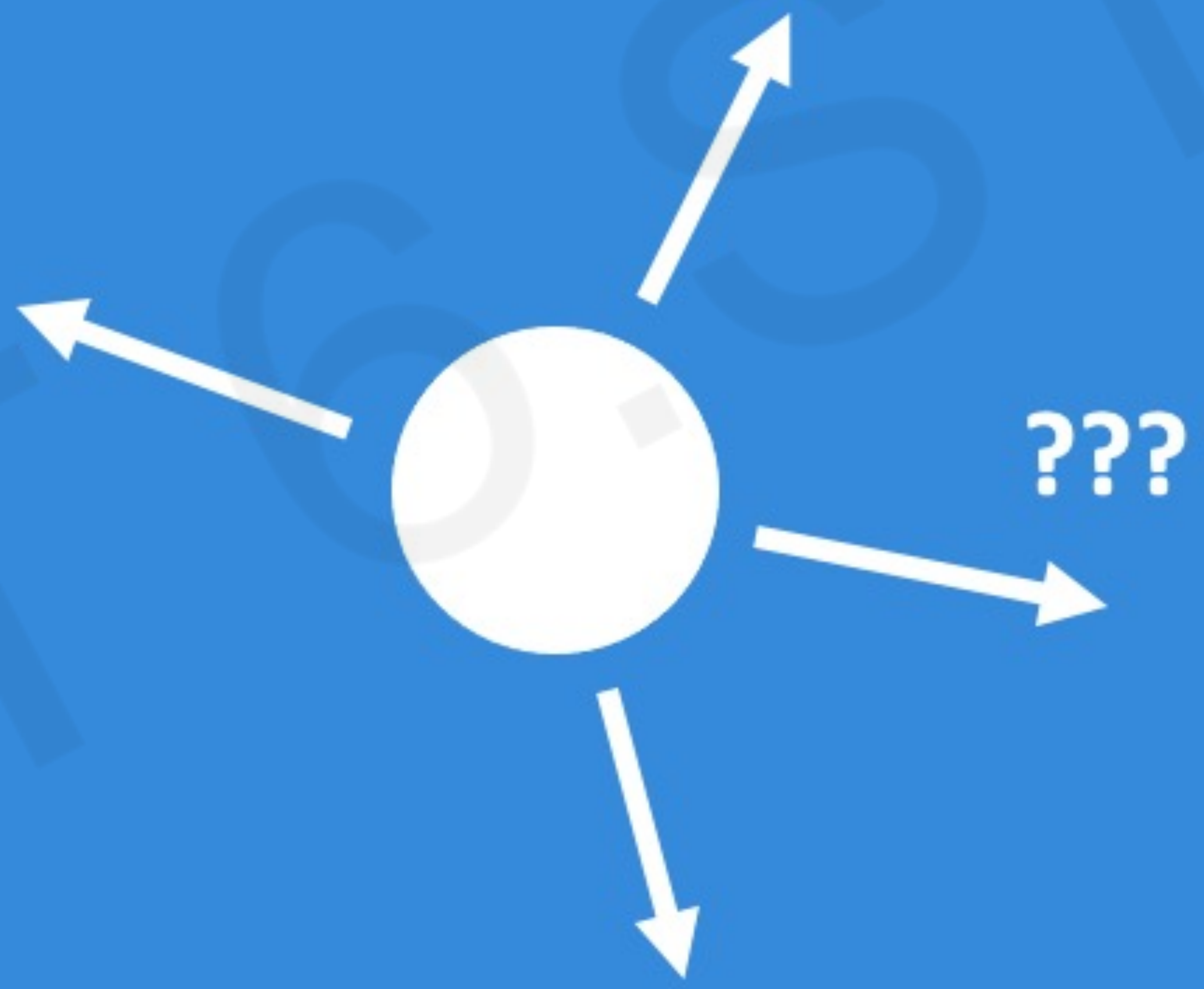

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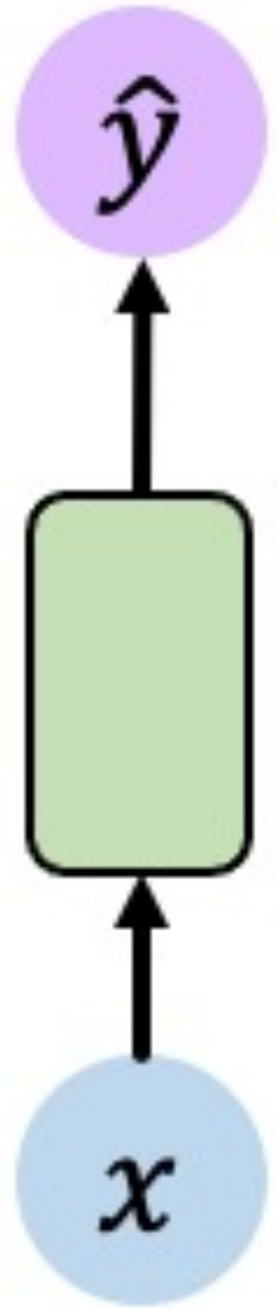
Sequences in the Wild

Audio

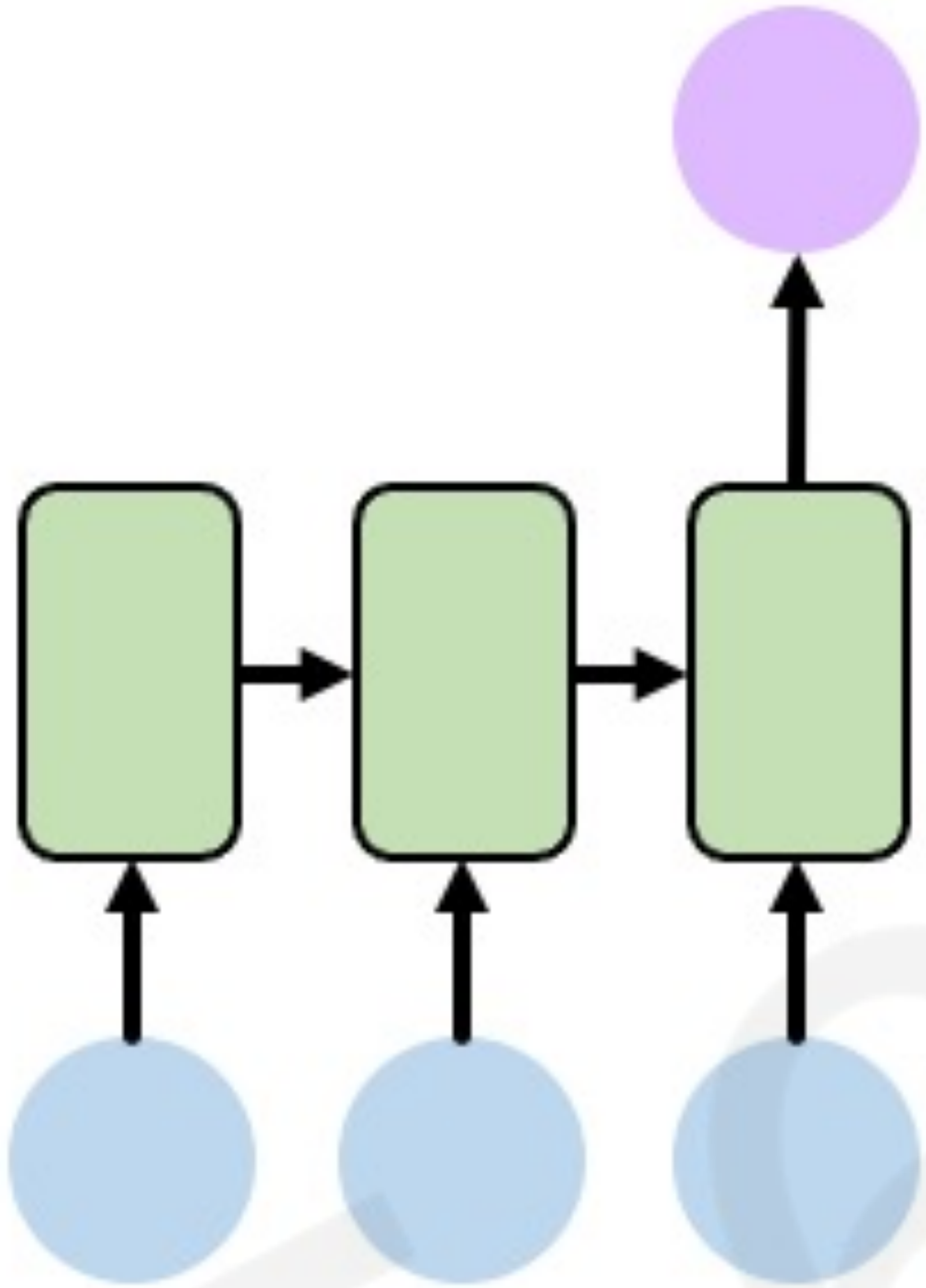
Sequences in the Wild

Sequence Modeling Applications

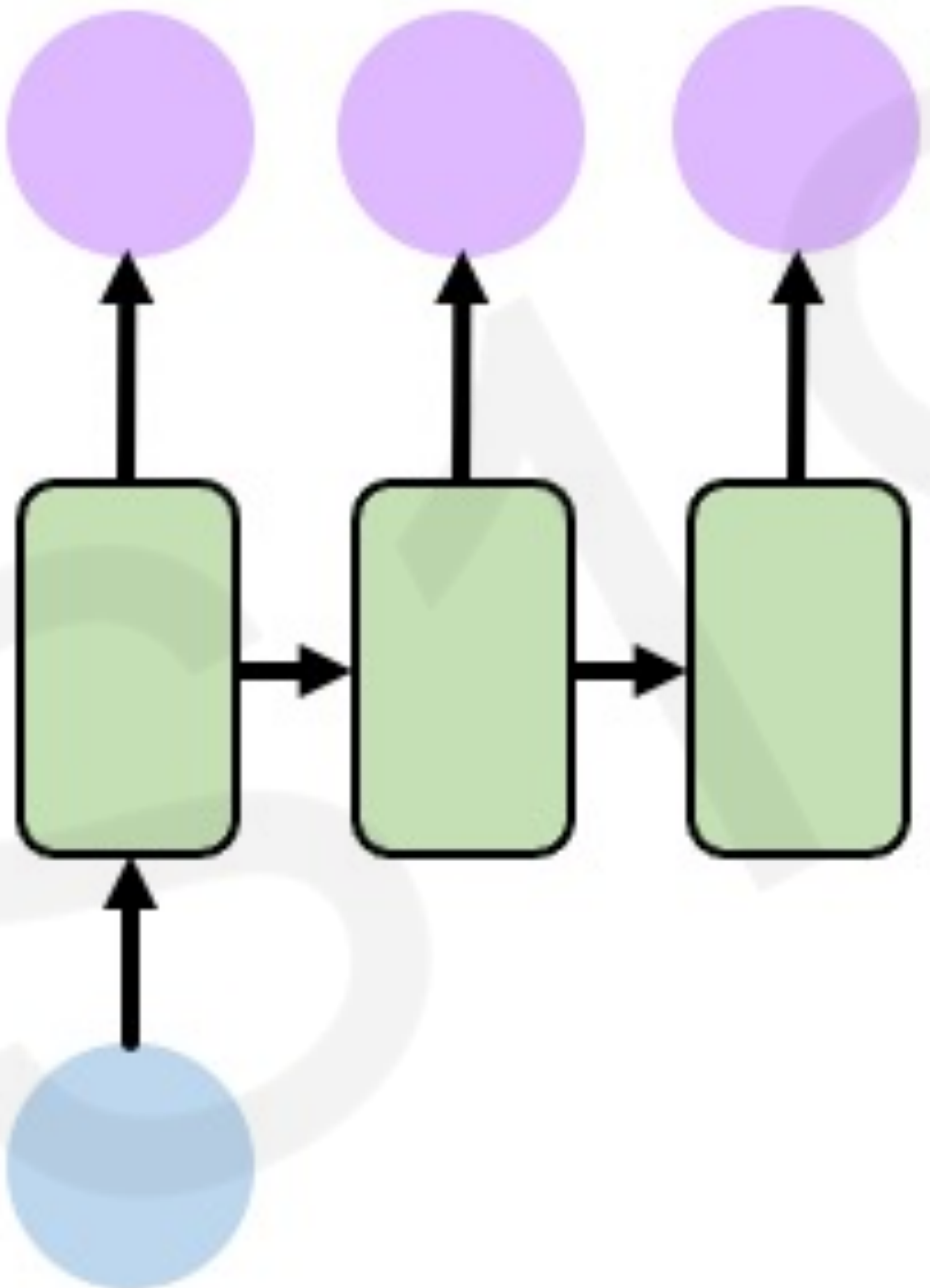


One to One
Binary Classification

"Will I pass this class?"
Student → Pass?

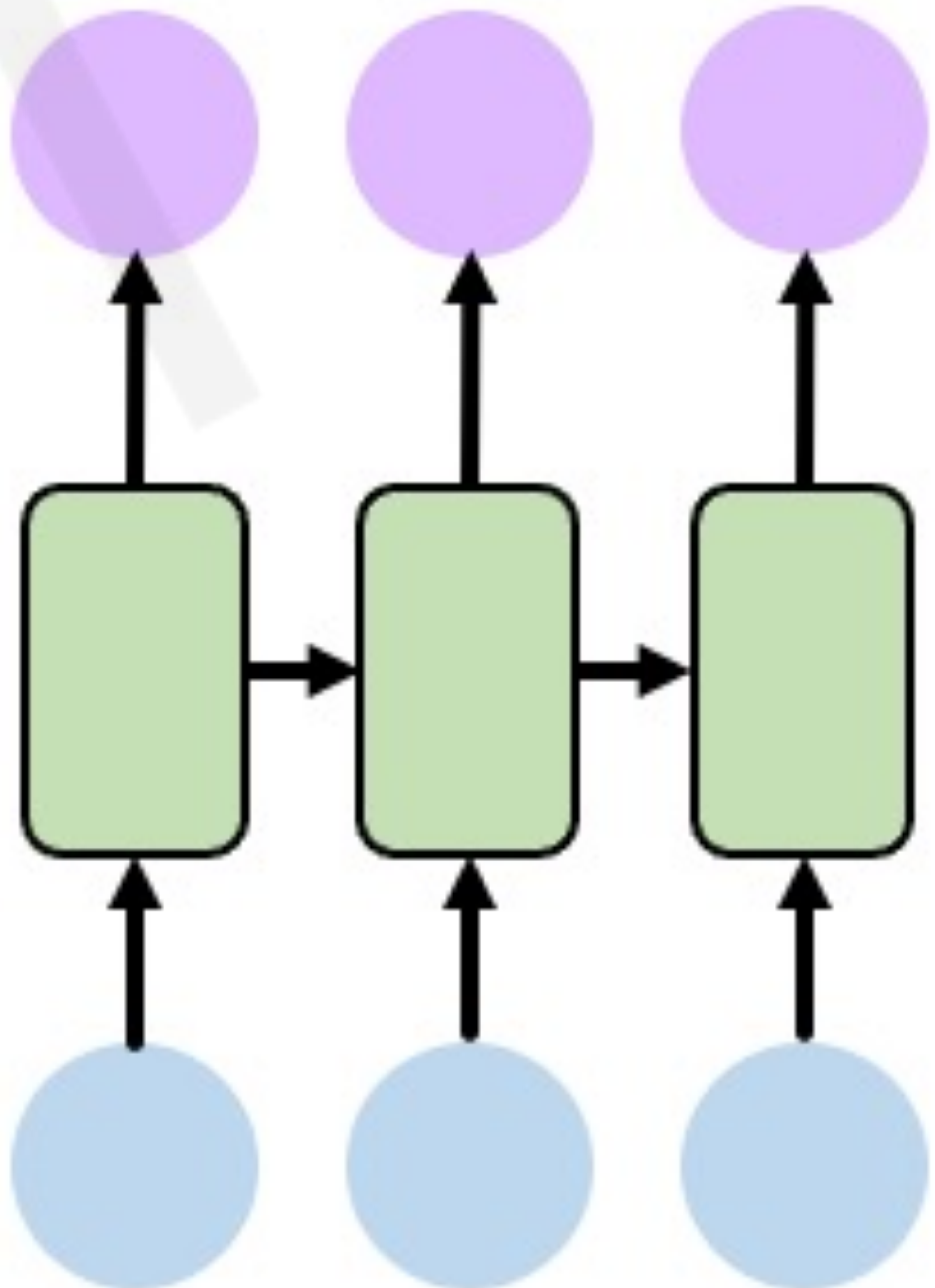


Many to One
Sentiment Classification



One to Many
Image Captioning

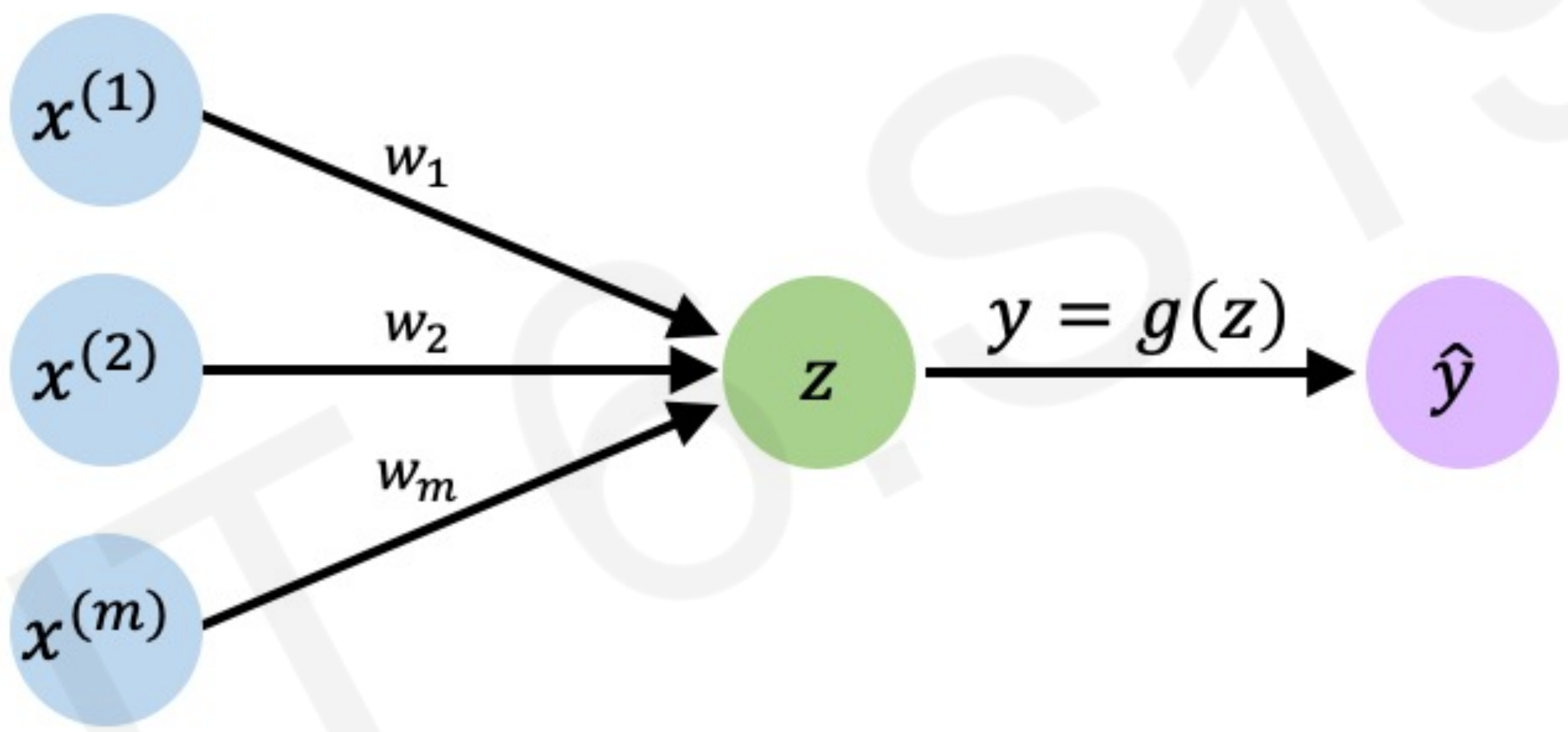
"A baseball player throws a ball."



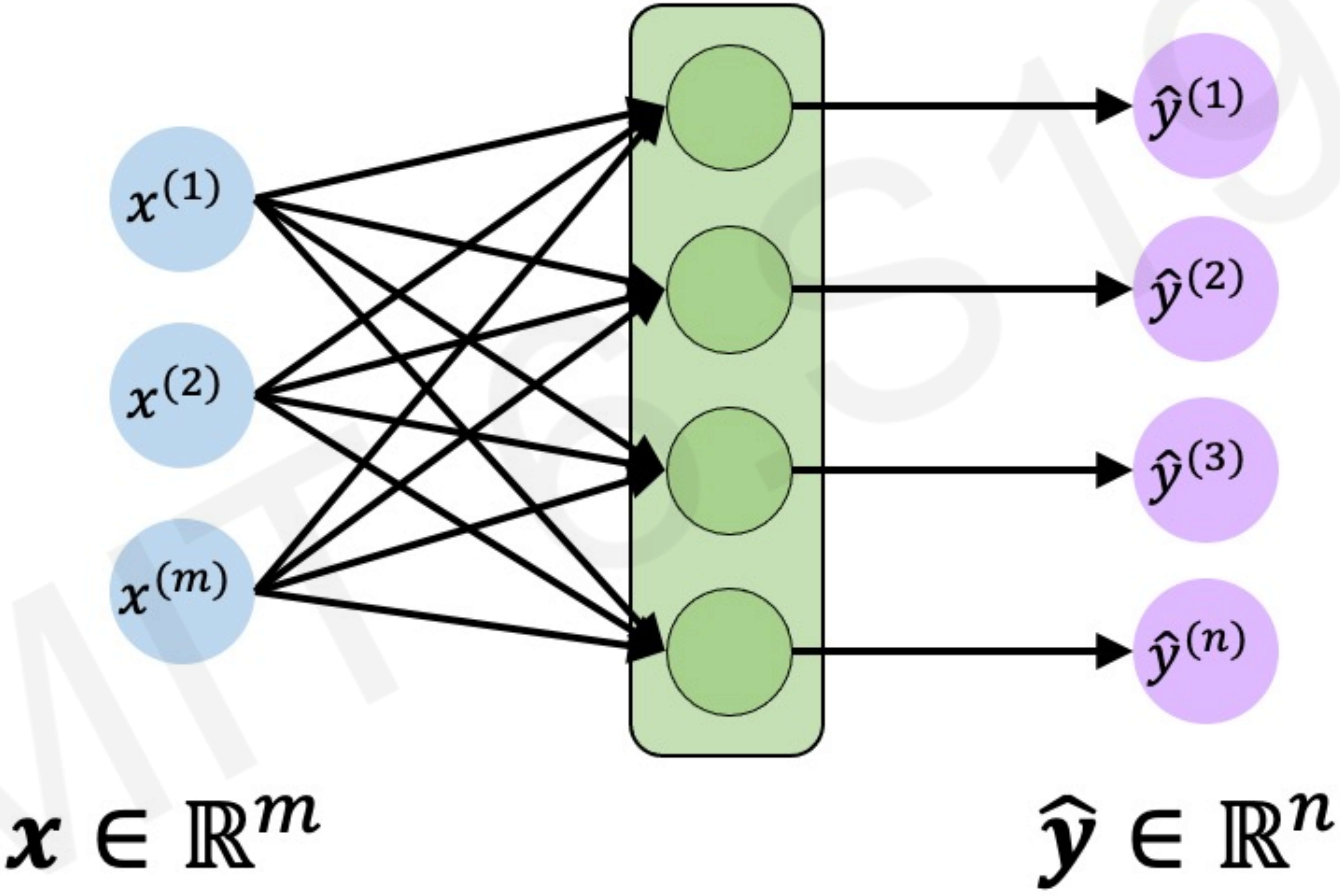
Many to Many
Machine Translation

Neurons with Recurrence

The Perceptron Revisited



Feed-Forward Networks Revisited



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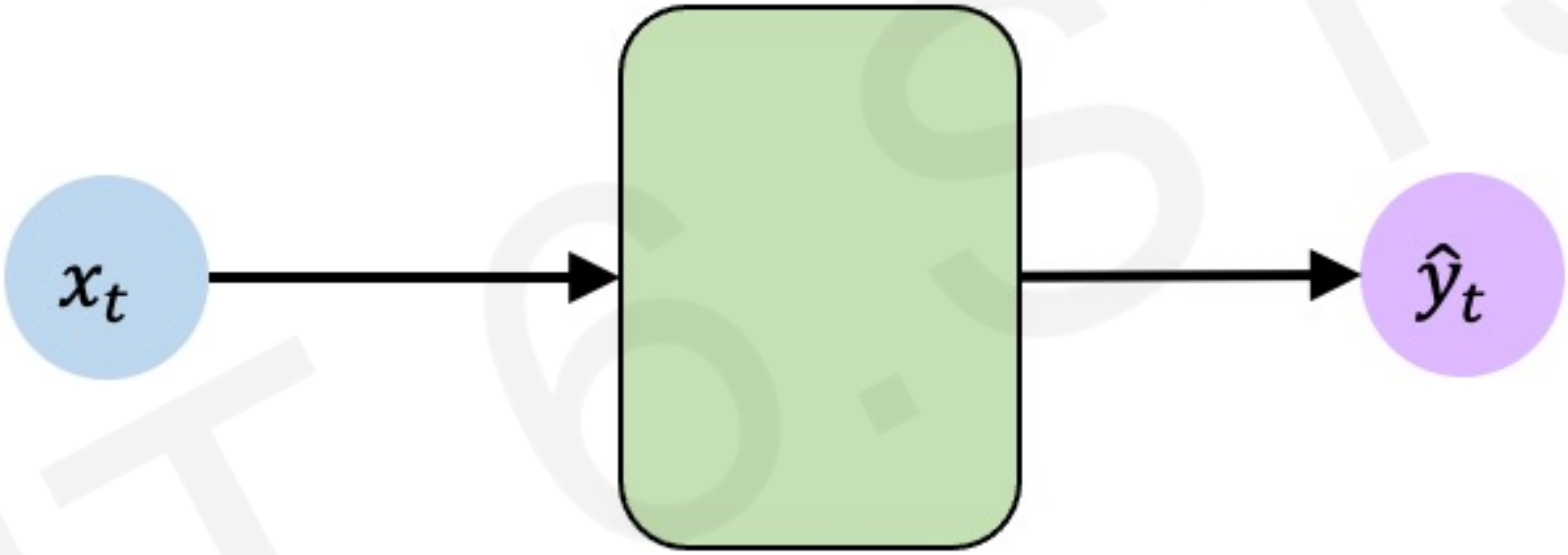
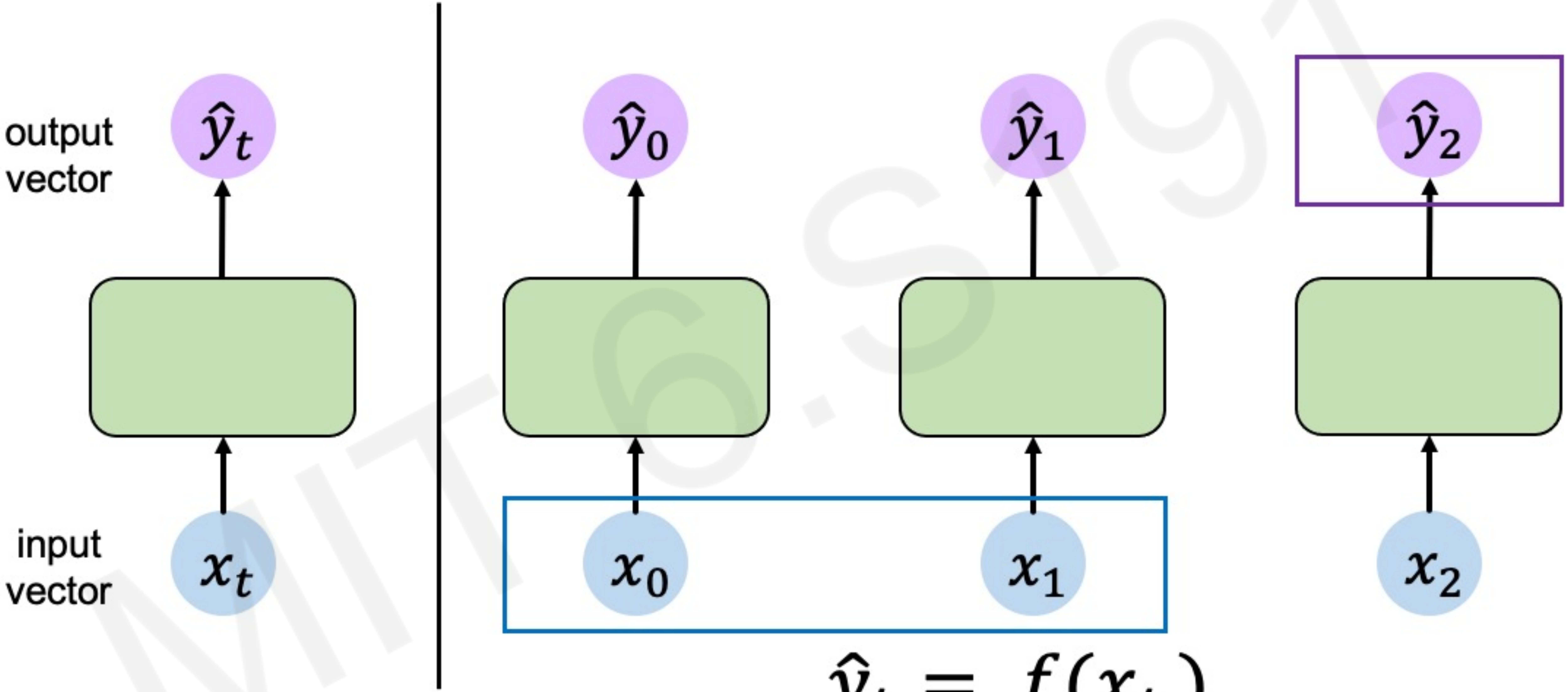


$\boldsymbol{x}_t \in \mathbb{R}^m$

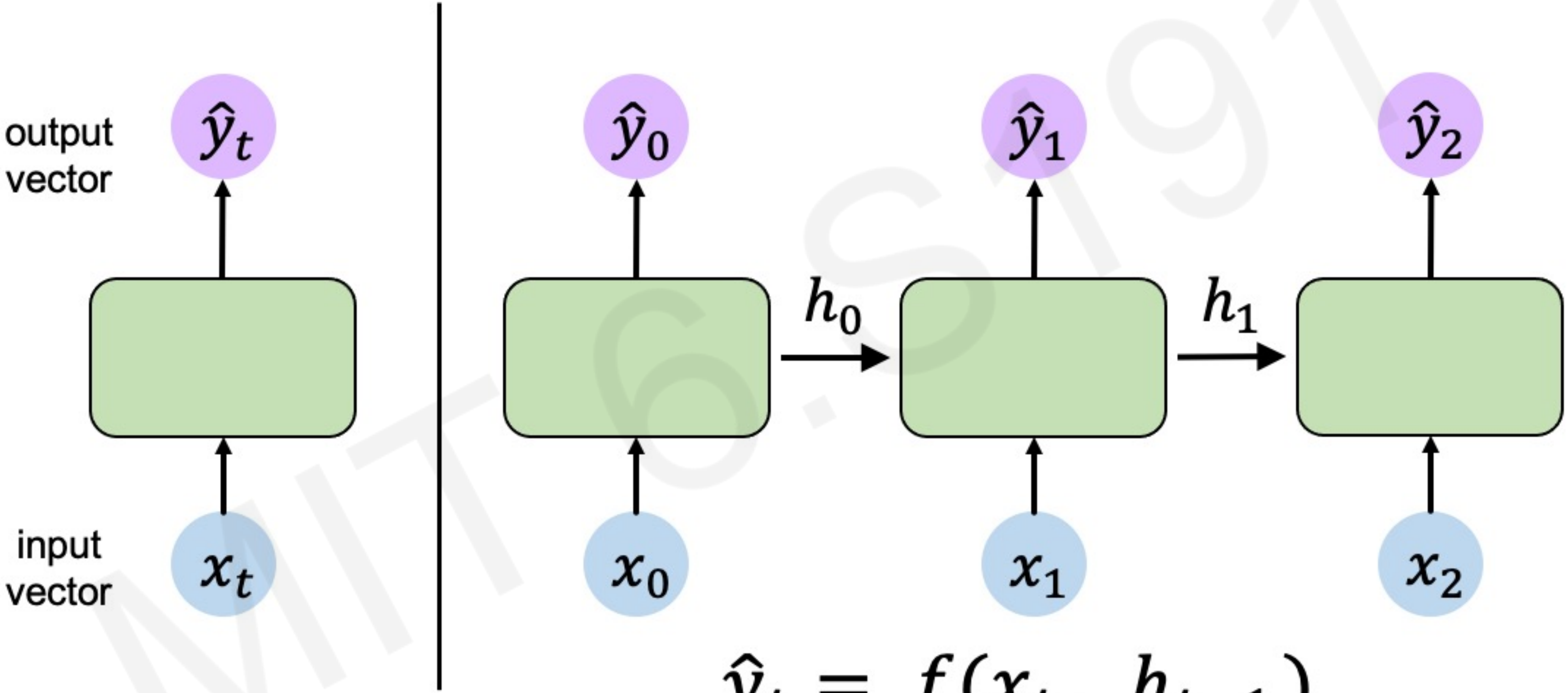
$\hat{\boldsymbol{y}}_t \in \mathbb{R}^n$

Handling Individual Time Steps



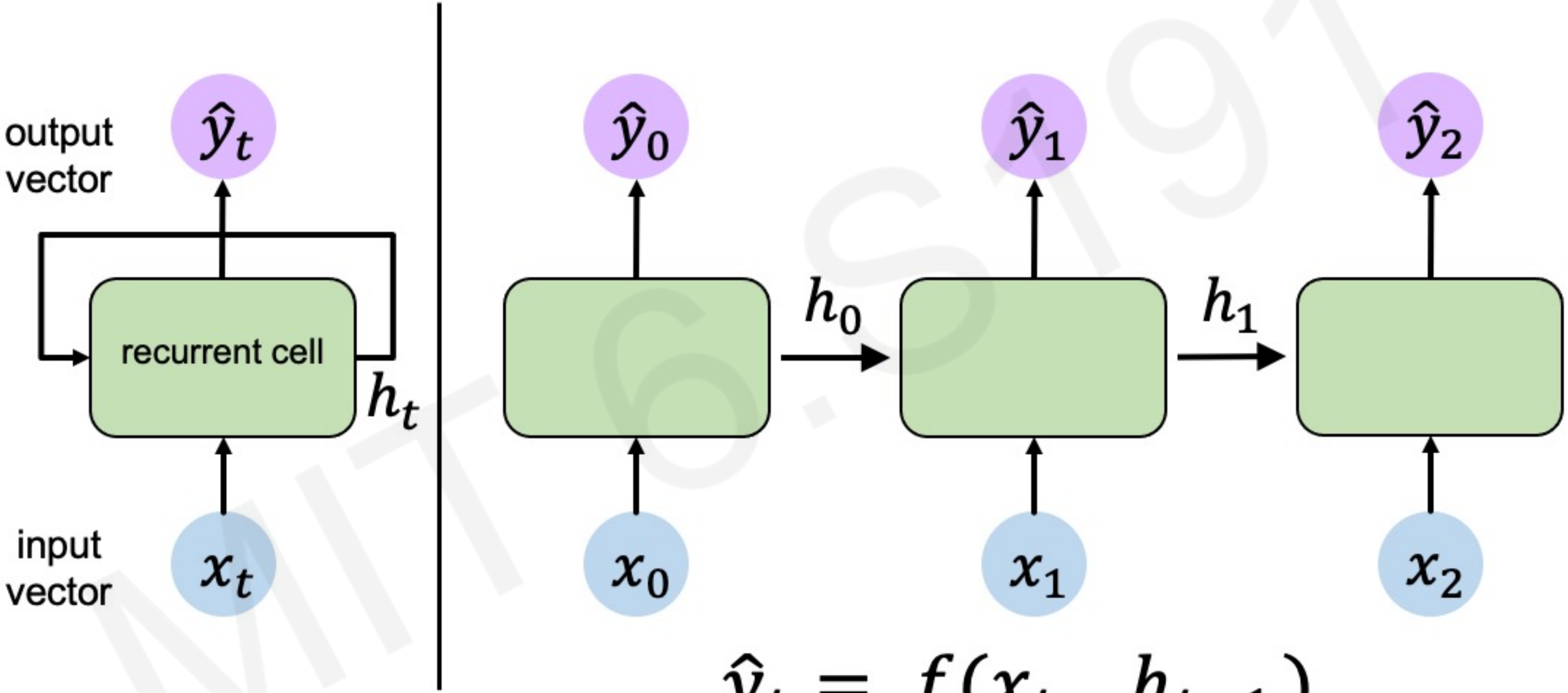
$$\hat{y}_t = f(x_t)$$

Neurons with Recurrence



$$\underbrace{\hat{y}_t}_{\text{output}} = f(\underbrace{x_t}_{\text{input}},\ \underbrace{h_{t-1}}_{\text{past memory}})$$

Neurons with Recurrence



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Recurrent Neural Networks (RNNs)

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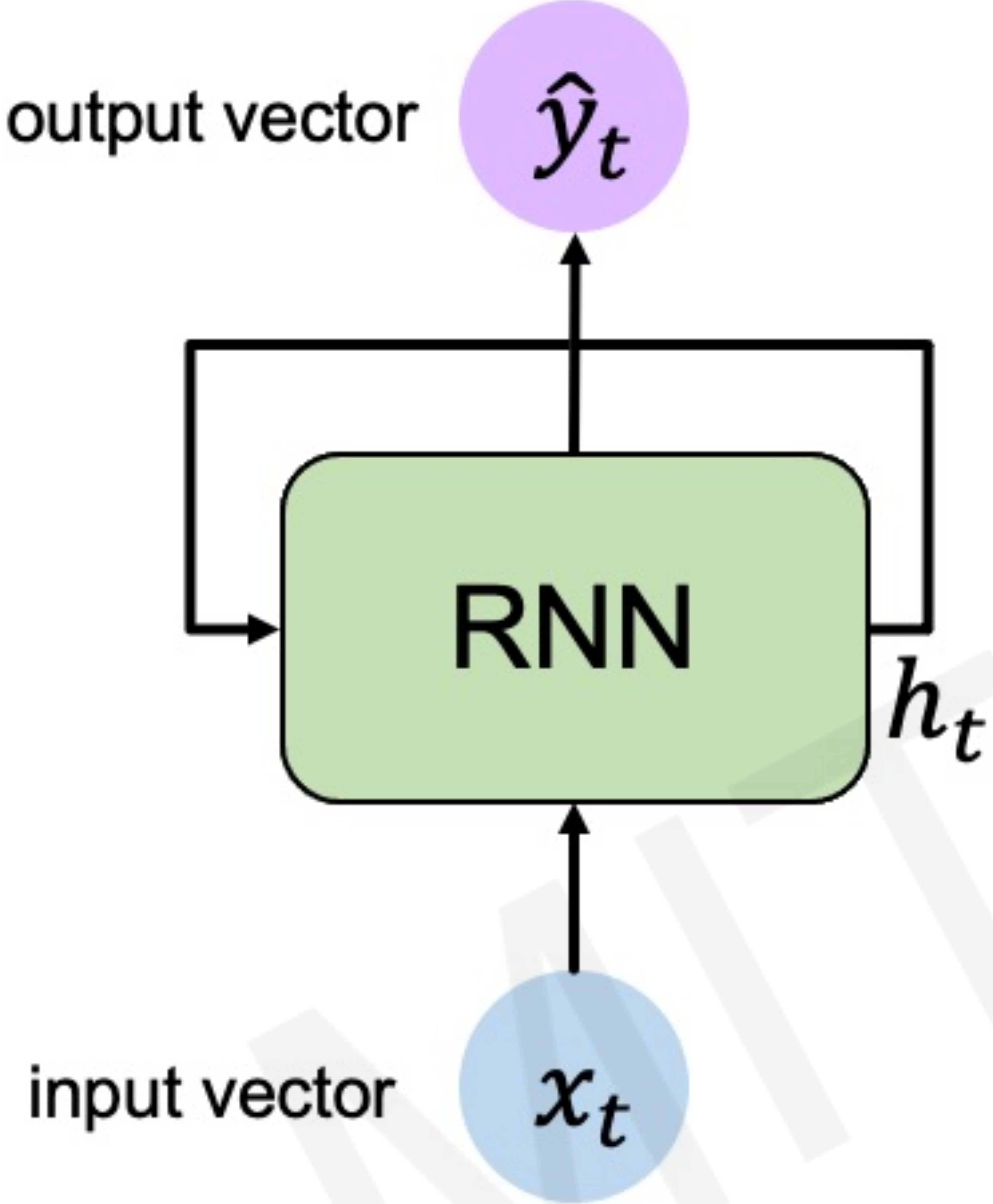


Apply a **recurrence relation** at every time step to process a sequence:

$$\boxed{h_t} = \boxed{f_W}(\boxed{x_t}, \boxed{h_{t-1}})$$

cell state — function with weights W — input — old state

Note: the same function and set of parameters are used at every time step

RNNs have a **state**, h_t, that is updated **at each time step** as a sequence is processed

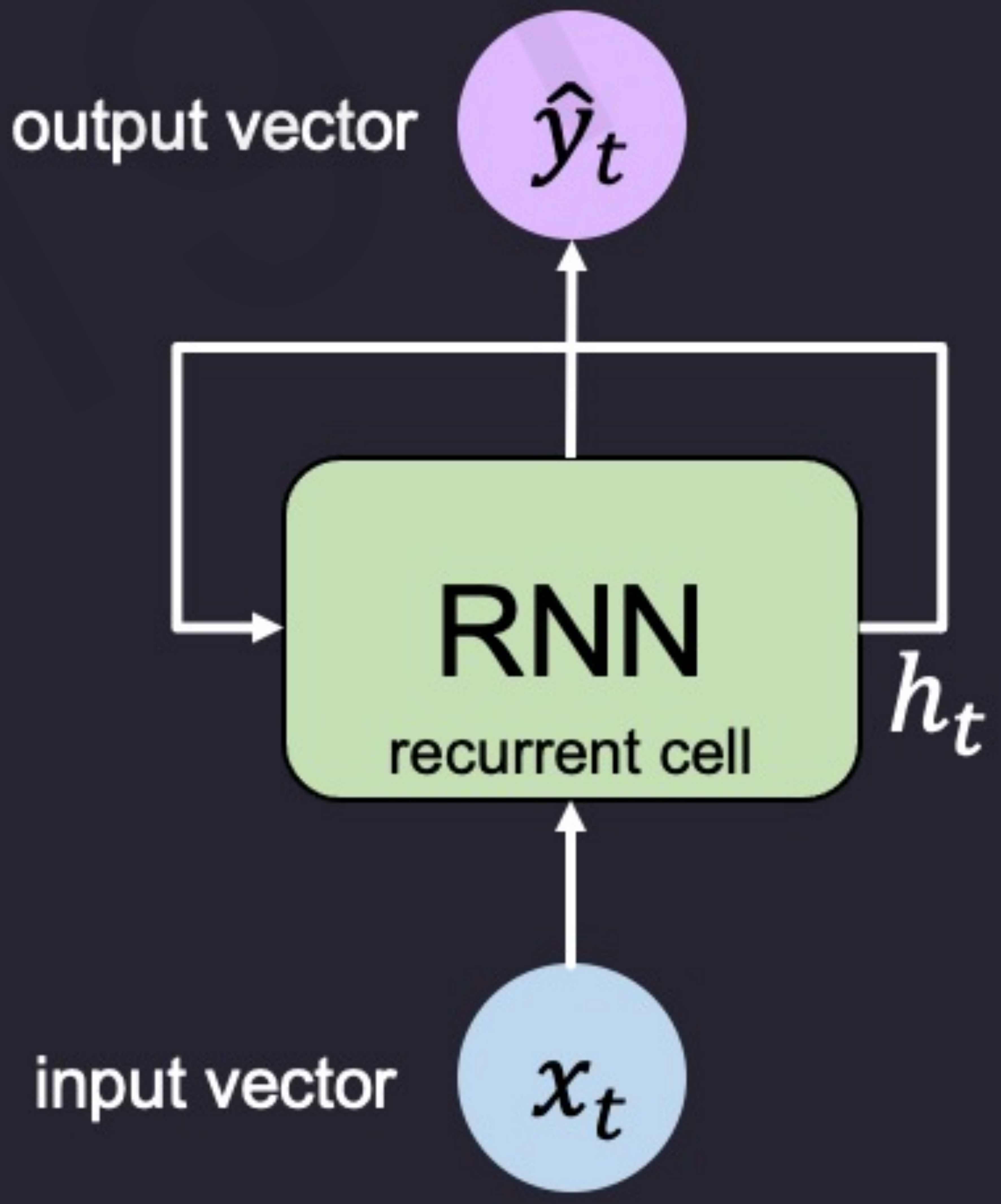
RNN Intuition

```
my_rnn = RNN()
hidden_state = [0, 0, 0, 0]

sentence = ["I", "love", "recurrent", "neural"]

for word in sentence:
    prediction, hidden_state = my_rnn(word, hidden_state)

next_word_prediction = prediction
# >>> "networks!"
```



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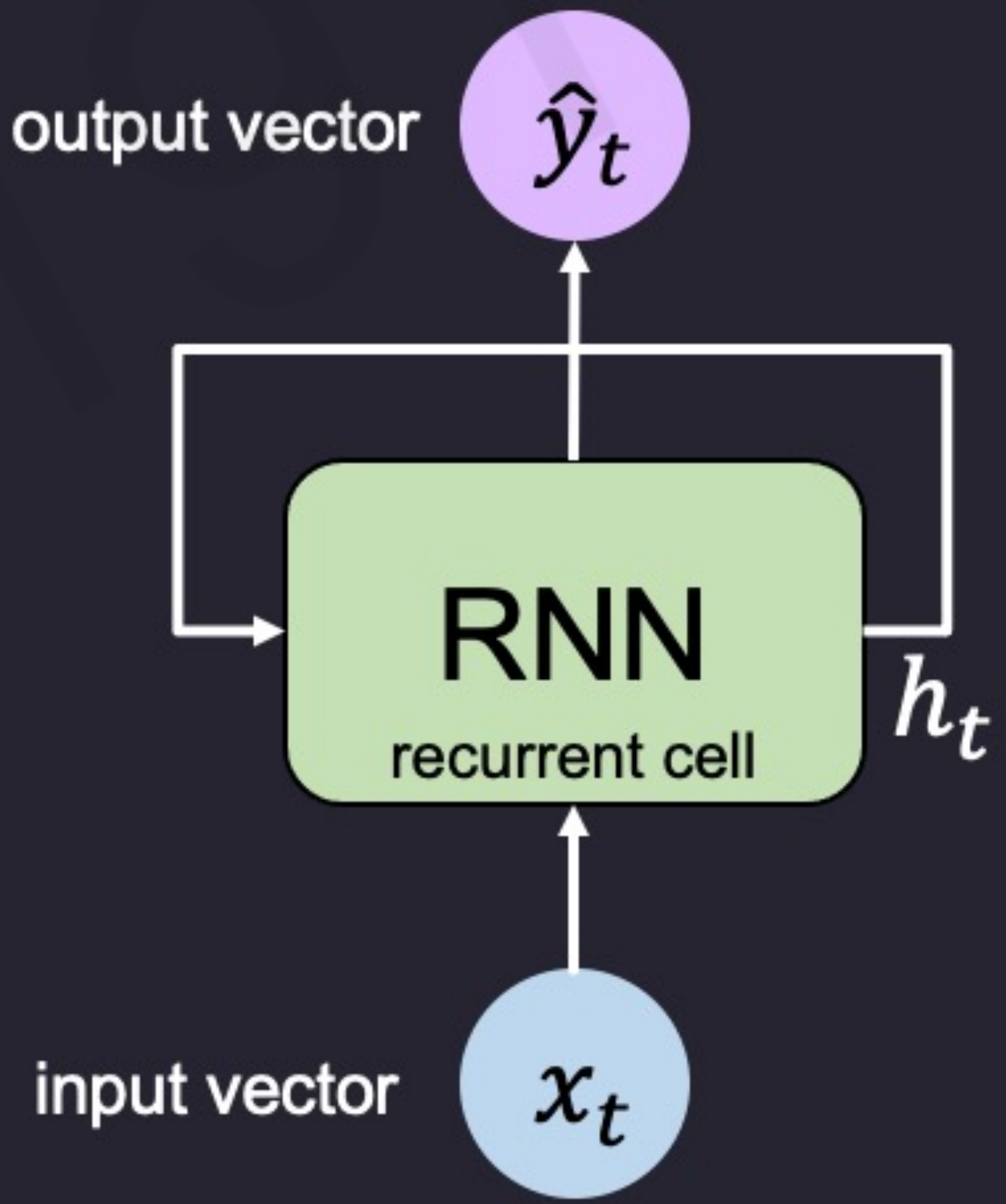

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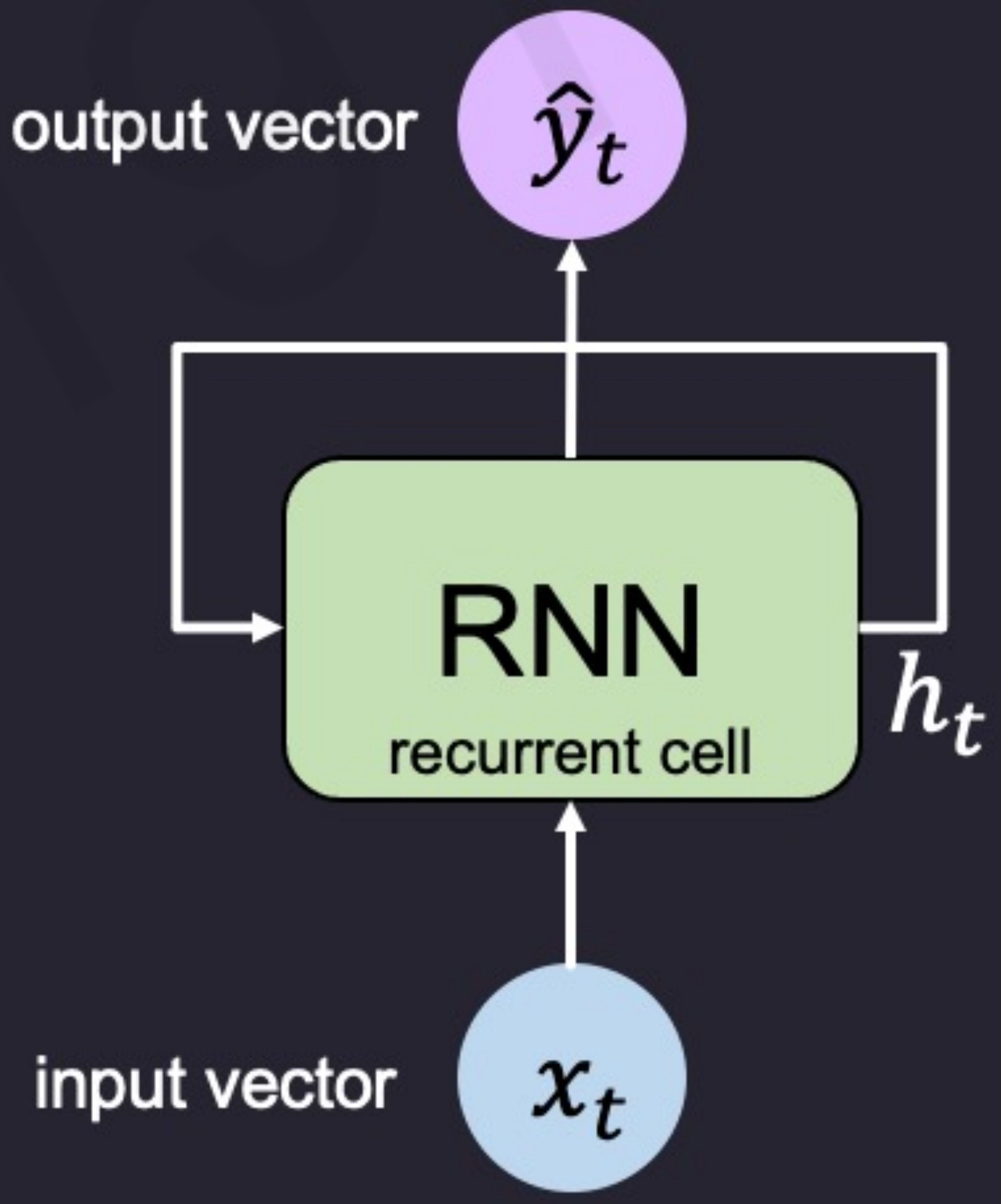
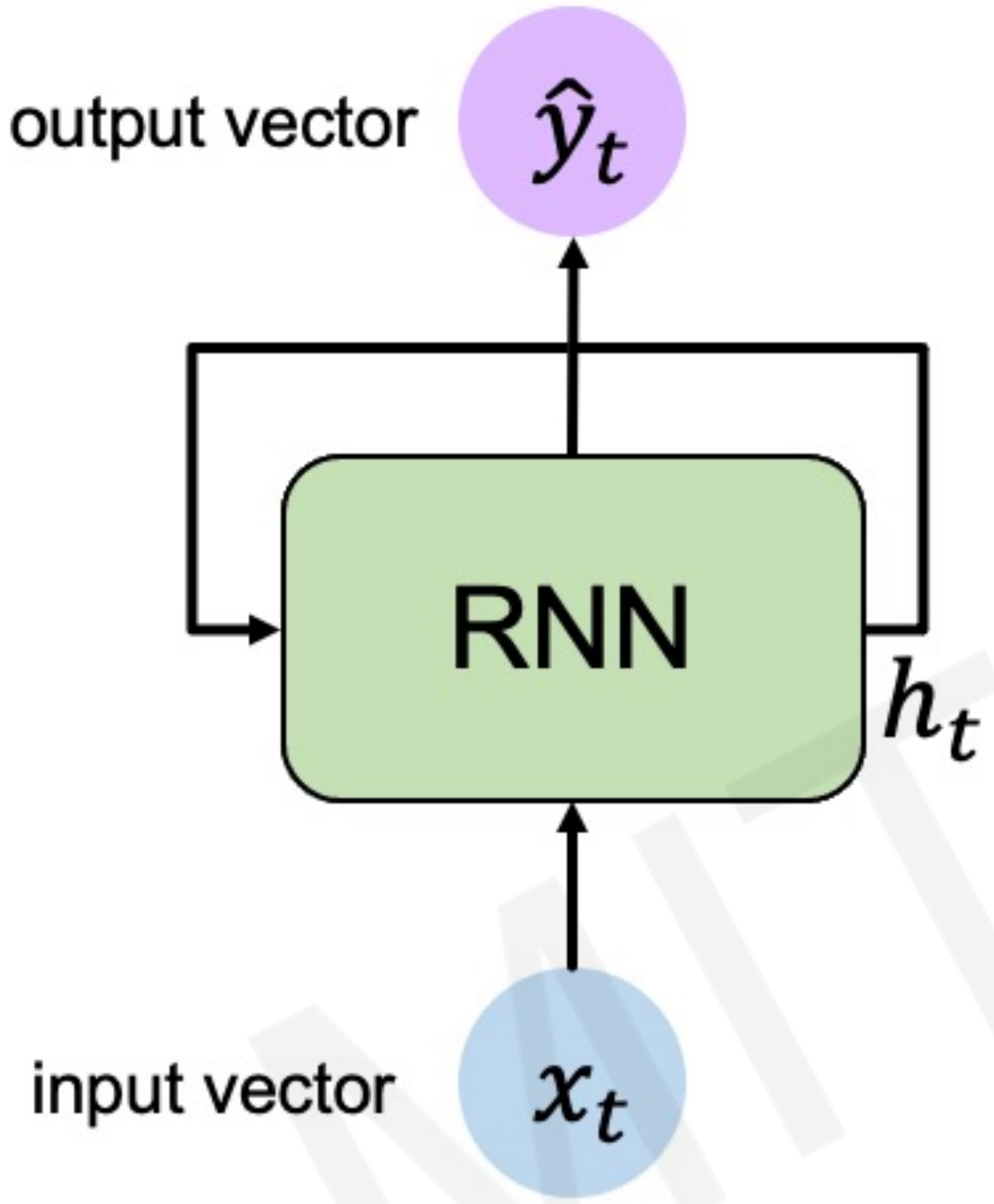


RNN State Update and Output



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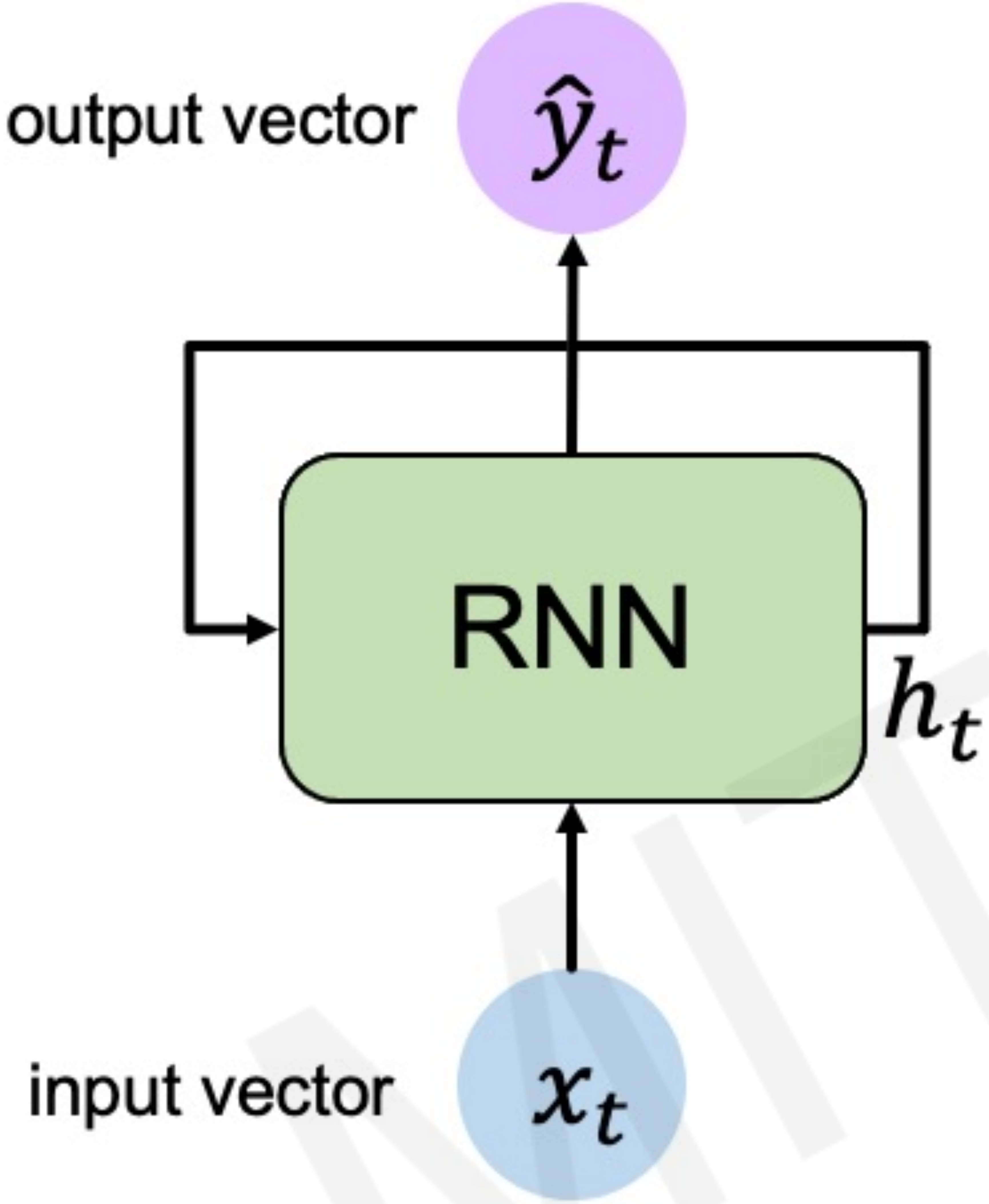
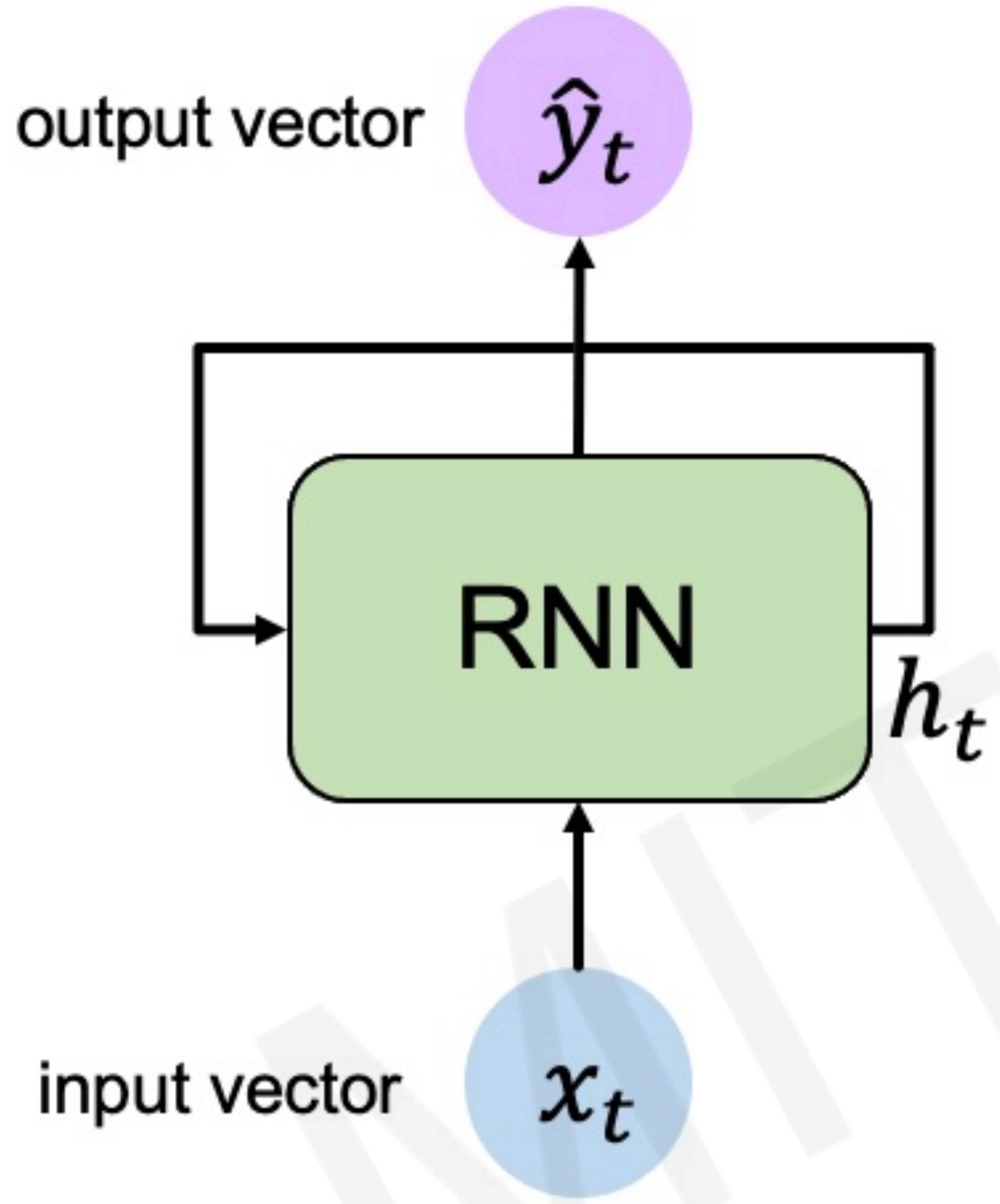


Input Vector

$$x_t$$

RNN State Update and Output



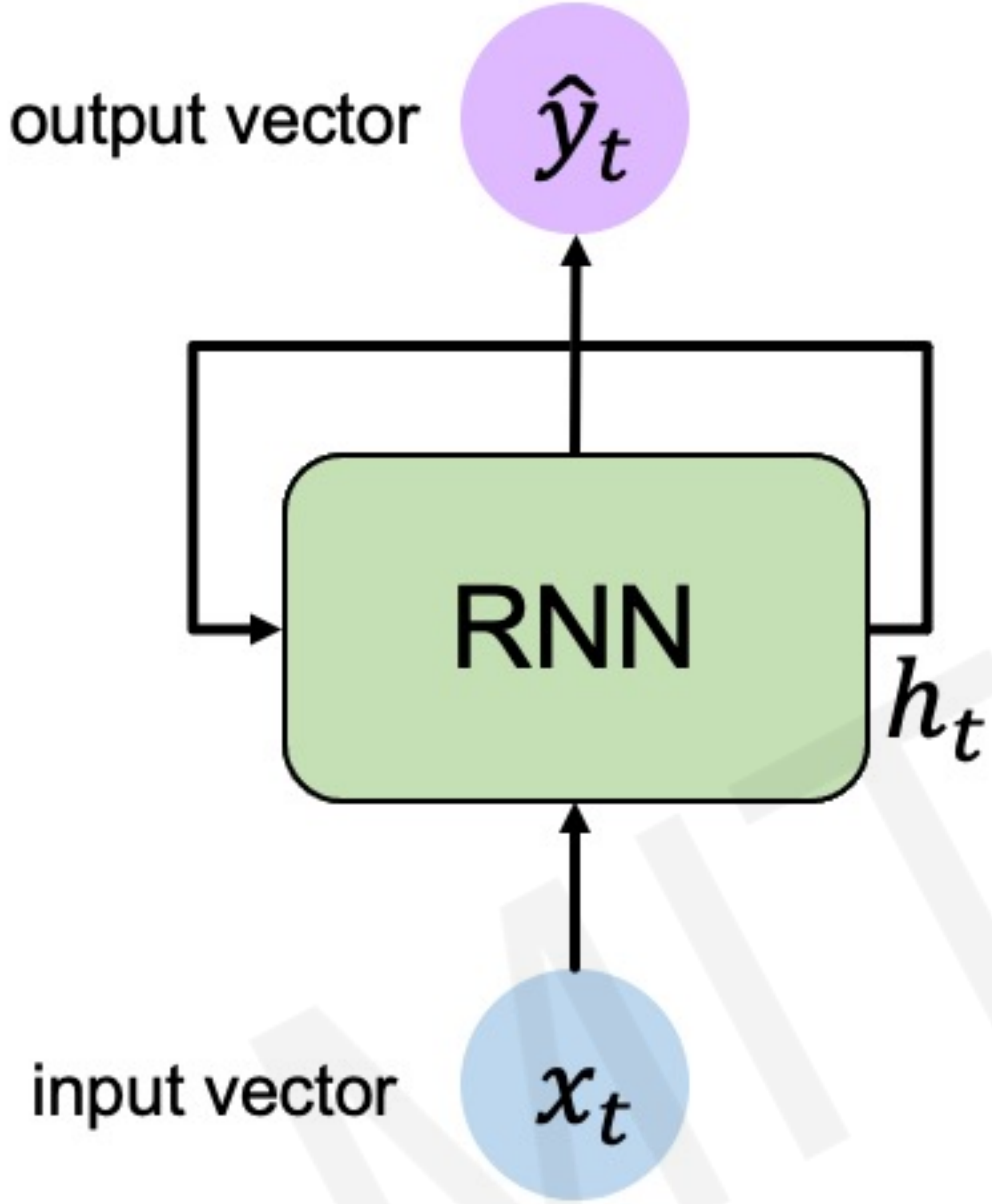
Update Hidden State

$$h_t = \tanh(\boldsymbol{W}_{hh}^T h_{t-1} + \boldsymbol{W}_{xh}^T x_t)$$

Input Vector

$$x_t$$

RNN State Update and Output



Output Vector

$$\hat{y}_t = \boldsymbol{W}_{\boldsymbol{hy}}^{\boldsymbol{T}} h_t$$

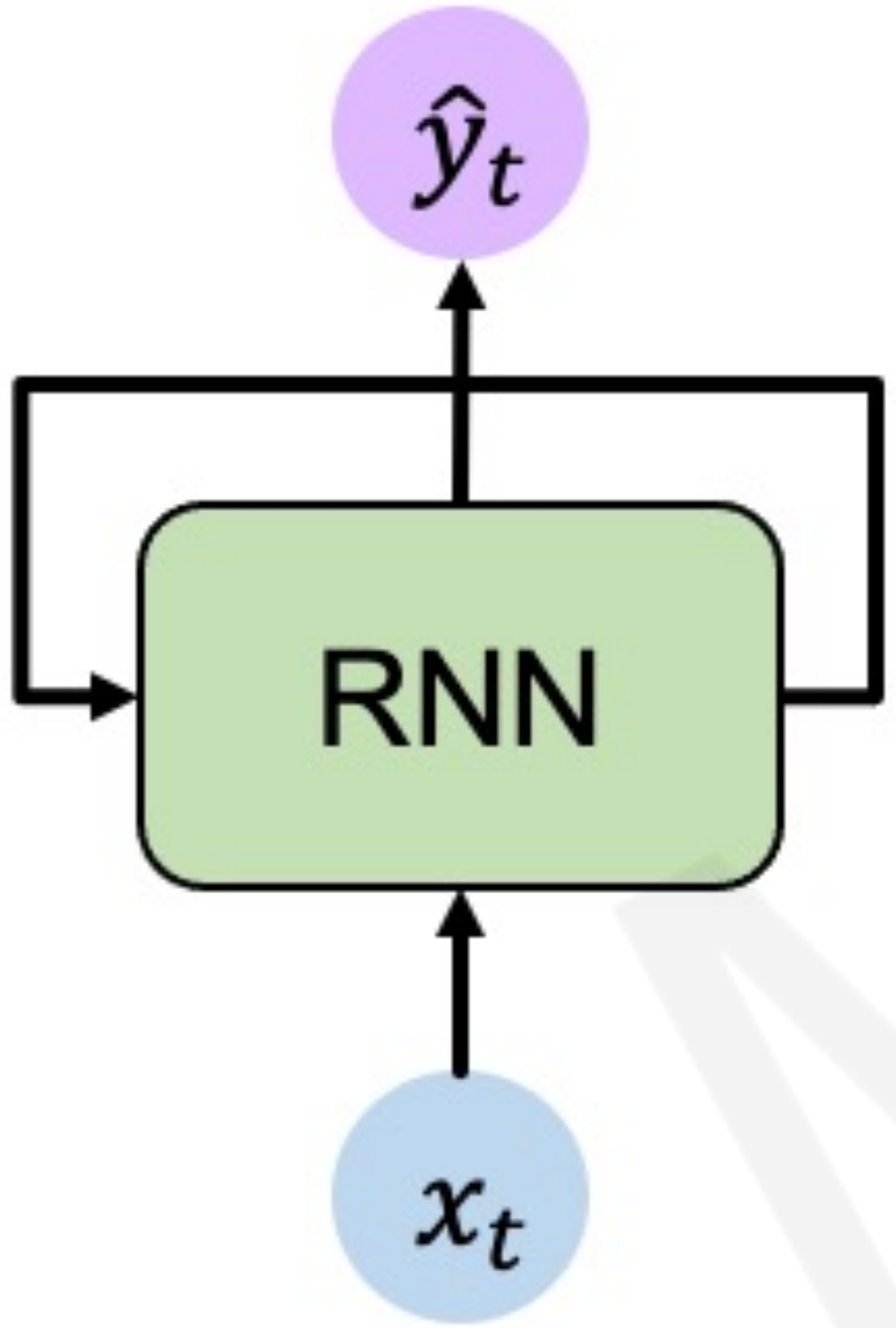
Update Hidden State

$$h_t = \tanh(\boldsymbol{W}_{\boldsymbol{hh}}^{\boldsymbol{T}} h_{t-1} + \boldsymbol{W}_{\boldsymbol{xh}}^{\boldsymbol{T}} x_t)$$

Input Vector

$$x_t$$

RNNs: Computational Graph Across Time

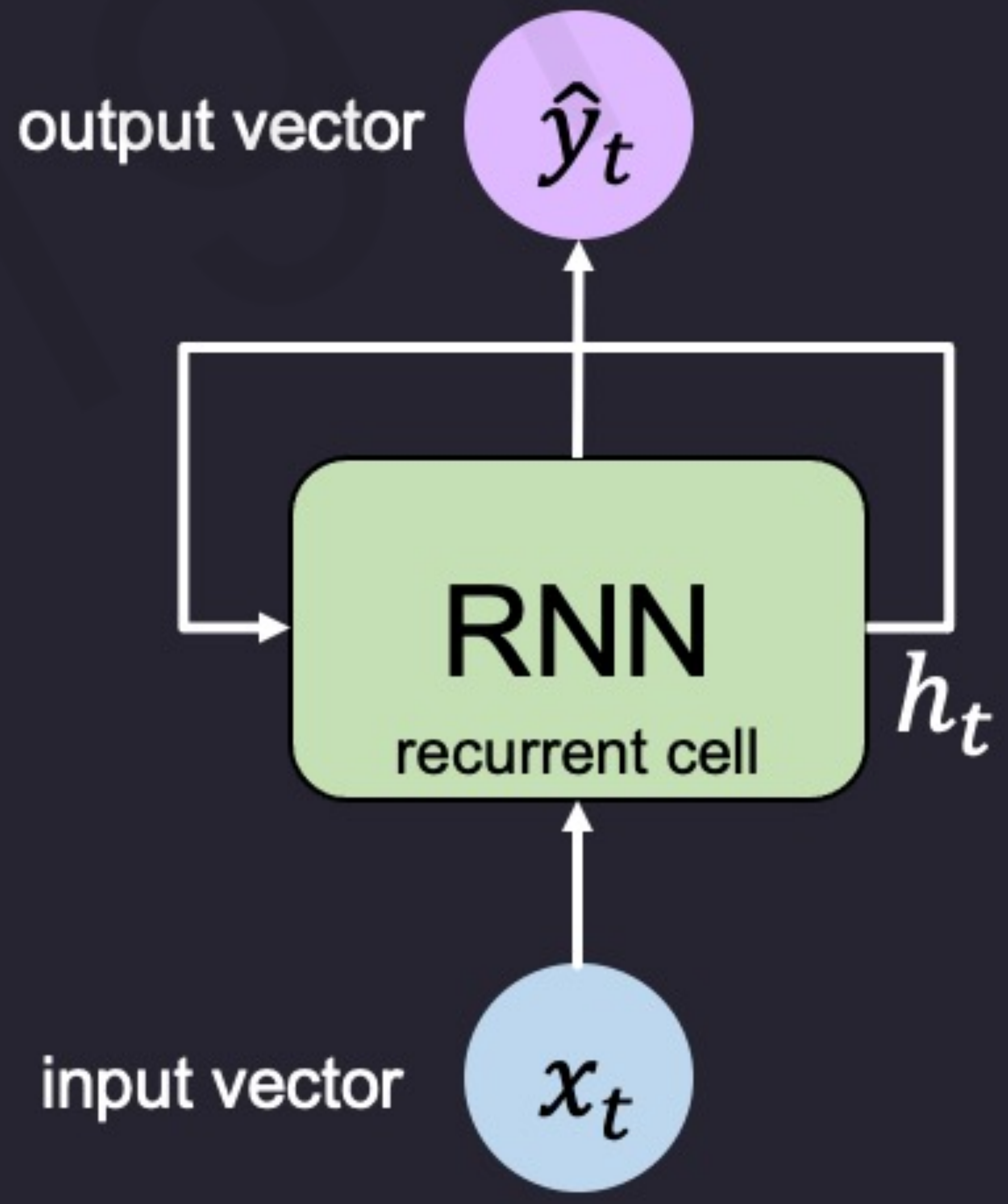


= Represent as computational graph unrolled across time

RNNs: Computational Graph Across Time

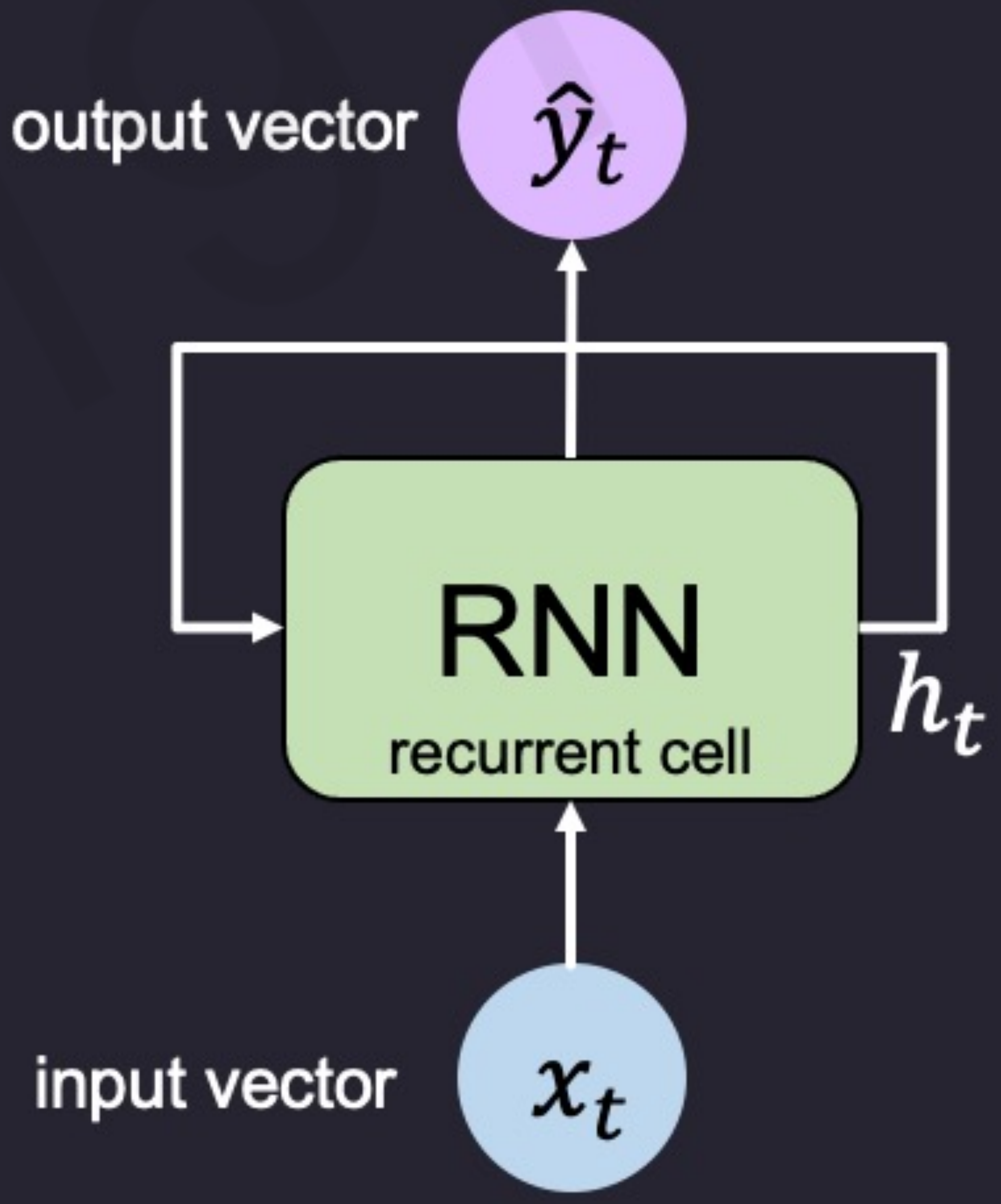
RNNs from Scratch

```python
class MyRNNCell(tf.keras.layers.Layer):
  def __init__(self, rnn_units, input_dim, output_dim):
    super(MyRNNCell, self).__init__()

    # Initialize weight matrices
    self.W_xh = self.add_weight([rnn_units, input_dim])
    self.W_hh = self.add_weight([rnn_units, rnn_units])
    self.W_hy = self.add_weight([output_dim, rnn_units])

    # Initialize hidden state to zeros
    self.h = tf.zeros([rnn_units, 1])

  def call(self, x):
    # Update the hidden state
    self.h = tf.math.tanh( self.W_hh * self.h + self.W_xh * x )

    # Compute the output
    output = self.W_hy * self.h

    # Return the current output and hidden state
    return output, self.h
```



RNN Implementation in TensorFlow

```
tf.keras.layers.SimpleRNN(rnn_units)
```



RNNs for Sequence Modeling

One to One
"Vanilla" NN
Binary classification

Many to One
Sentiment Classification

One to Many
Text Generation
Image Captioning

Many to Many
Translation & Forecasting
Music Generation

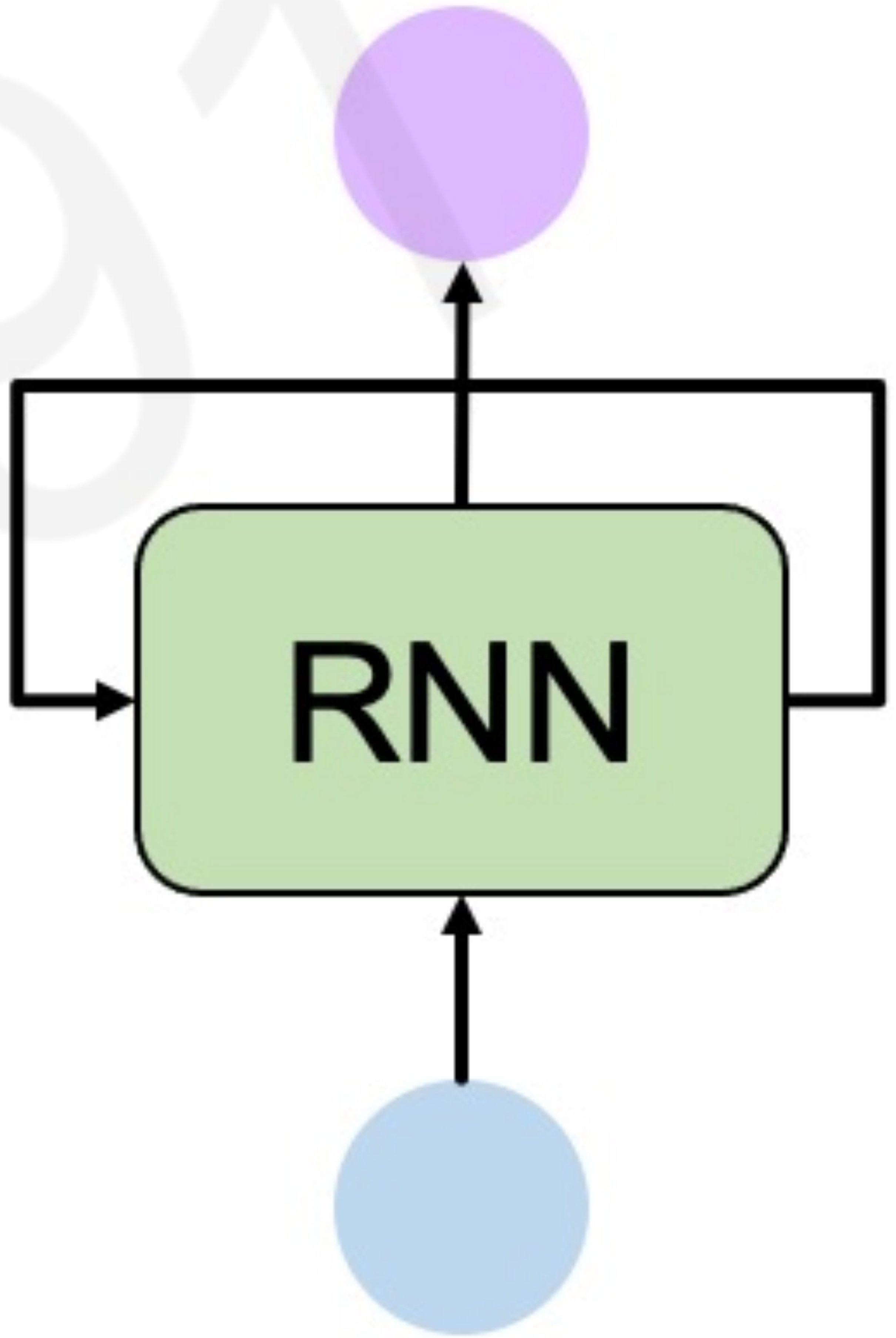
… and many other architectures and applications

Software Lab!

Sequence Modeling: Design Criteria

To model sequences, we need to:

1. Handle **variable-length** sequences
2. Track **long-term** dependencies
3. Maintain information about **order**
4. **Share parameters** across the sequence



Recurrent Neural Networks (RNNs) meet these sequence modeling design criteria

A Sequence Modeling Problem: Predict the Next Word

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"This morning I took my cat for a walk."

A Sequence Modeling Problem: Predict the Next Word

"This morning I took my cat for a walk."

given these words

A Sequence Modeling Problem: Predict the Next Word

"This morning I took my cat for a walk."

given these words

predict the next word

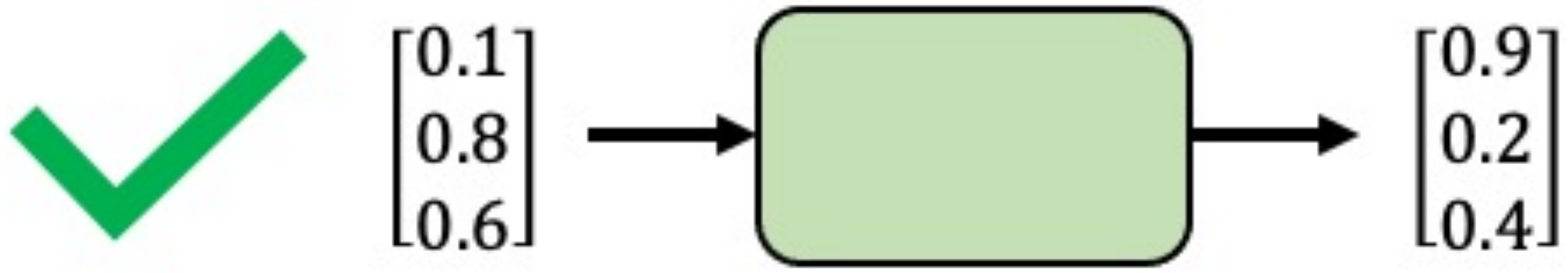
A Sequence Modeling Problem: Predict the Next Word

"This morning I took my cat for a walk."

given these words — predict the next word

Representing Language to a Neural Network

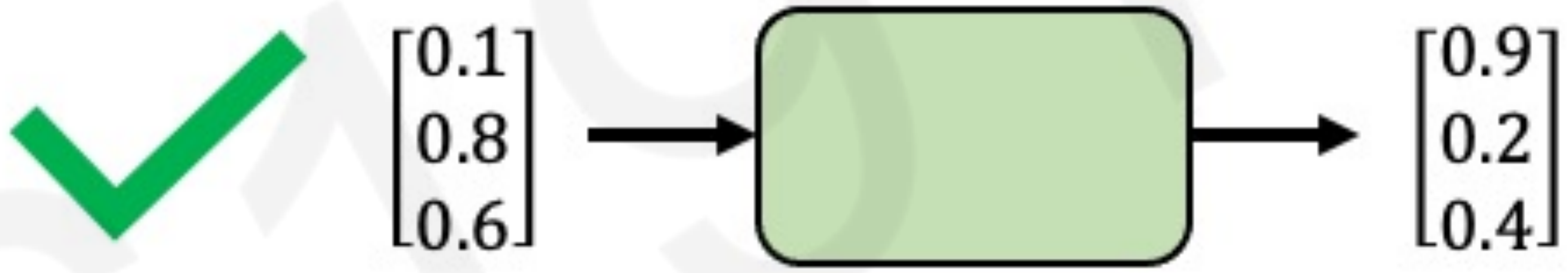
Neural networks cannot interpret words



Neural networks require numerical inputs

Encoding Language for a Neural Network

Neural networks cannot interpret words



Neural networks require numerical inputs

Embedding: transform indexes into a vector of fixed size.

this cat for took my walk I a morning

1. Vocabulary:
Corpus of words

a → 1
cat → 2
… …
walk → N

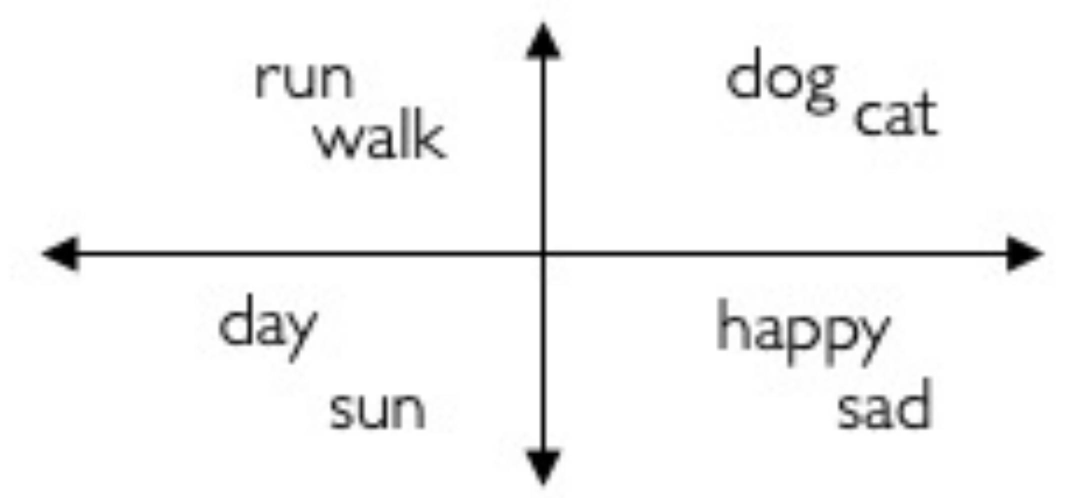
2. Indexing:
Word to index

One-hot embedding

"cat" = [0, 1, 0, 0, 0, 0]

i-th index

Learned embedding



3. Embedding:
Index to fixed-sized vector

Handle Variable Sequence Lengths

The food was great

vs.

We visited a restaurant for lunch

vs.

We were hungry but cleaned the house before eating

Model Long-Term Dependencies

"**France** is where I grew up, but I now live in Boston. I speak fluent ___."

J'aime 6.S191!

We need information from **the distant past** to accurately predict the correct word.

Capture Differences in Sequence Order

The food was good, not bad at all.

vs.

The food was bad, not good at all.

Sequence Modeling: Design Criteria

To model sequences, we need to:

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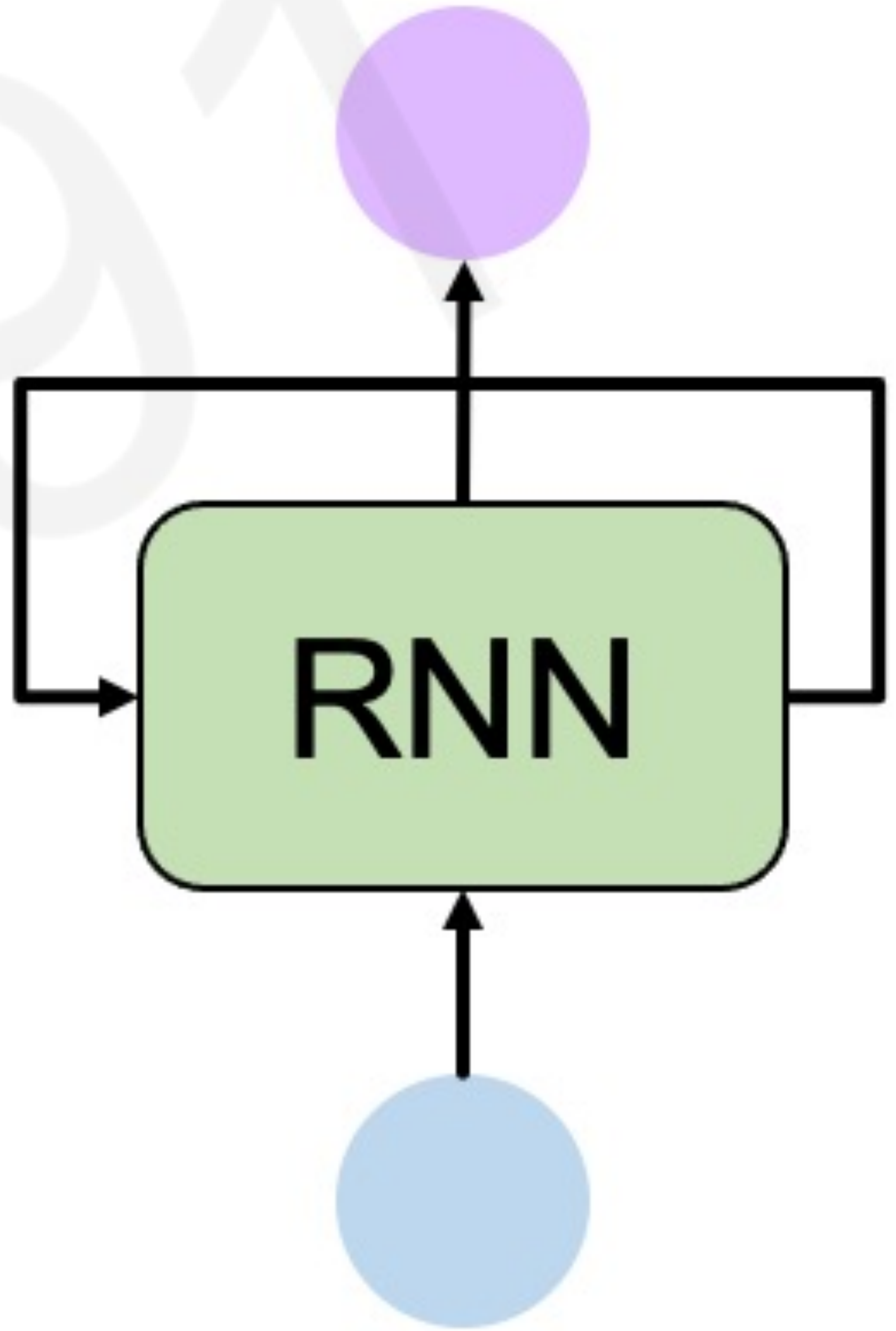
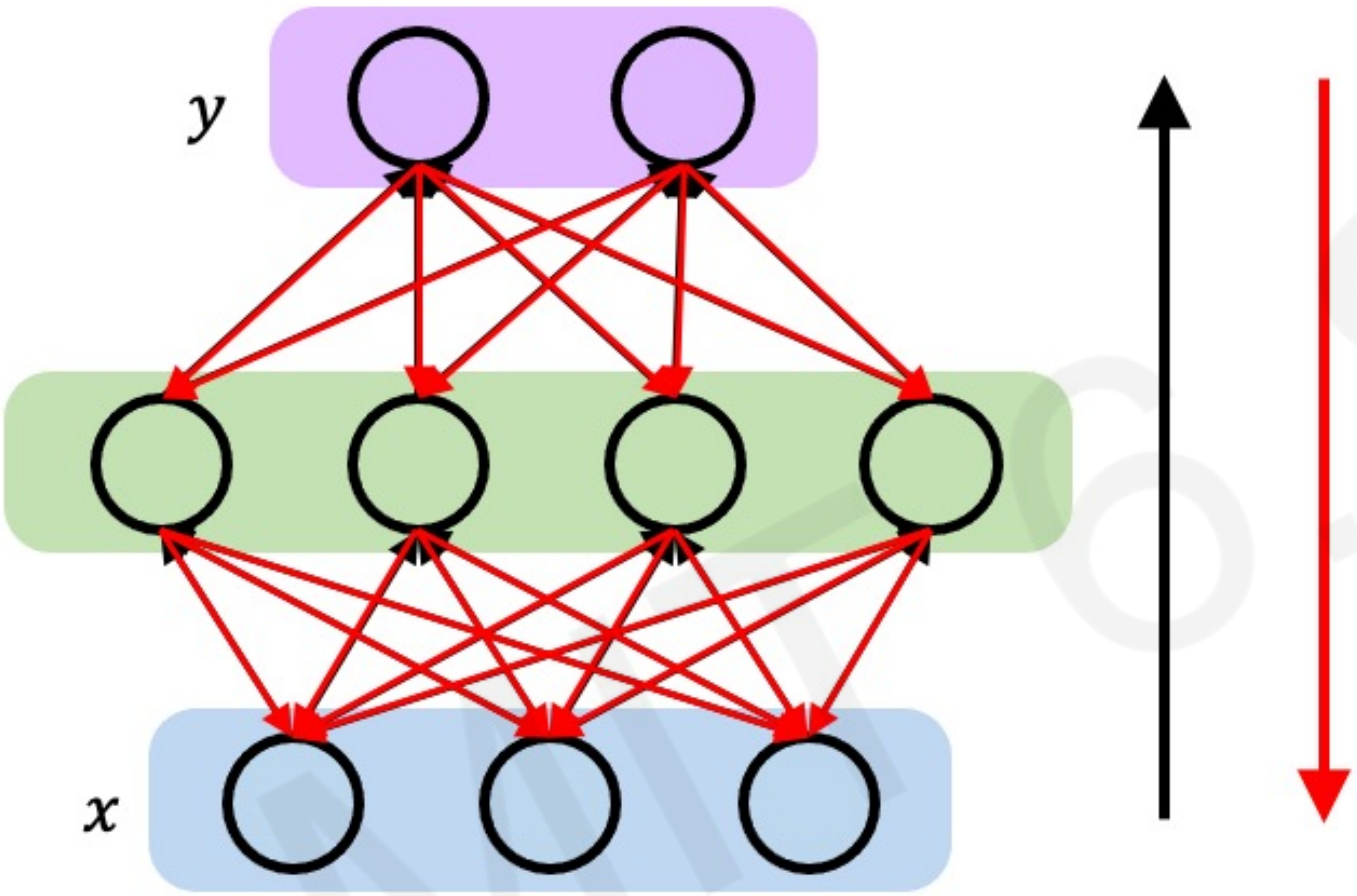


Recurrent Neural Networks (RNNs) meet these sequence modeling design criteria

Backpropagation Through Time (BPTT)

Recall: Backpropagation in Feed Forward Models



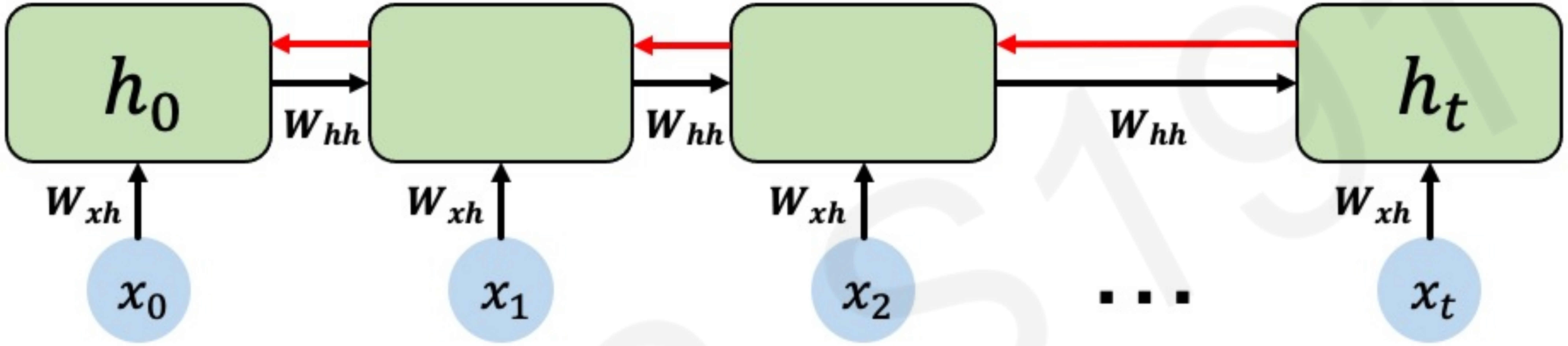
Backpropagation algorithm:

1. Take the derivative (gradient) of the loss with respect to each parameter
2. Shift parameters in order to minimize loss

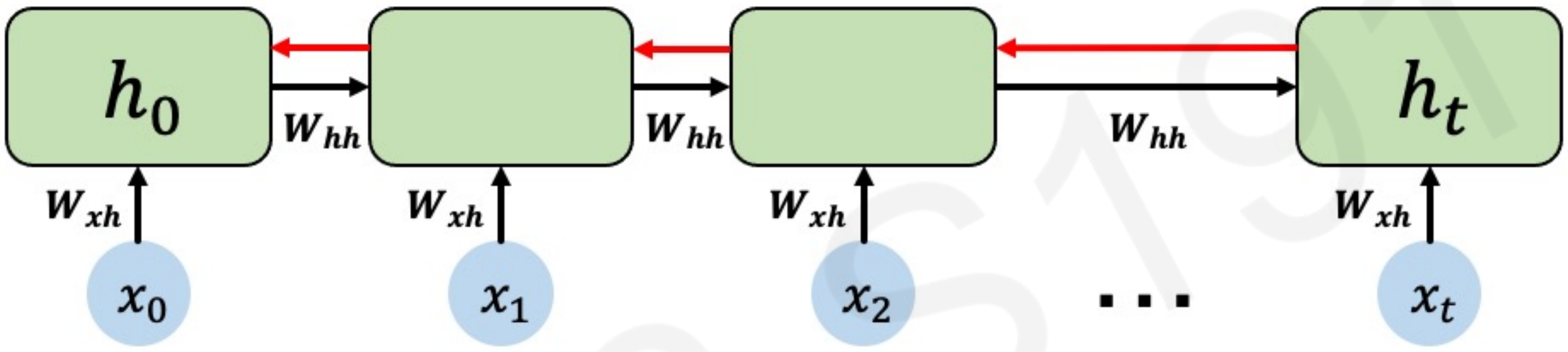
RNNs: Backpropagation Through Time

RNNs: Backpropagation Through Time

Standard RNN Gradient Flow

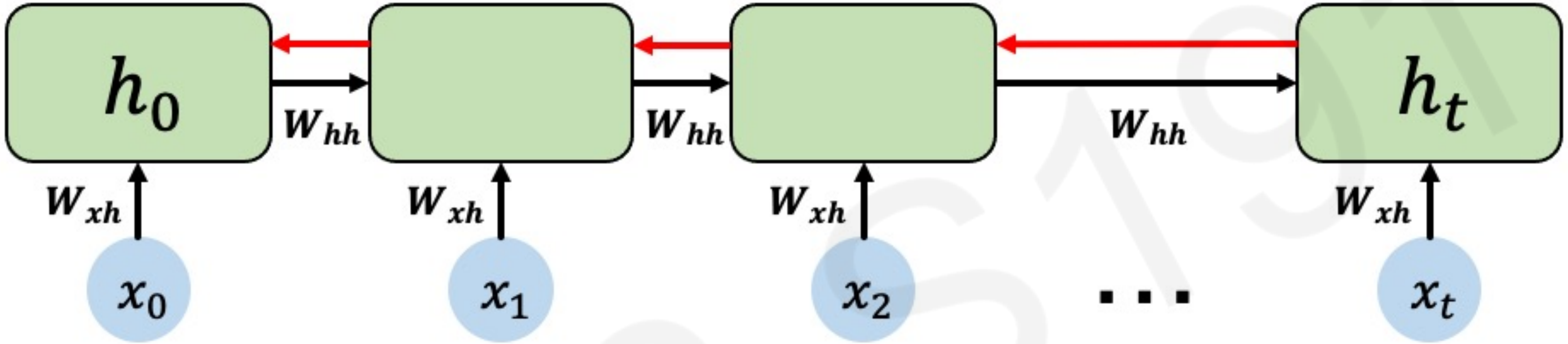


Standard RNN Gradient Flow



Computing the gradient wrt h_0 involves **many factors of** W_{hh} + **repeated gradient computation**!

Standard RNN Gradient Flow: Exploding Gradients

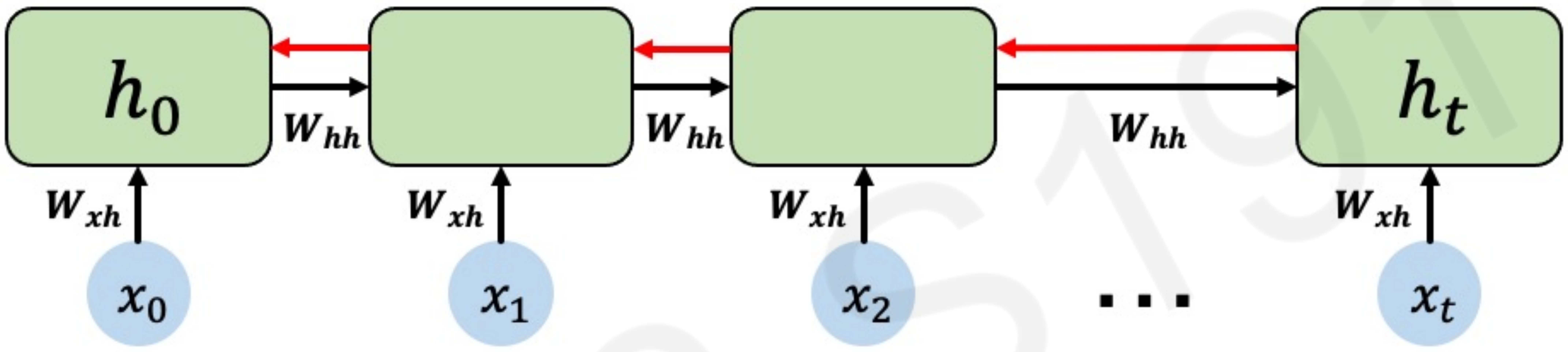


Computing the gradient wrt h_0 involves **many factors of W_{hh} + repeated gradient computation!**

Many values > 1:
exploding gradients

Gradient clipping to scale big gradients

Standard RNN Gradient Flow: Vanishing Gradients



Computing the gradient wrt h_0 involves **many factors of W_{hh} + repeated gradient computation!**

Many values > 1:
exploding gradients

Gradient clipping to scale big gradients

Many values < 1:
vanishing gradients

1. **Activation function**
2. **Weight initialization**
3. **Network architecture**

The Problem of Long-Term Dependencies

Why are vanishing gradients a problem?

Multiply many **small numbers** together

↓

Errors due to further back time steps have smaller and smaller gradients

↓

Bias parameters to capture short-term dependencies

The Problem of Long-Term Dependencies

"The clouds are in the ___"

Why are vanishing gradients a problem?

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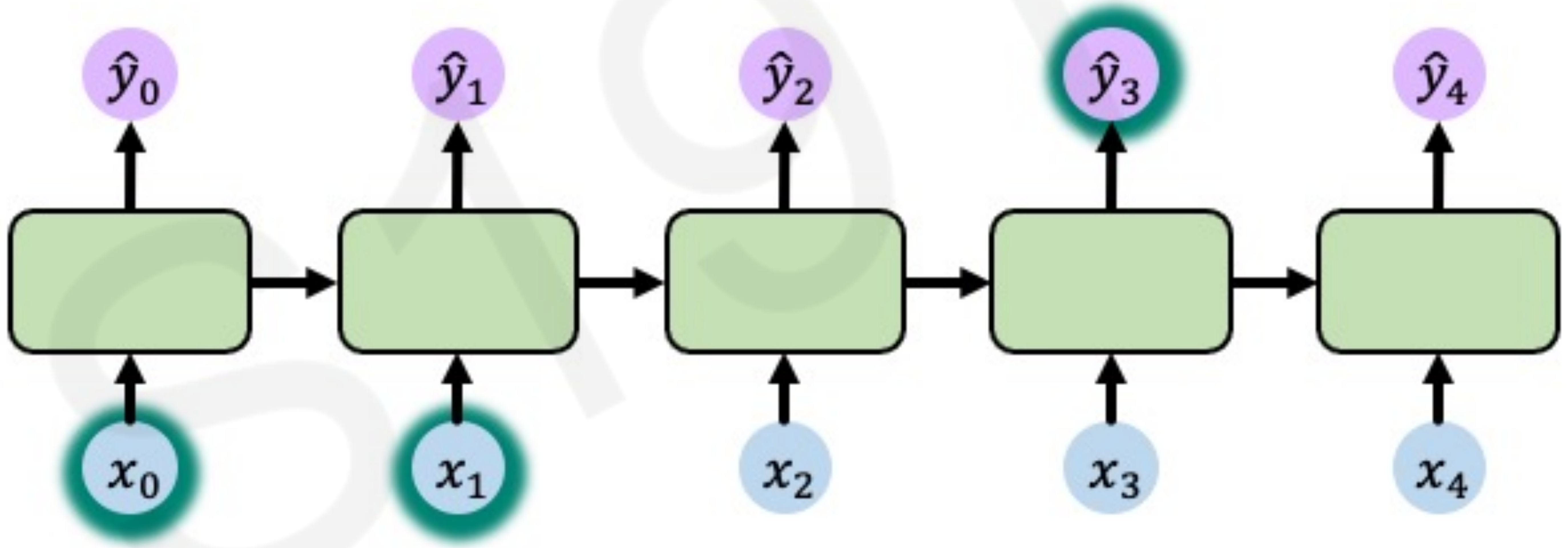

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Bias parameters to capture short-term dependencies

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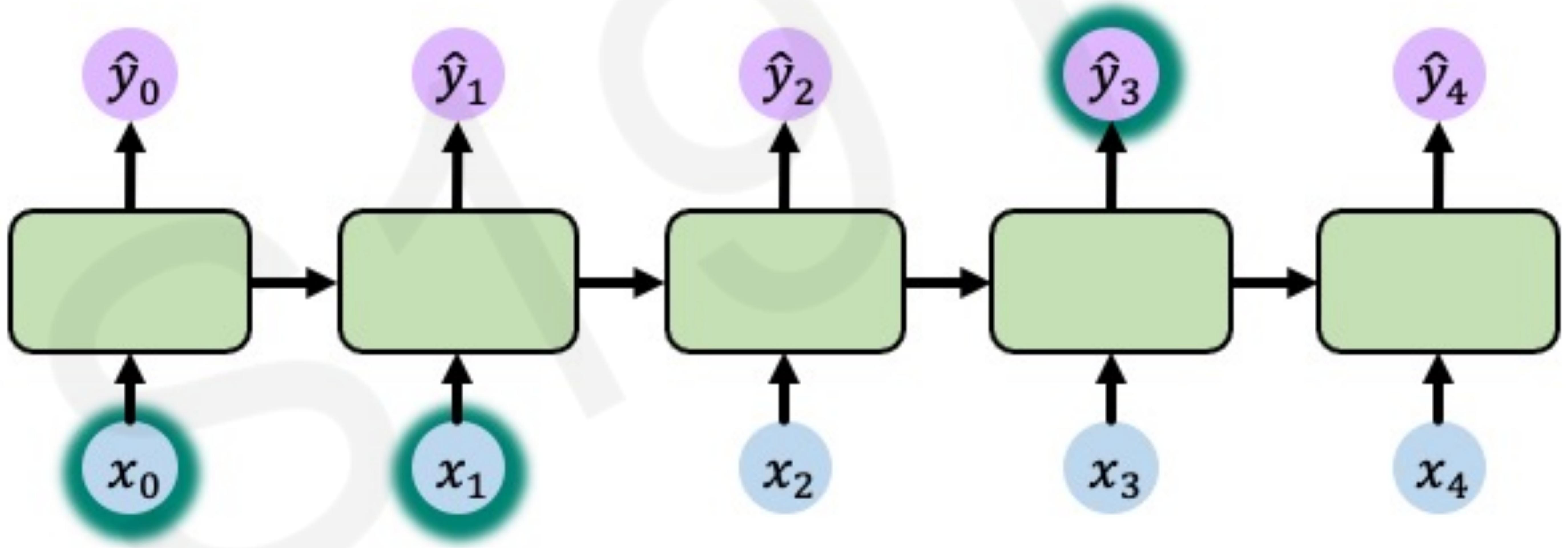

"I grew up in France, … and I speak fluent___ "

The Problem of Long-Term Dependencies

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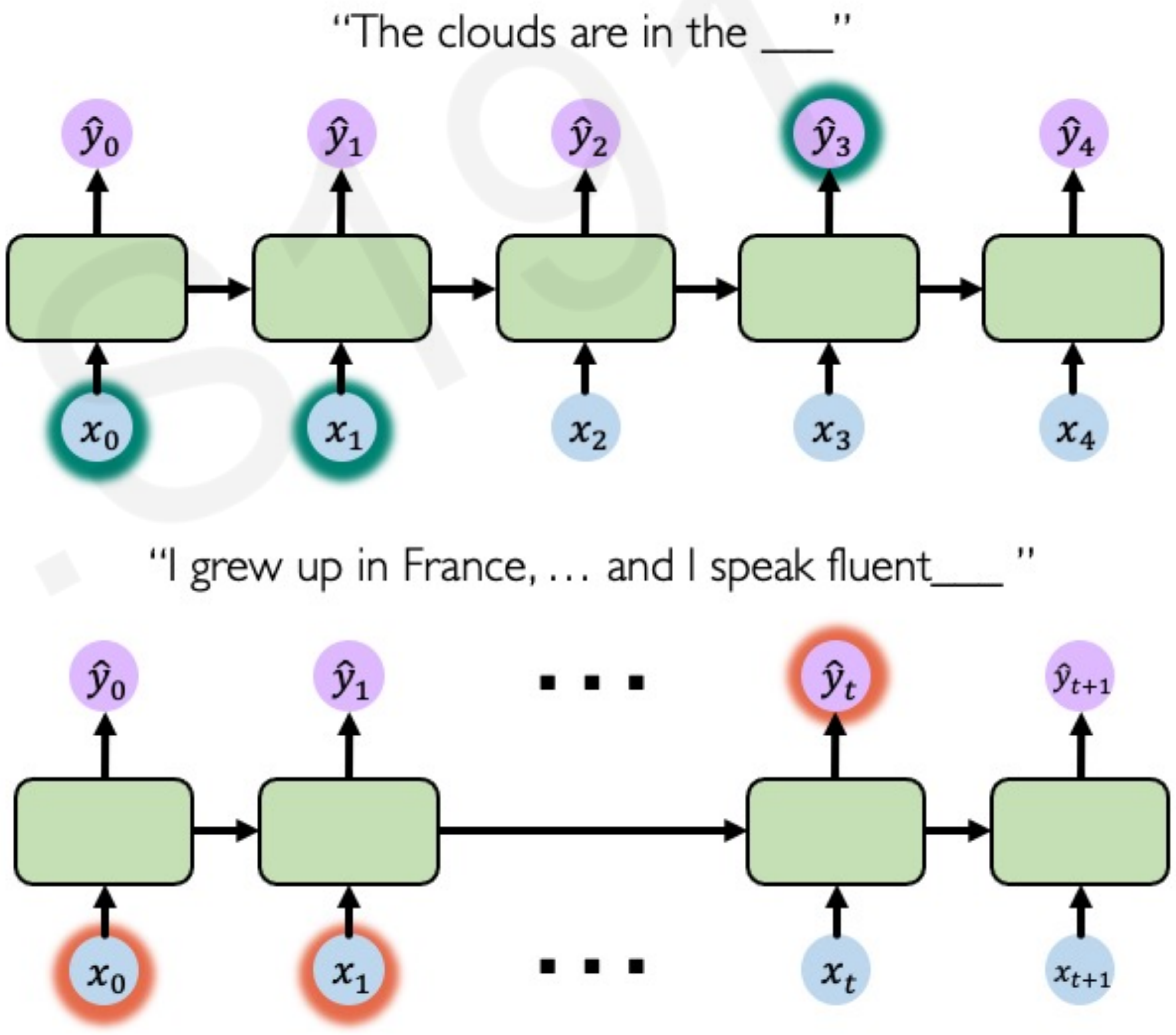
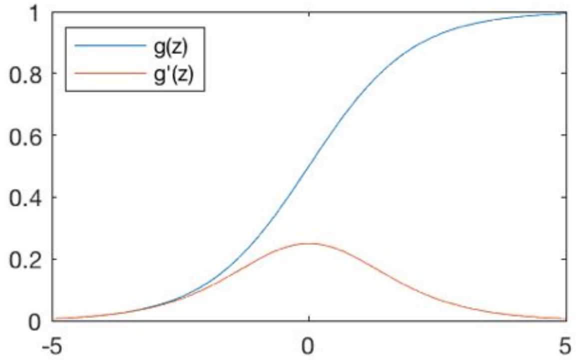
Bias parameters to capture short-term dependencies



Common Activation Functions

Sigmoid Function

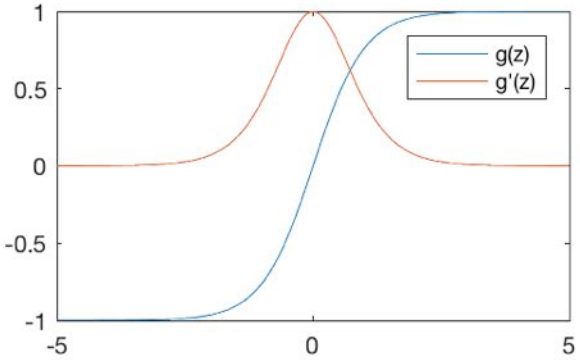


$$g(z) = \frac{1}{1 + e^{-z}}$$

$$g'(z) = g(z)(1 - g(z))$$

`tf.nn.sigmoid(z)`

Hyperbolic Tangent

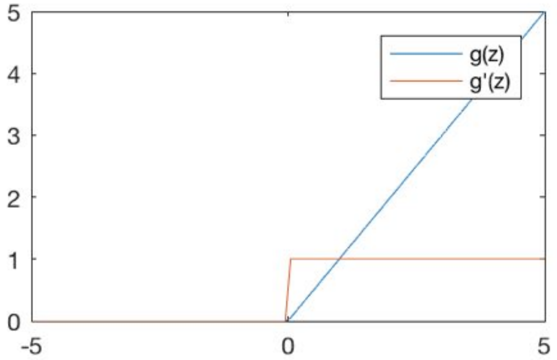


$$g(z) = \frac{e^{z} - e^{-z}}{e^{z} + e^{-z}}$$

$$g'(z) = 1 - g(z)^2$$

`tf.nn.tanh(z)`

Rectified Linear Unit (ReLU)



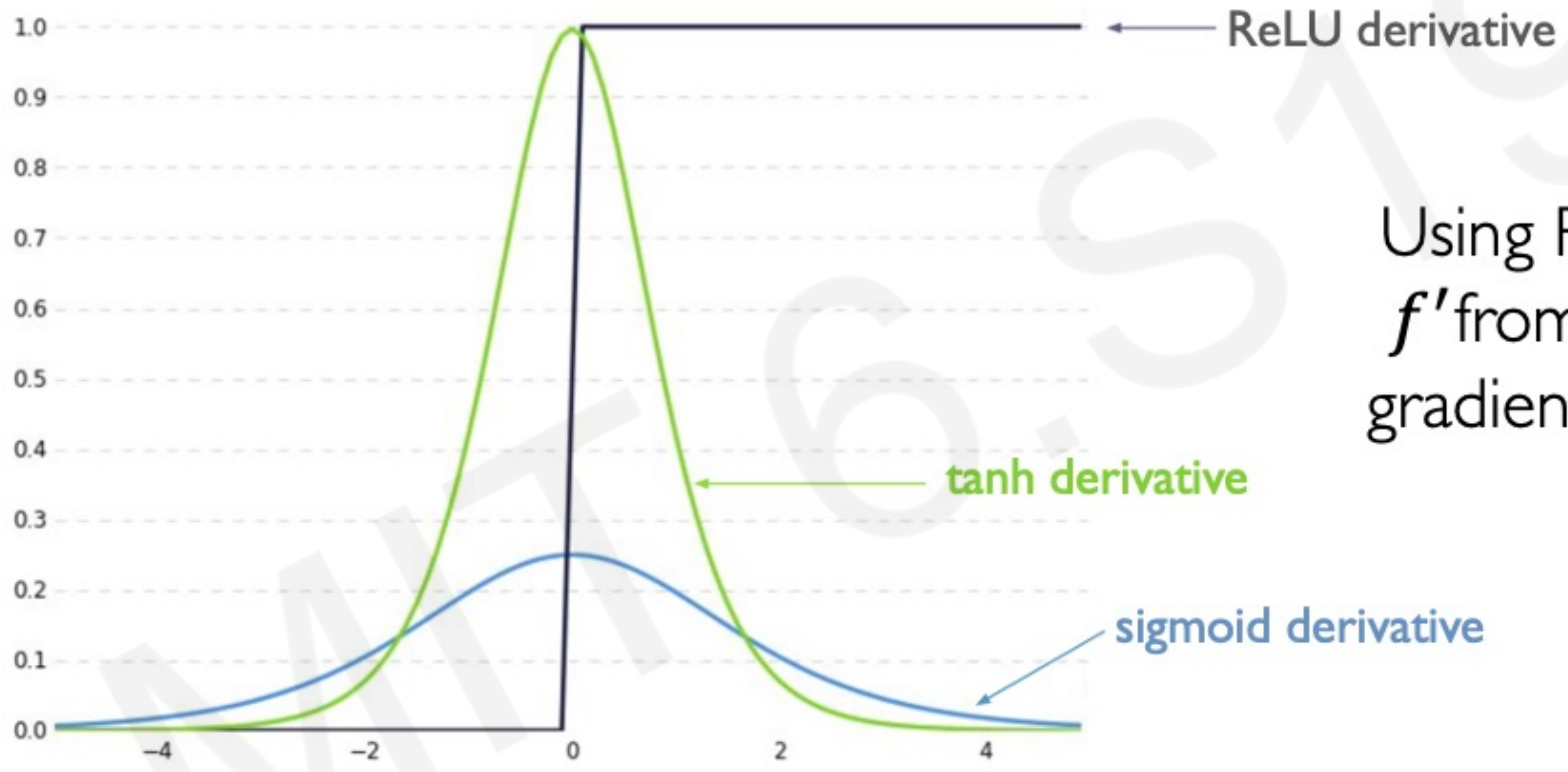
$$g(z) = \max(0, z)$$

$$g'(z) = \begin{cases} 1, & z > 0 \\ 0, & \text{otherwise} \end{cases}$$

`tf.nn.relu(z)`

NOTE: All activation functions are **non-linear**

Trick #1: Activation Functions



Using ReLU prevents f' from shrinking the gradients when $x > 0$

Trick #2: Parameter Initialization

Initialize **weights** to identity matrix

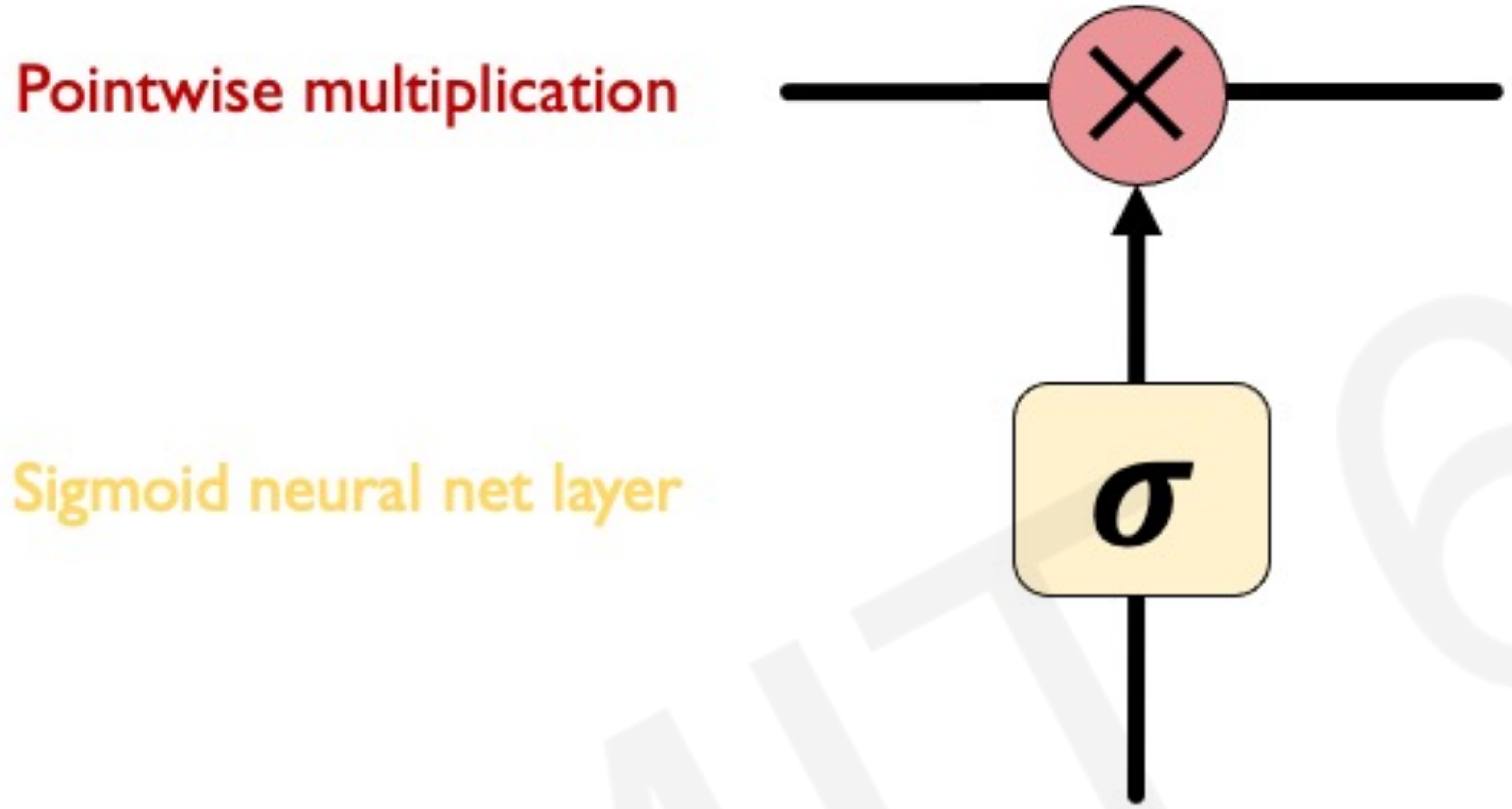
Initialize **biases** to zero

$$I_n = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{pmatrix}$$

This helps prevent the weights from shrinking to zero.

Trick #3: Gated Cells

Idea: use **gates** to selectively **add** or **remove** information within **each recurrent unit with**



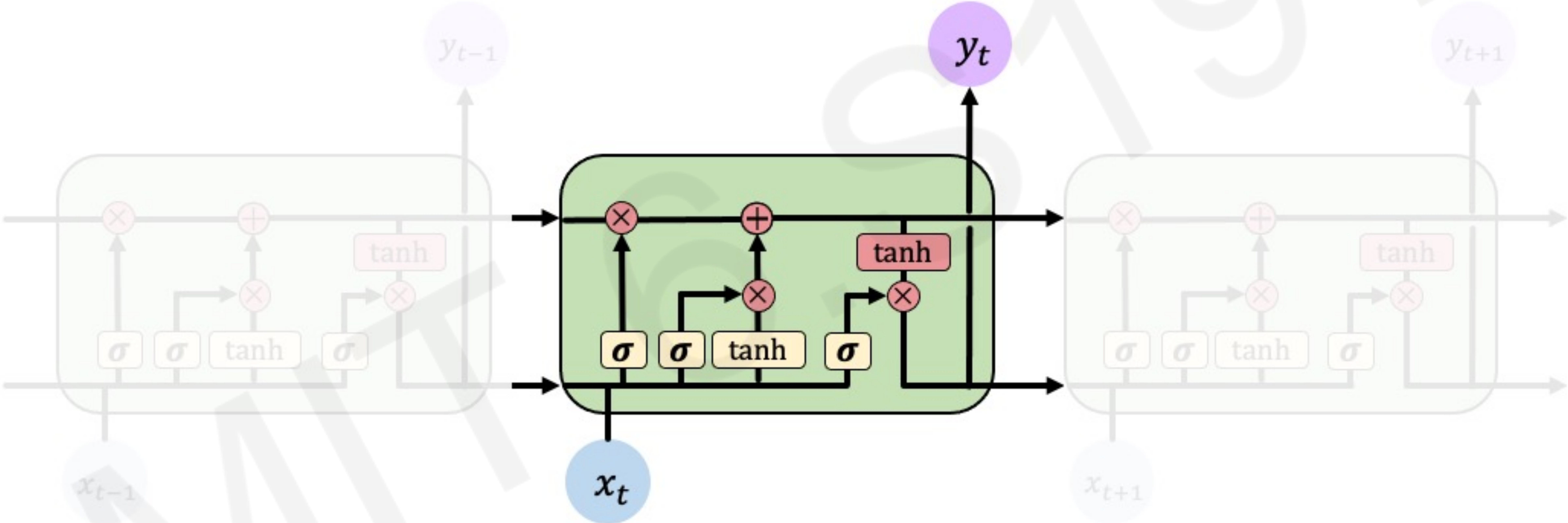
Gates optionally let information through the cell

Long Short Term Memory (LSTMs) networks rely on a gated cell to track information throughout many time steps.

Long Short Term Memory (LSTMs)

Gated LSTM cells **control information flow:**

1) Forget 2) Store 3) Update 4) Output

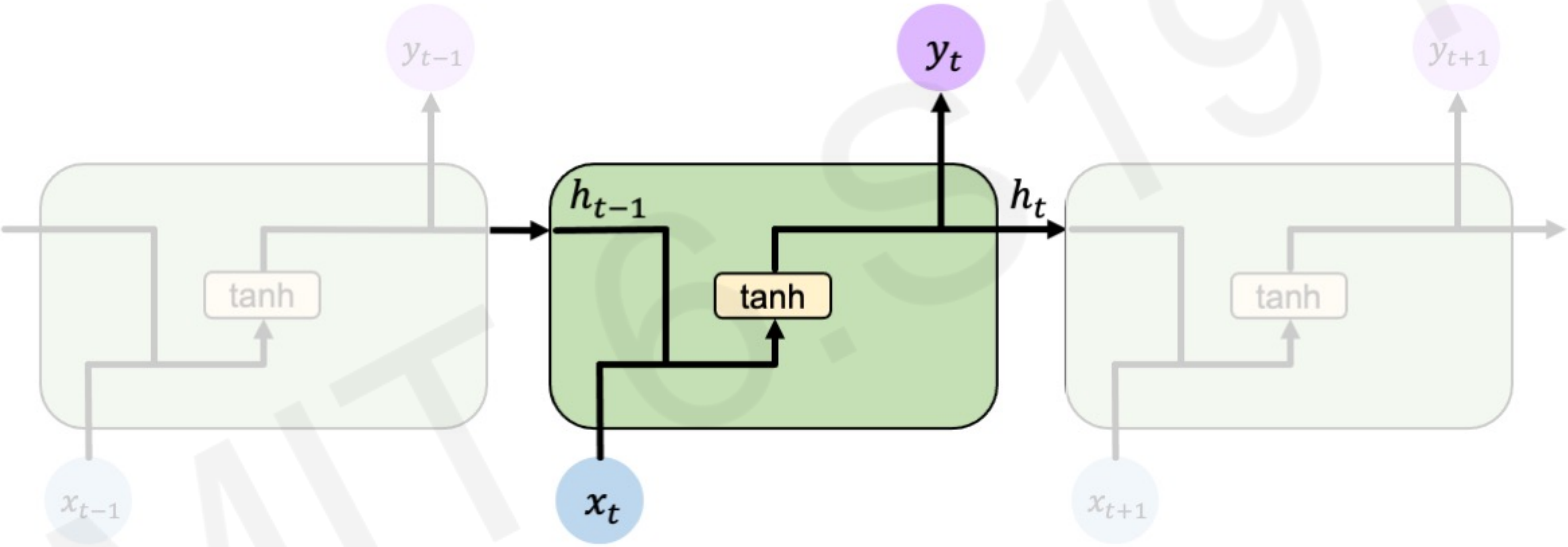


LSTM cells are able to track information throughout many timesteps

```
tf.keras.layers.LSTM(num_units)
```

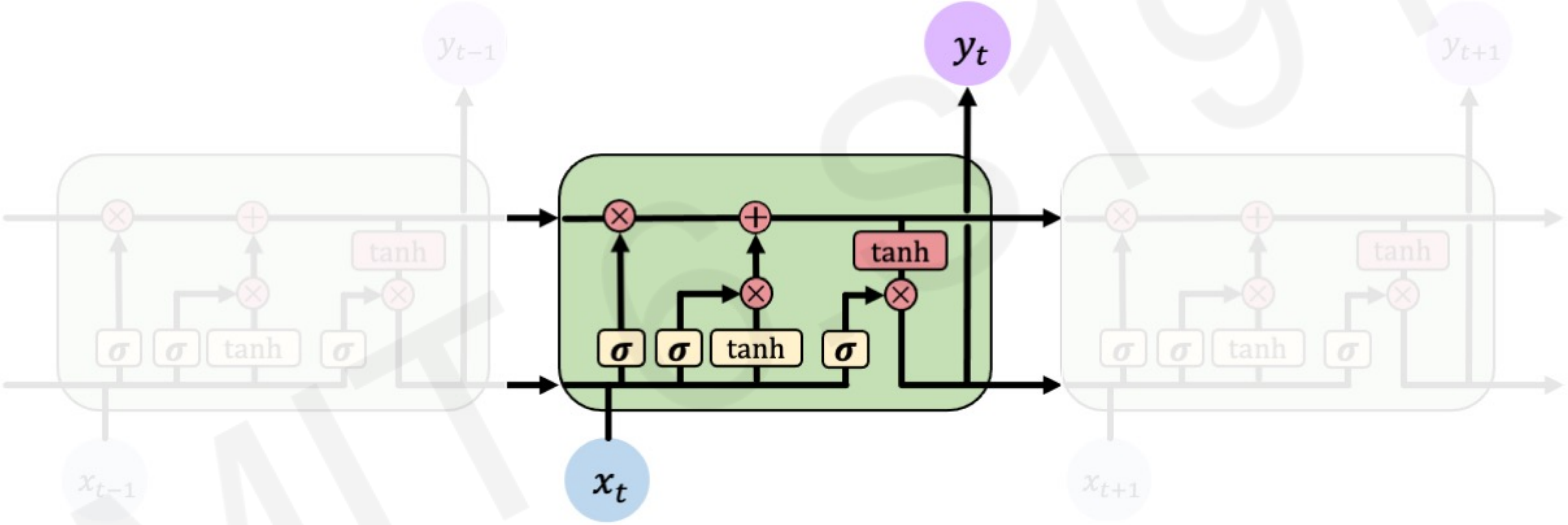
Standard RNN

In a standard RNN, repeating modules contain a **simple computation node**



Long Short Term Memory (LSTMs)

LSTM modules contain **computational blocks** that **control information flow**

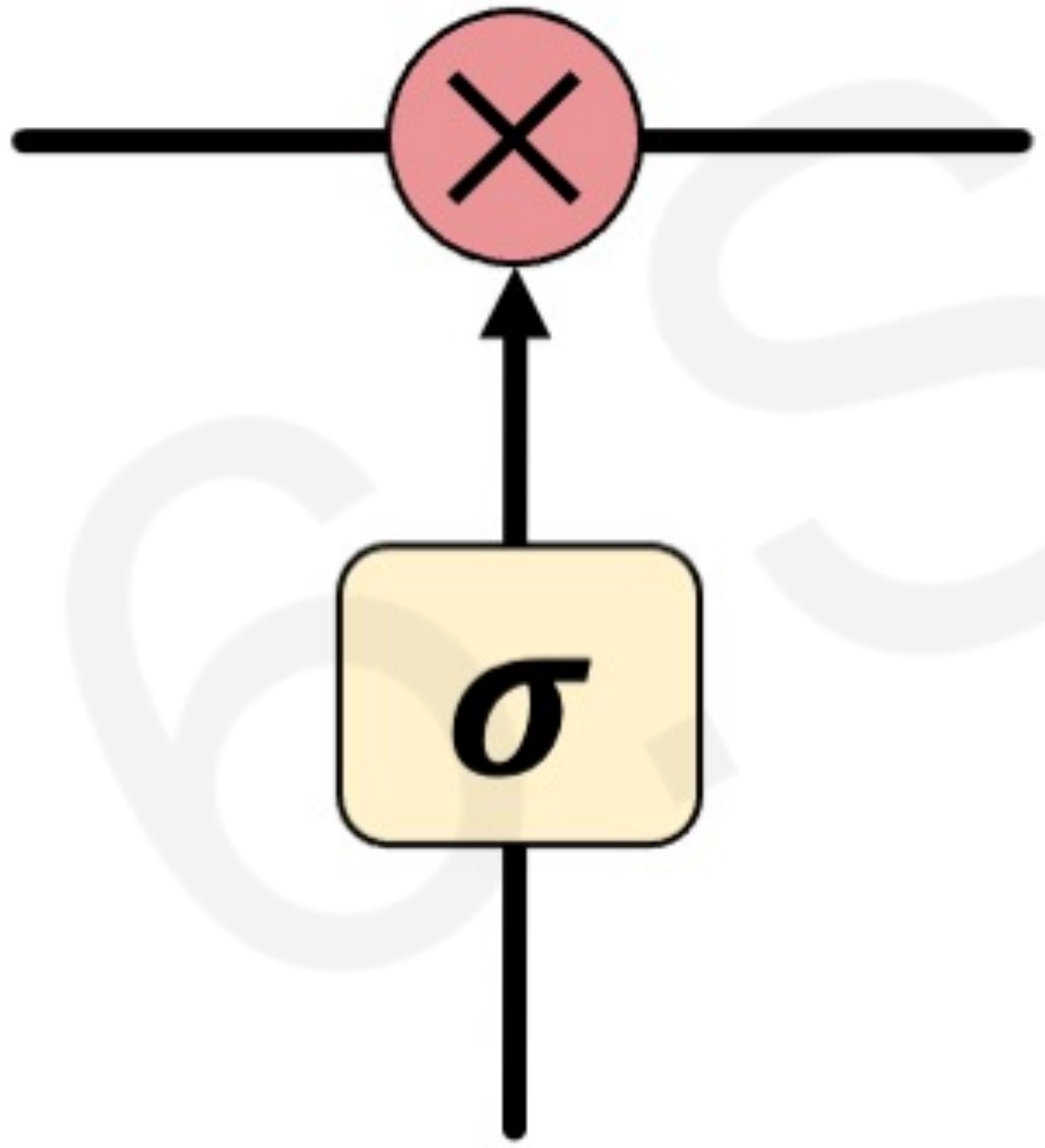


LSTM cells are able to track information throughout many timesteps

```
tf.keras.layers.LSTM(num_units)
```

Long Short Term Memory (LSTMs)

Information is **added** or **removed** through structures called **gates**

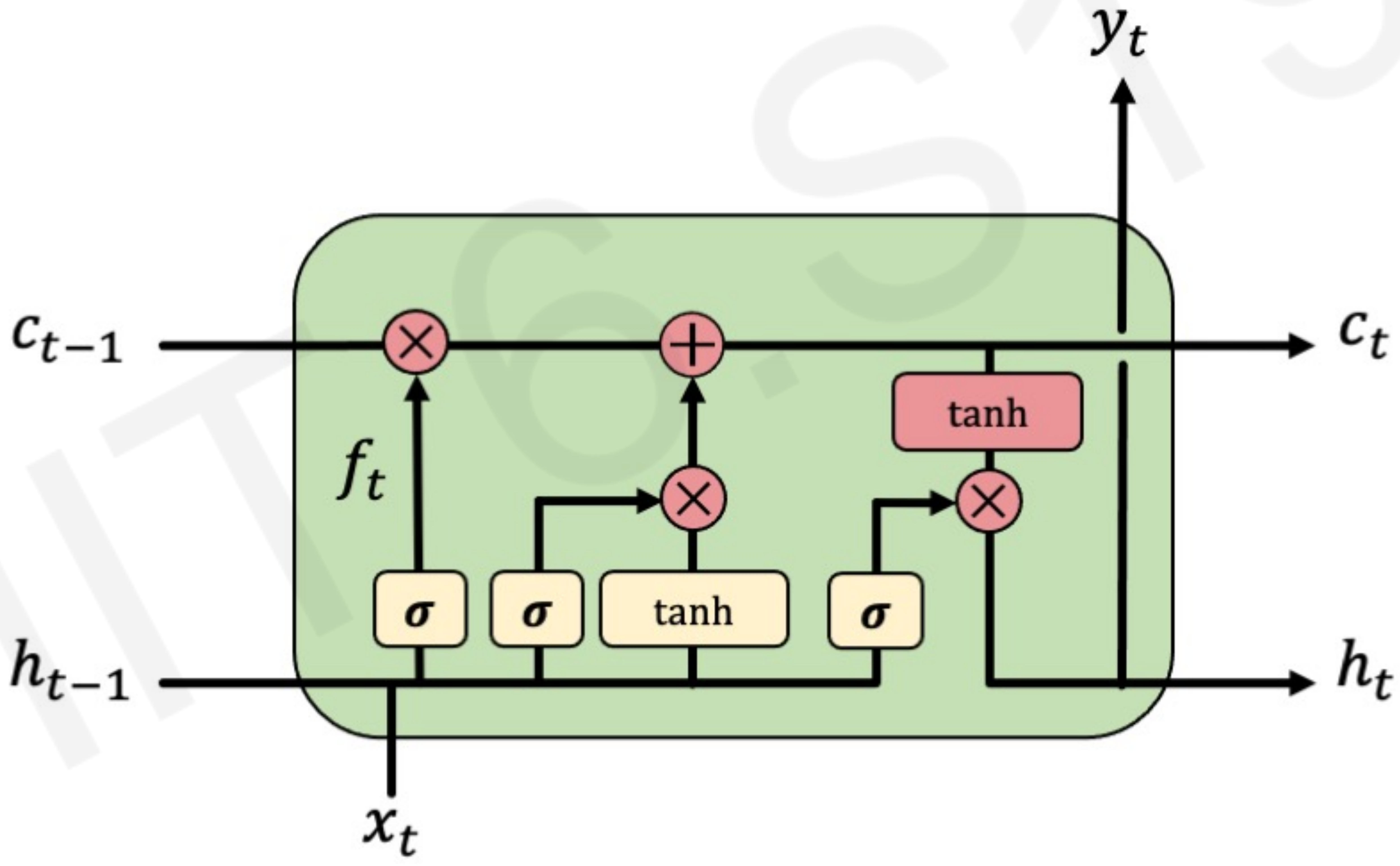


Gates optionally let information through, for example via a sigmoid neural net layer and pointwise multiplication

Long Short Term Memory (LSTMs)

How do LSTMs work?

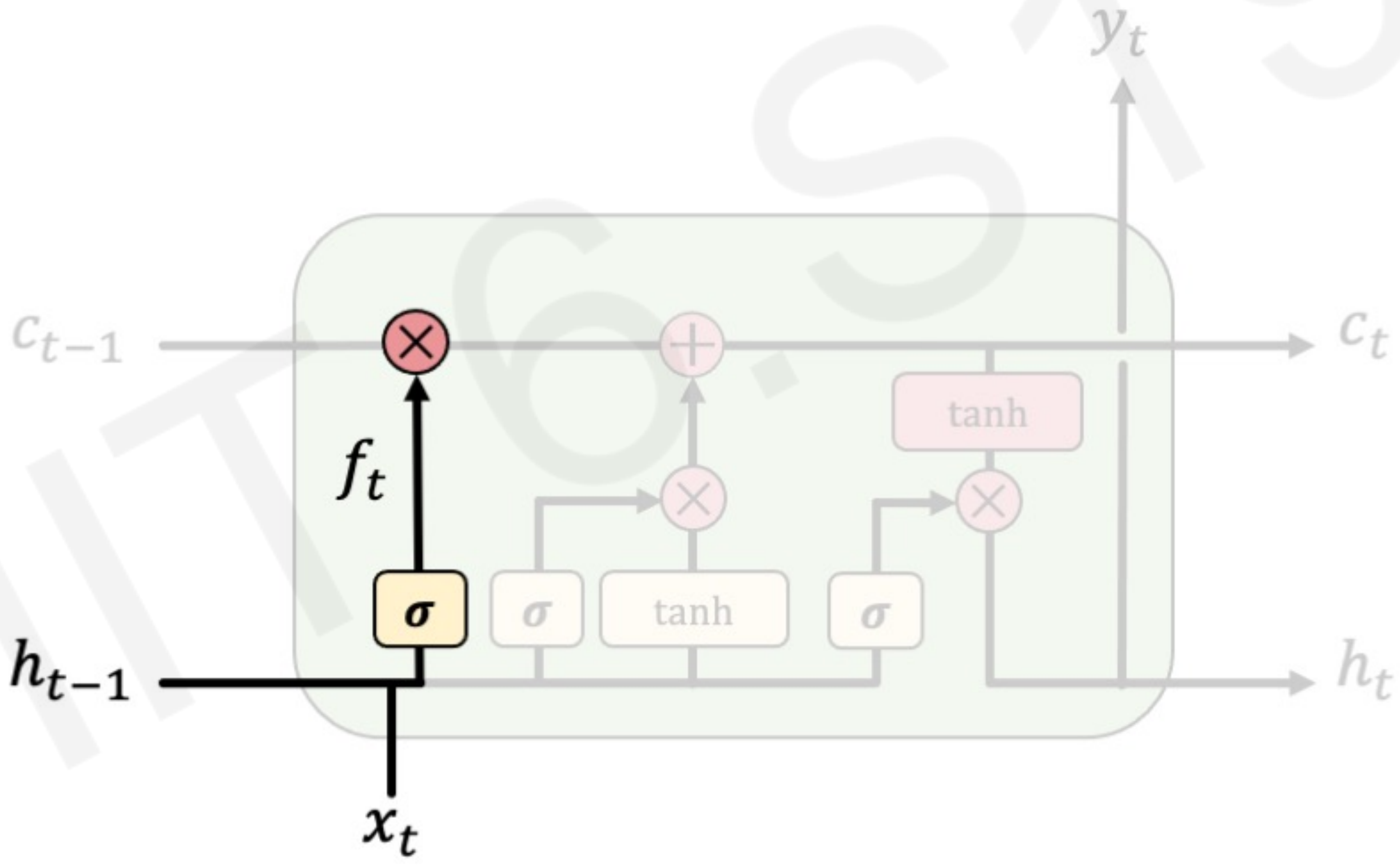
1) Forget   2) Store   3) Update   4) Output



Long Short Term Memory (LSTMs)

1) Forget 2) Store 3) Update 4) Output

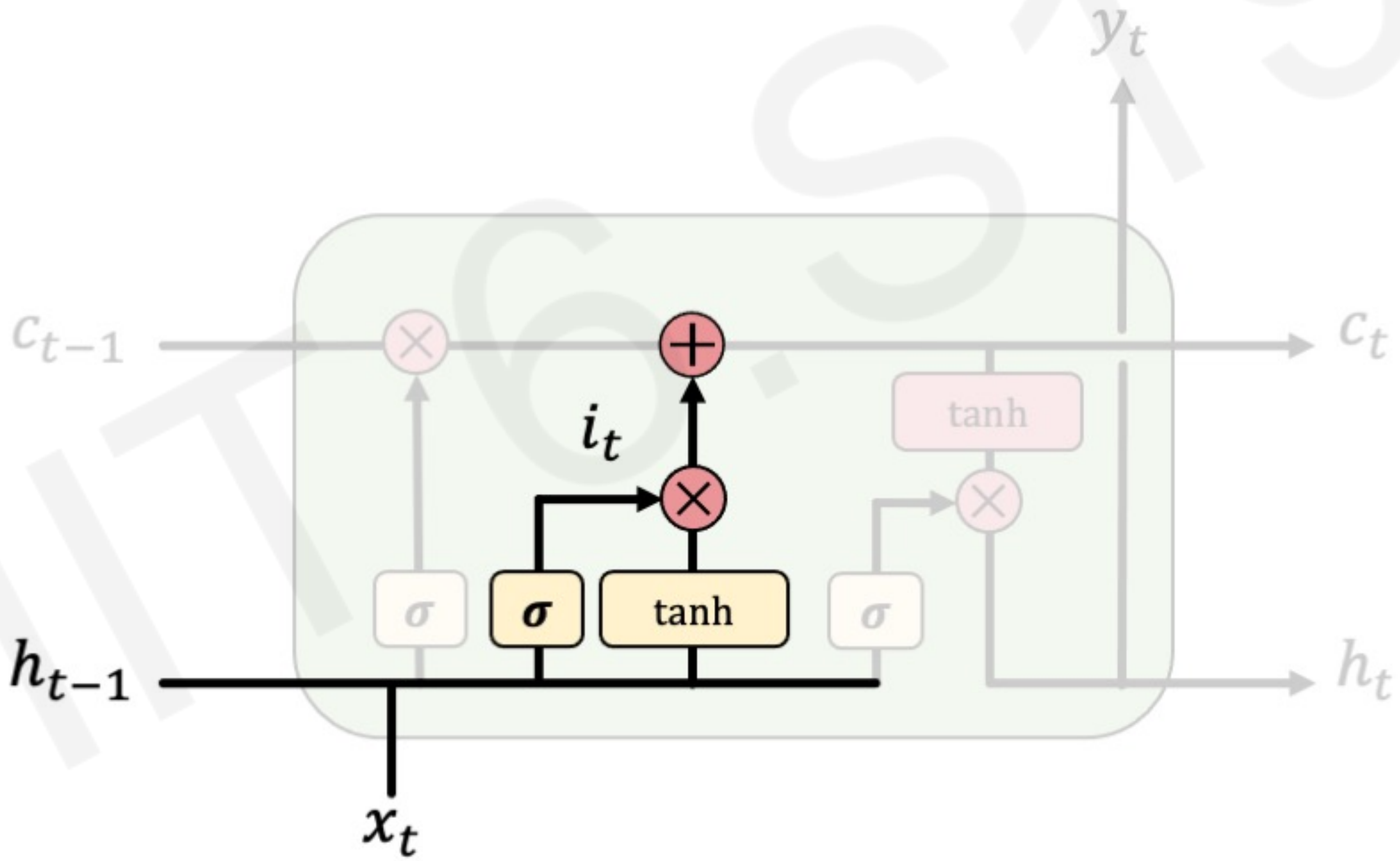
LSTMs **forget irrelevant** parts of the previous state



Long Short Term Memory (LSTMs)

1) Forget **2) Store** 3) Update 4) Output

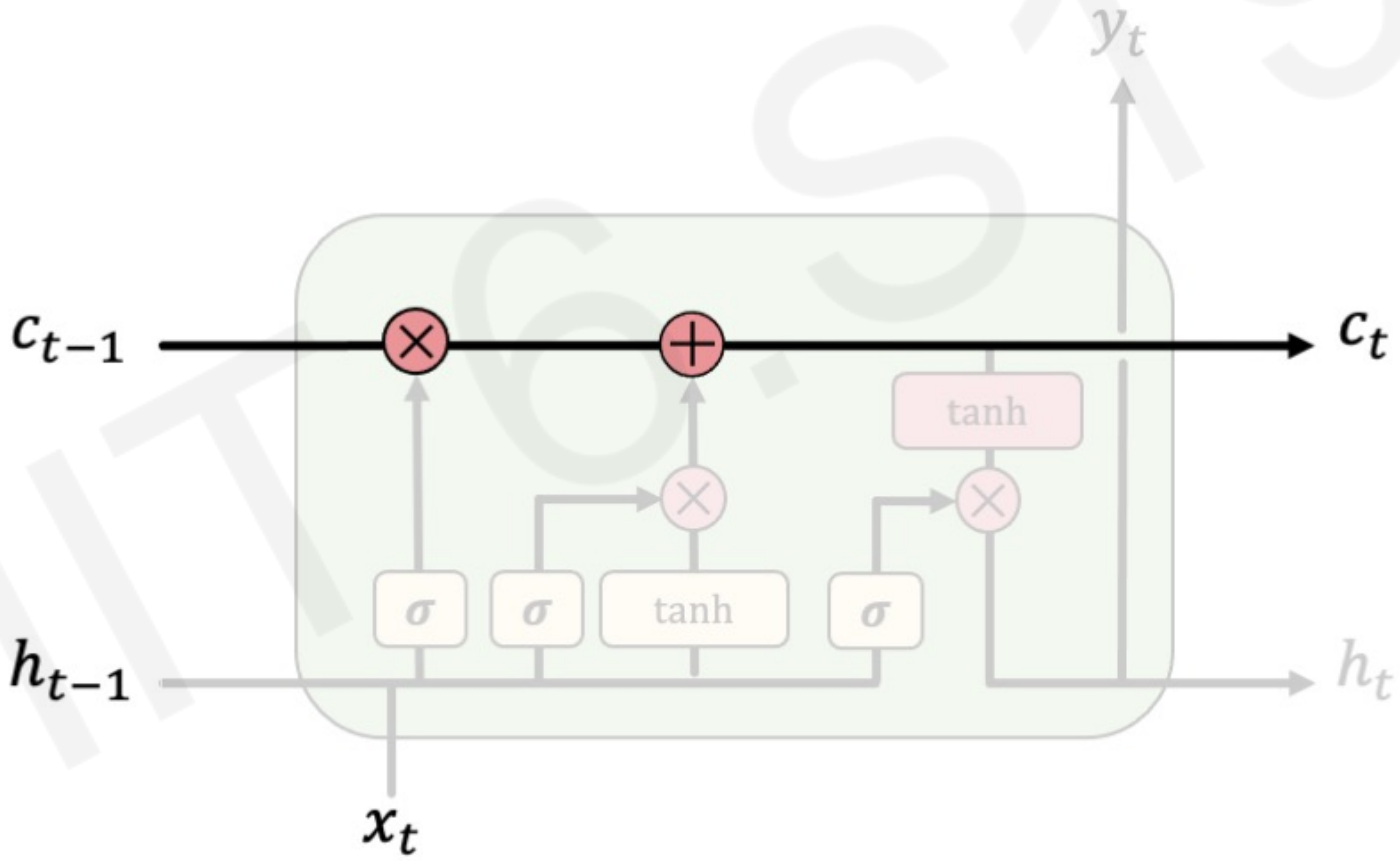
LSTMs **store relevant** new information into the cell state



Long Short Term Memory (LSTMs)

1) Forget 2) Store **3) Update** 4) Output

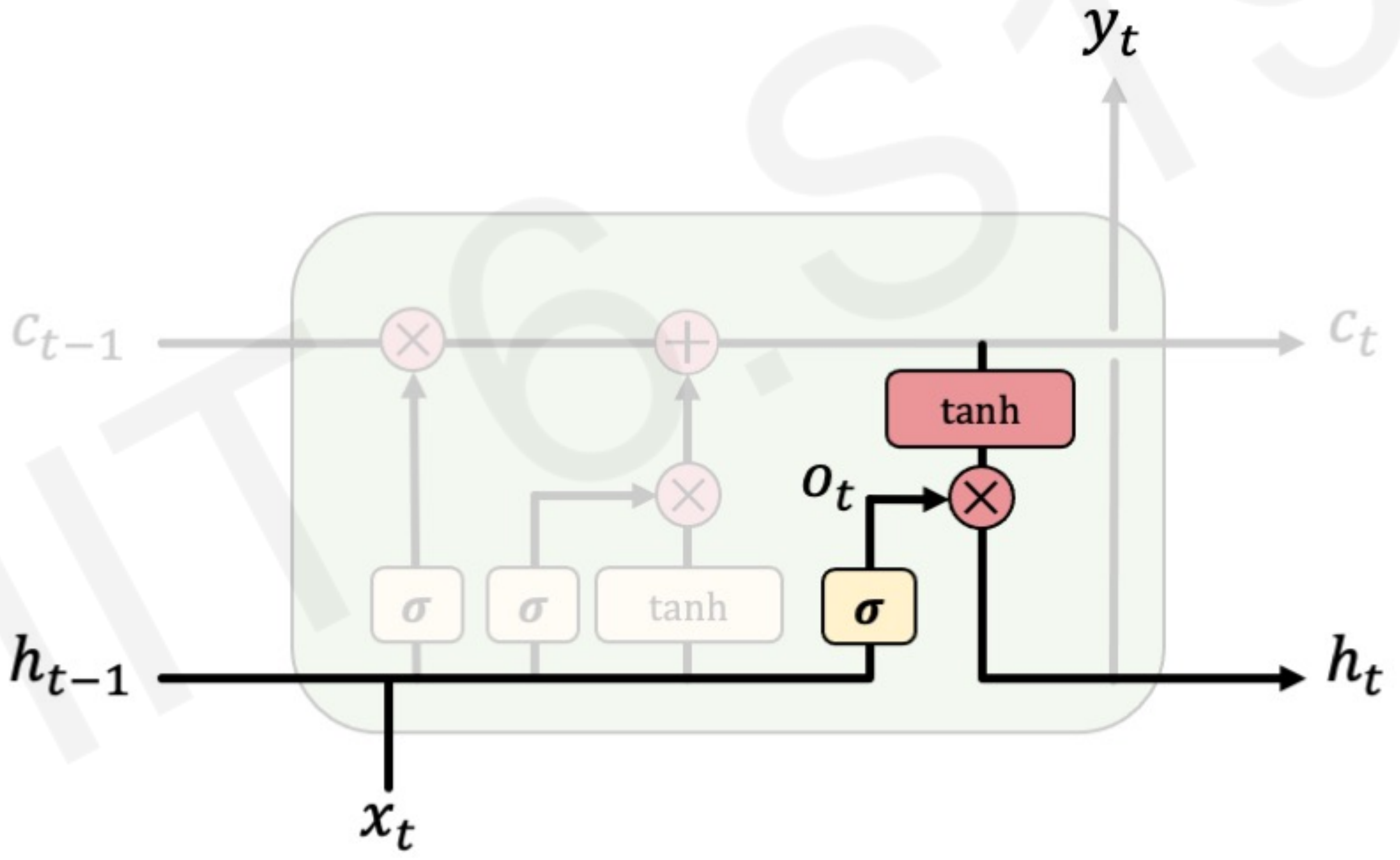
LSTMs **selectively update** cell state values



Long Short Term Memory (LSTMs)

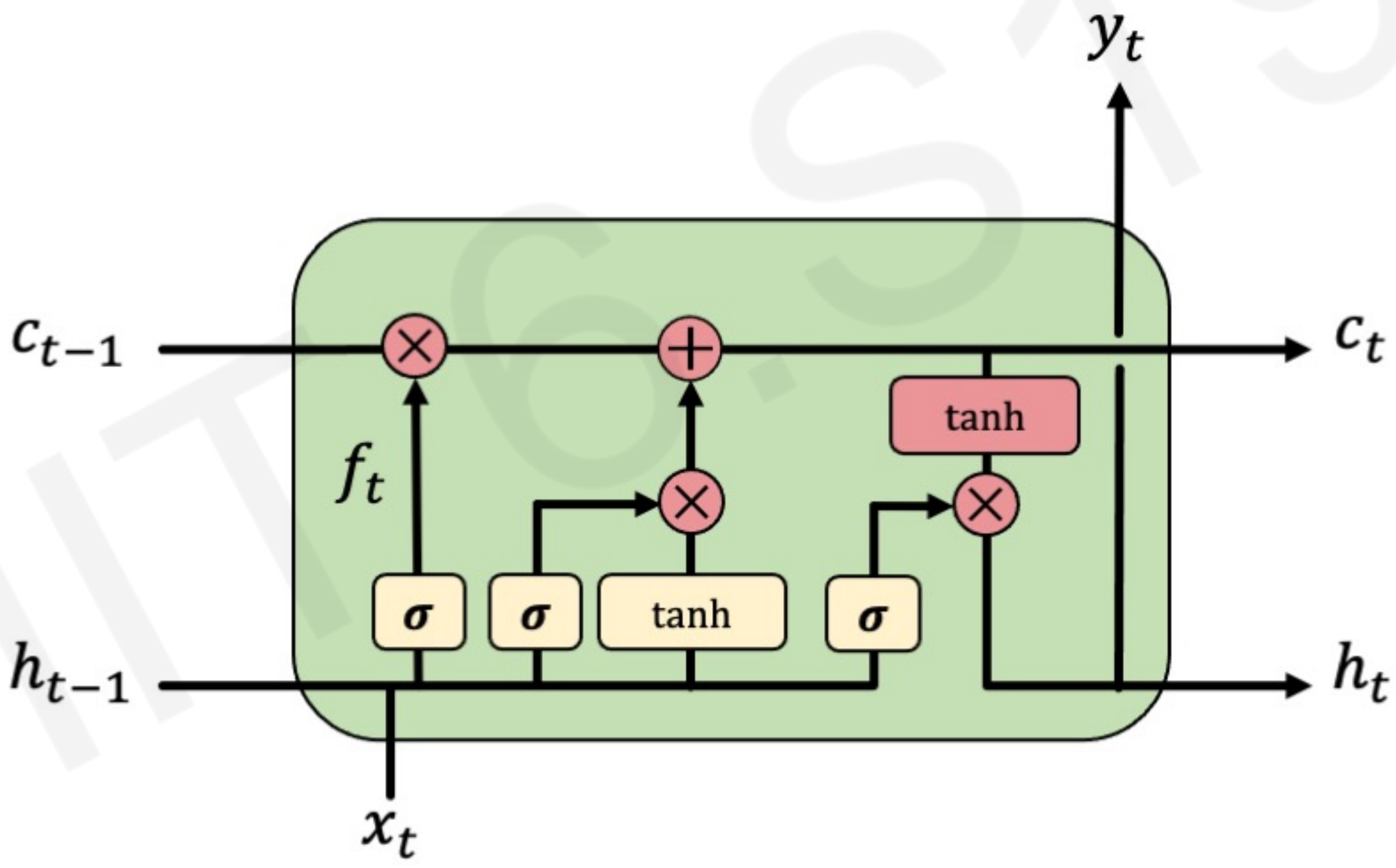
1) Forget 2) Store 3) Update **4) Output**

The **output gate** controls what information is sent to the next time step



Long Short Term Memory (LSTMs)

1) Forget 2) Store 3) Update 4) Output



LSTM Gradient Flow

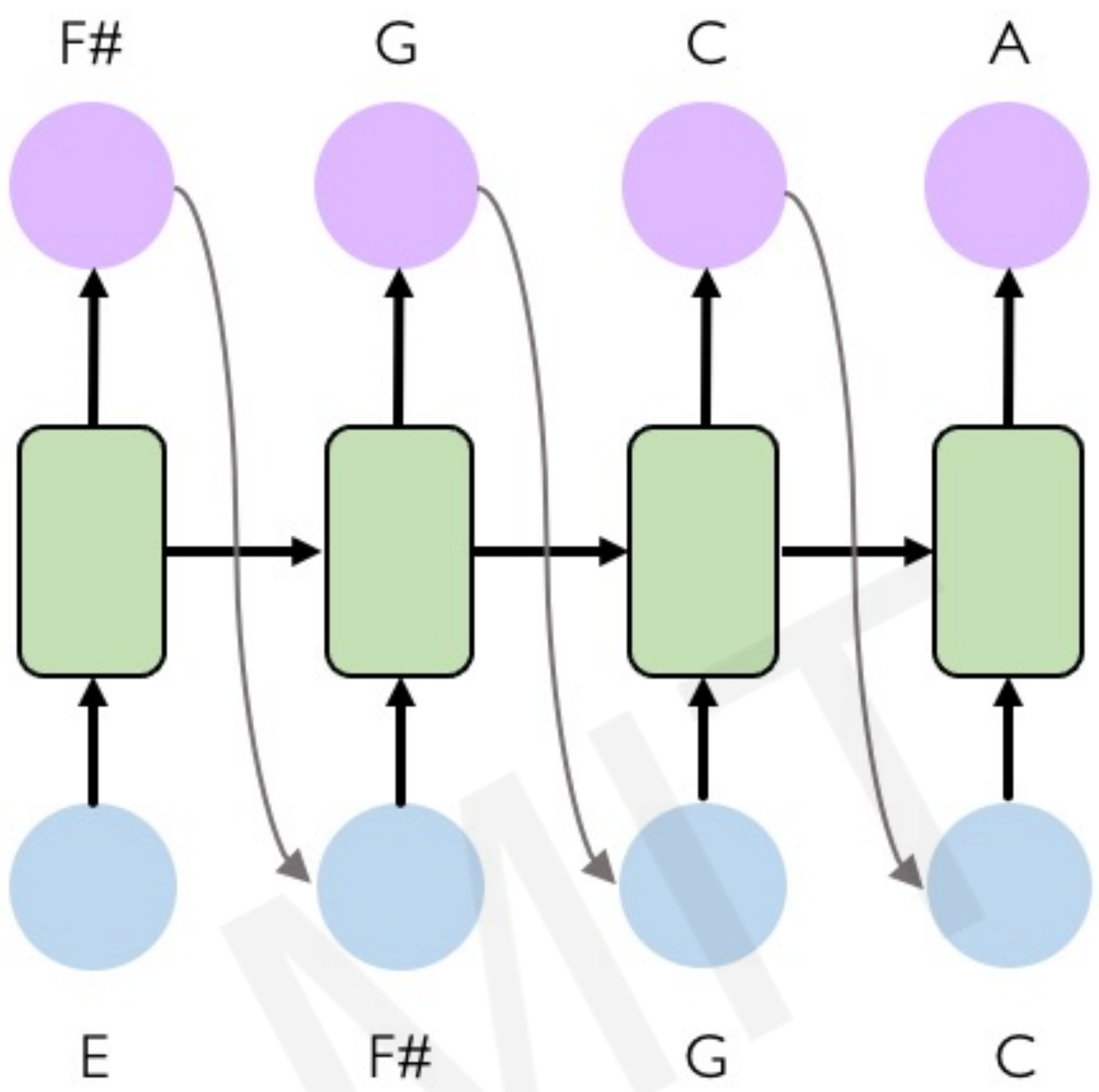
Uninterrupted gradient flow!

LSTMs: Key Concepts

1. Maintain a **cell state**
2. Use **gates** to control the **flow of information**
   - **Forget** gate gets rid of irrelevant information
   - **Store** relevant information from current input
   - Selectively **update** cell state
   - **Output** gate returns a filtered version of the cell state
3. Backpropagation through time with partially **uninterrupted gradient flow**

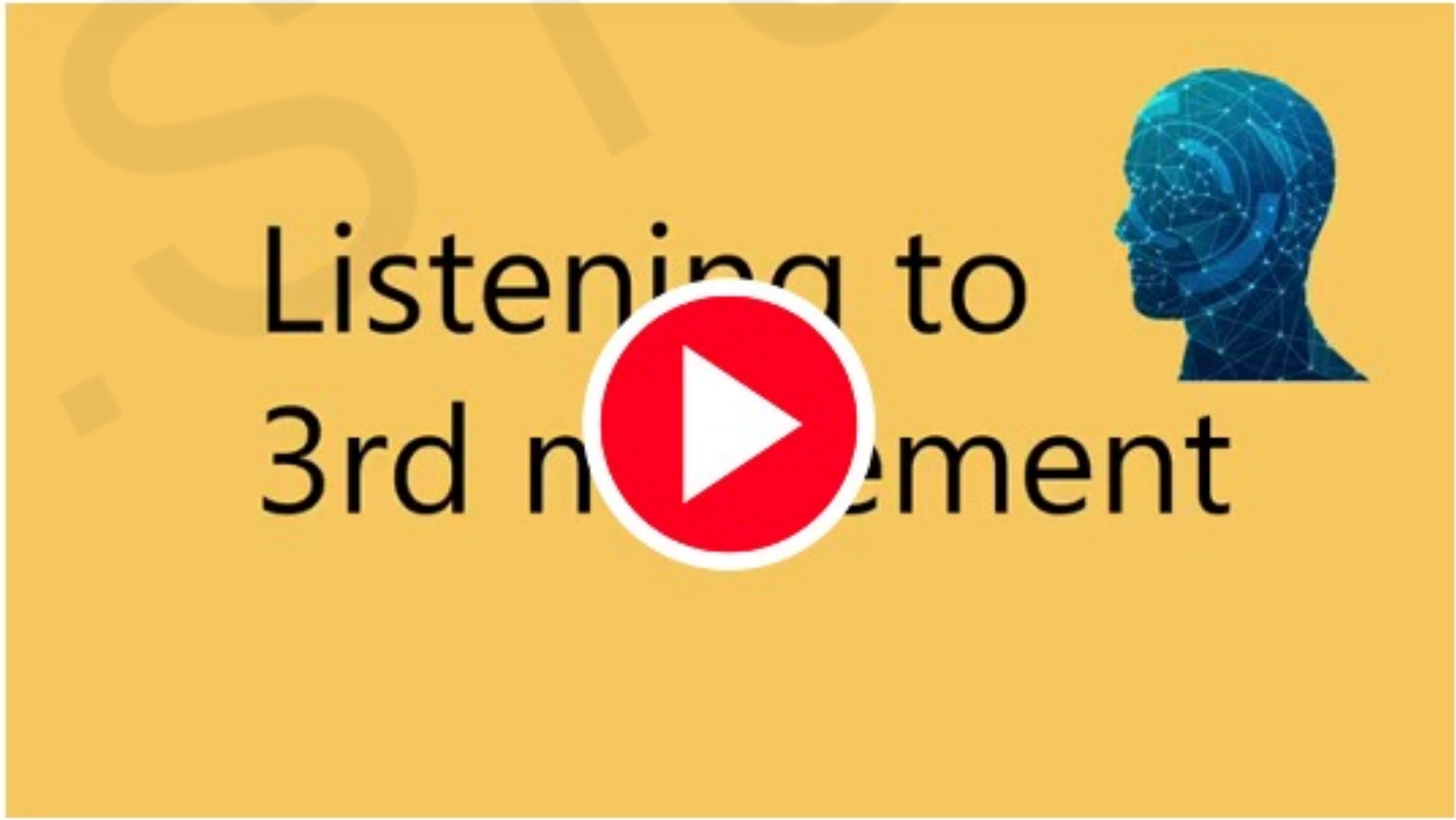
RNN Applications & Limitations

Example Task: Music Generation



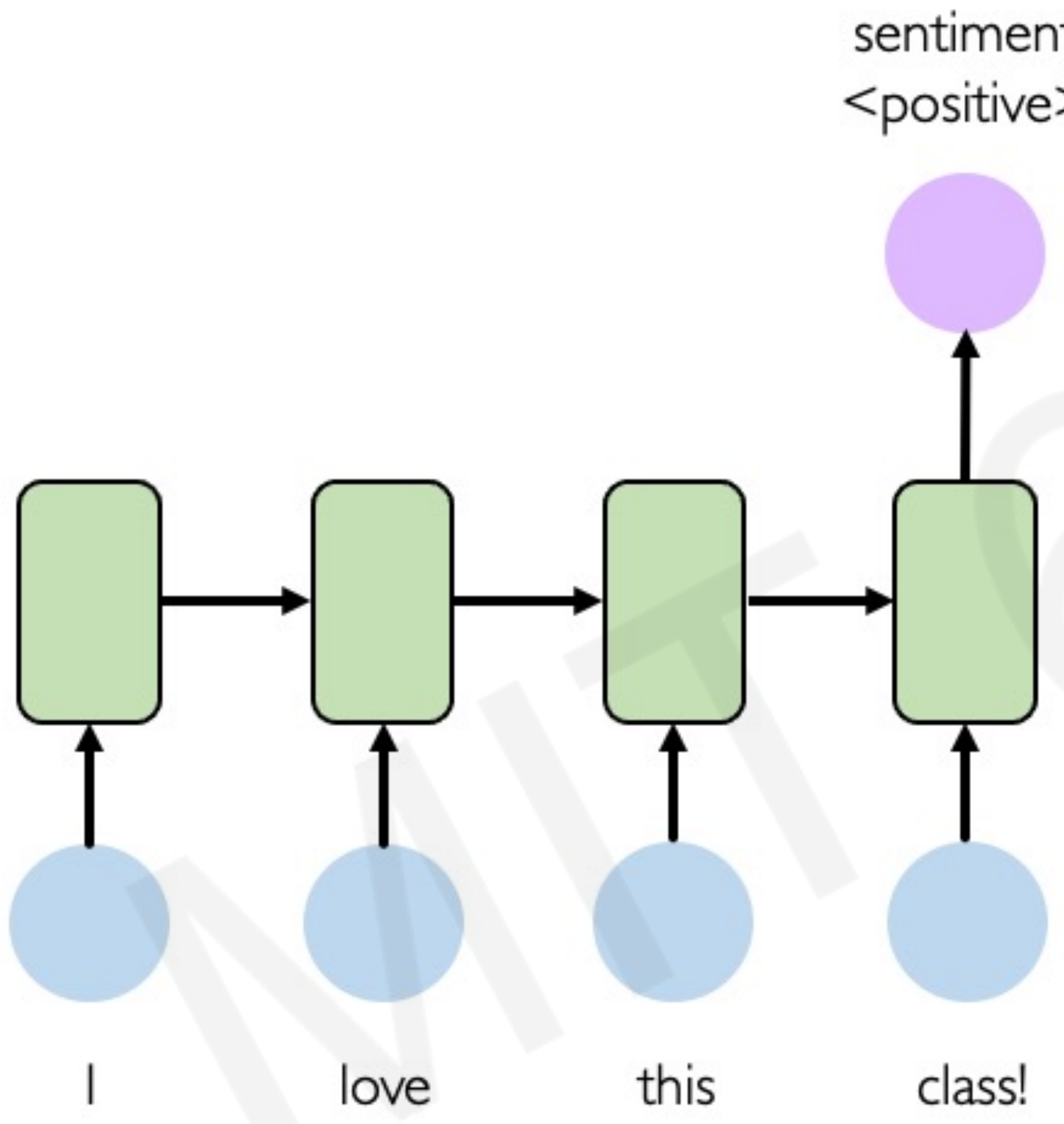
Input: sheet music

Output: next character in sheet music



Software Lab!

Example Task: Sentiment Classification

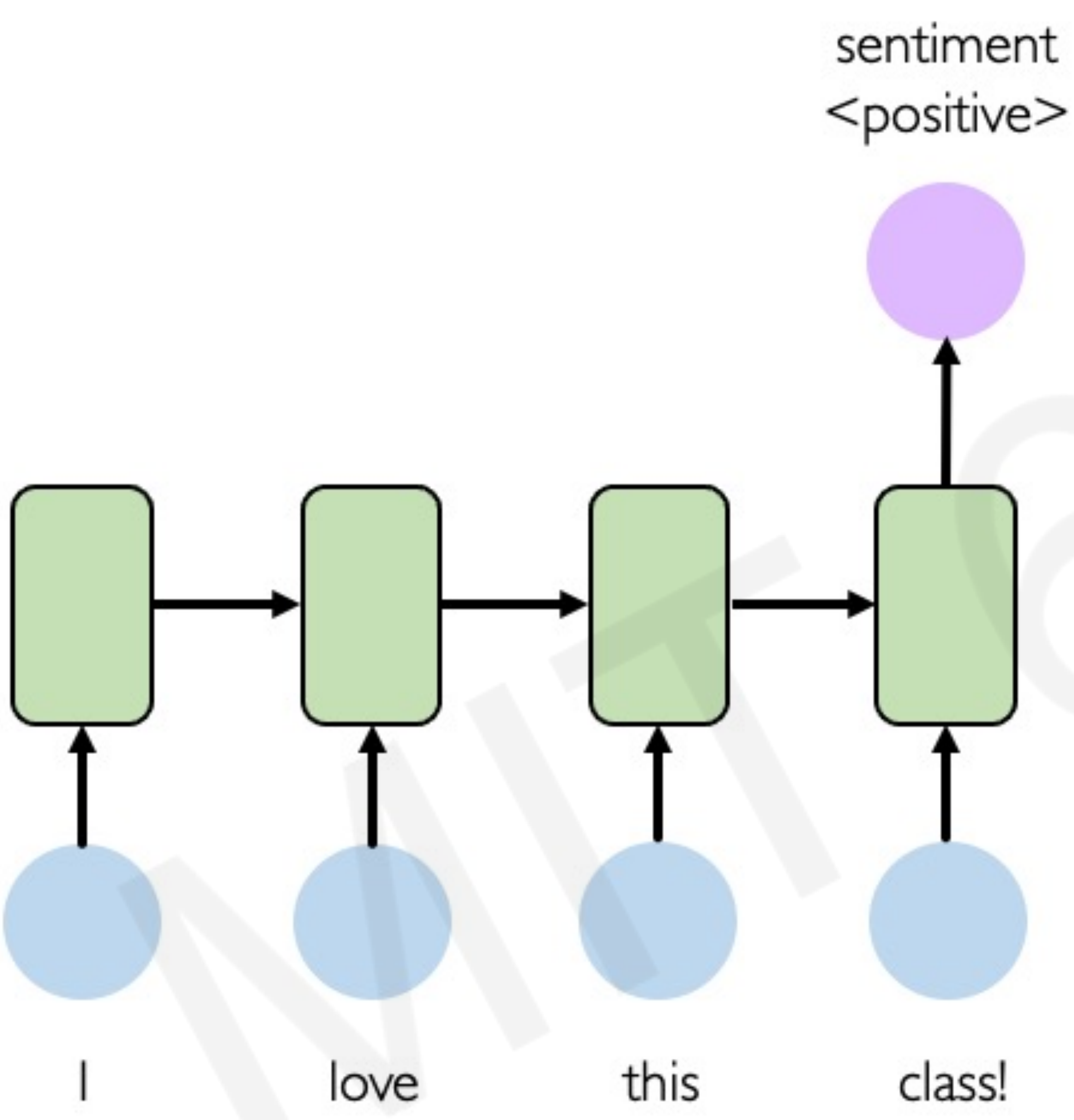


Input: sequence of words

Output: probability of having positive sentiment

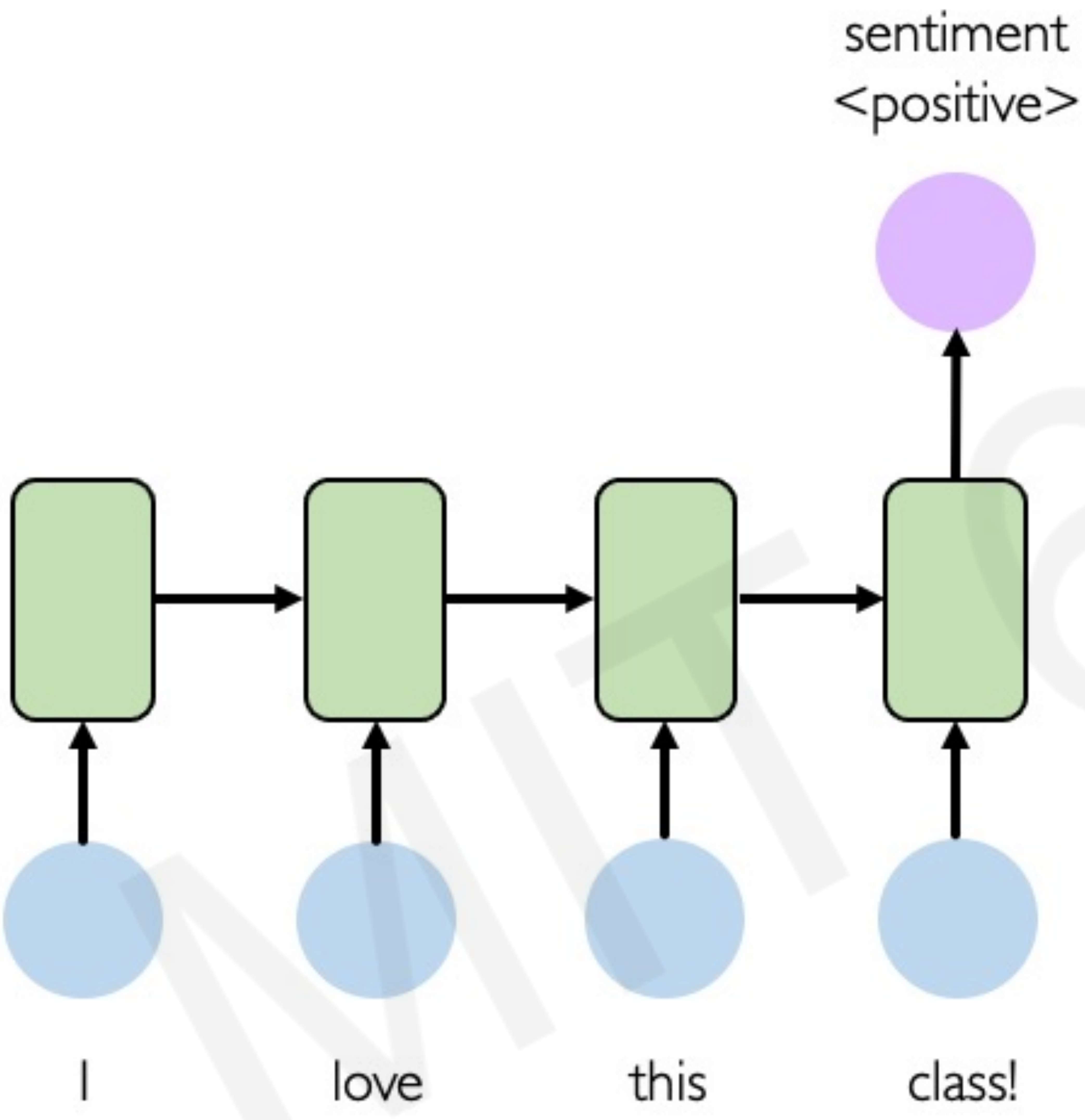
```
loss = tf.nn.softmax_cross_entropy_with_logits(y, predicted)
```

Example Task: Sentiment Classification



Tweet sentiment classification

Limitations of Recurrent Models



Limitations of RNNs

- Encoding bottleneck
- Slow, no parallelization
- Not long memory

Goal of Sequence Modeling

RNNs: recurrence to model sequence dependencies

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Limitations of RNNs

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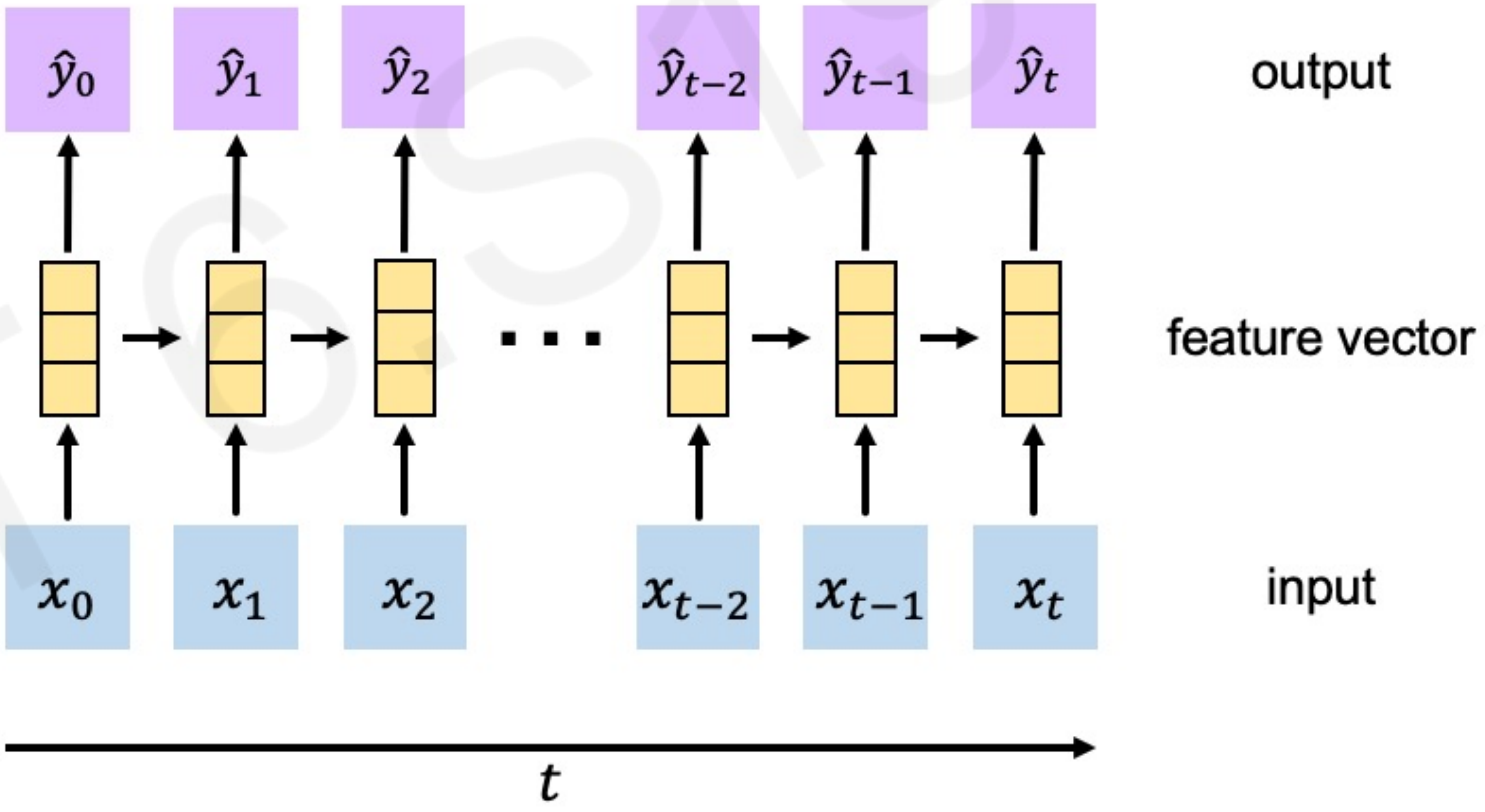
RNNs: recurrence to model sequence dependencies

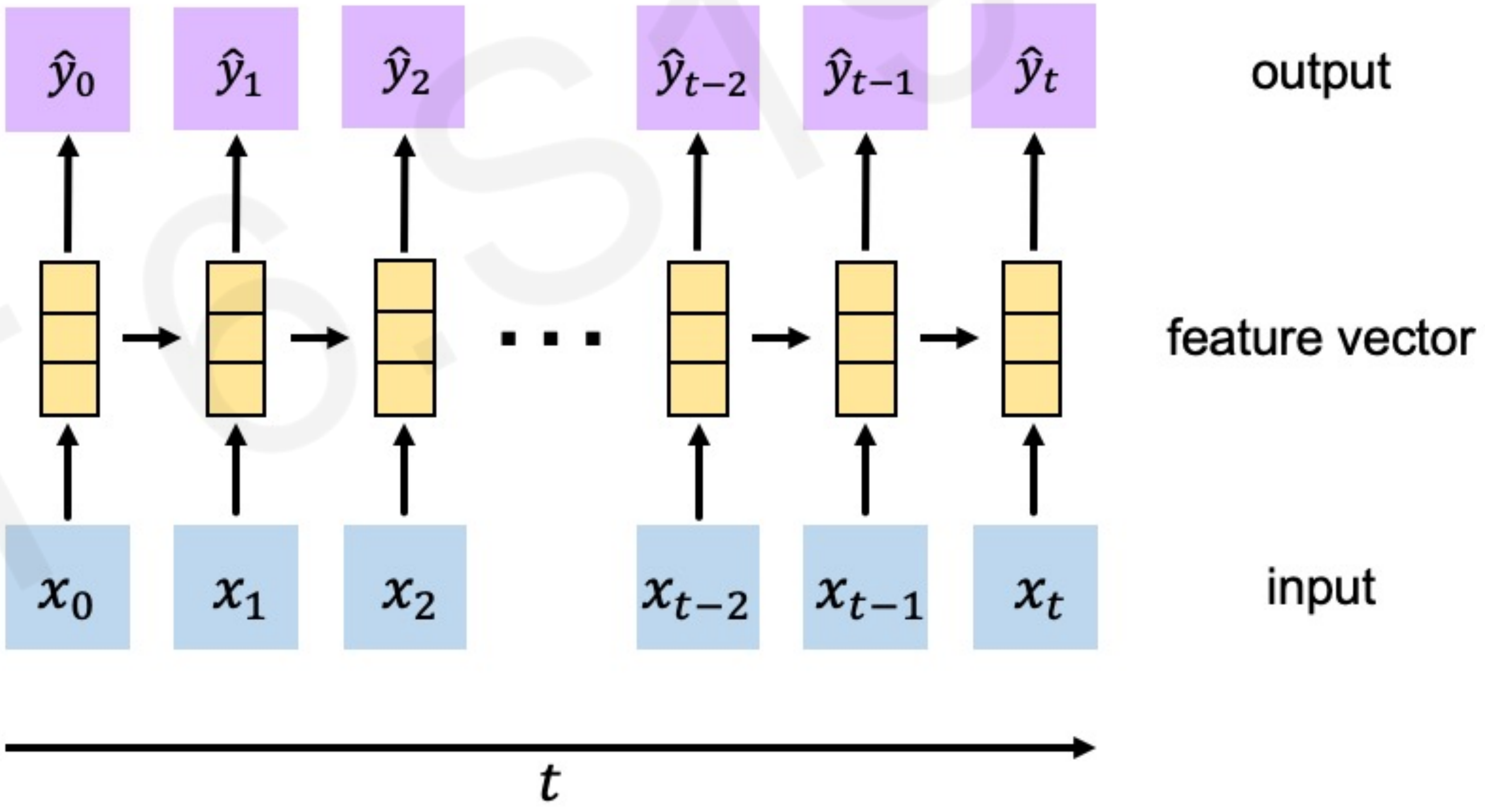


Goal of Sequence Modeling

Can we eliminate the need for recurrence entirely?

Desired Capabilities

- Continuous stream
- Parallelization
- Long memory



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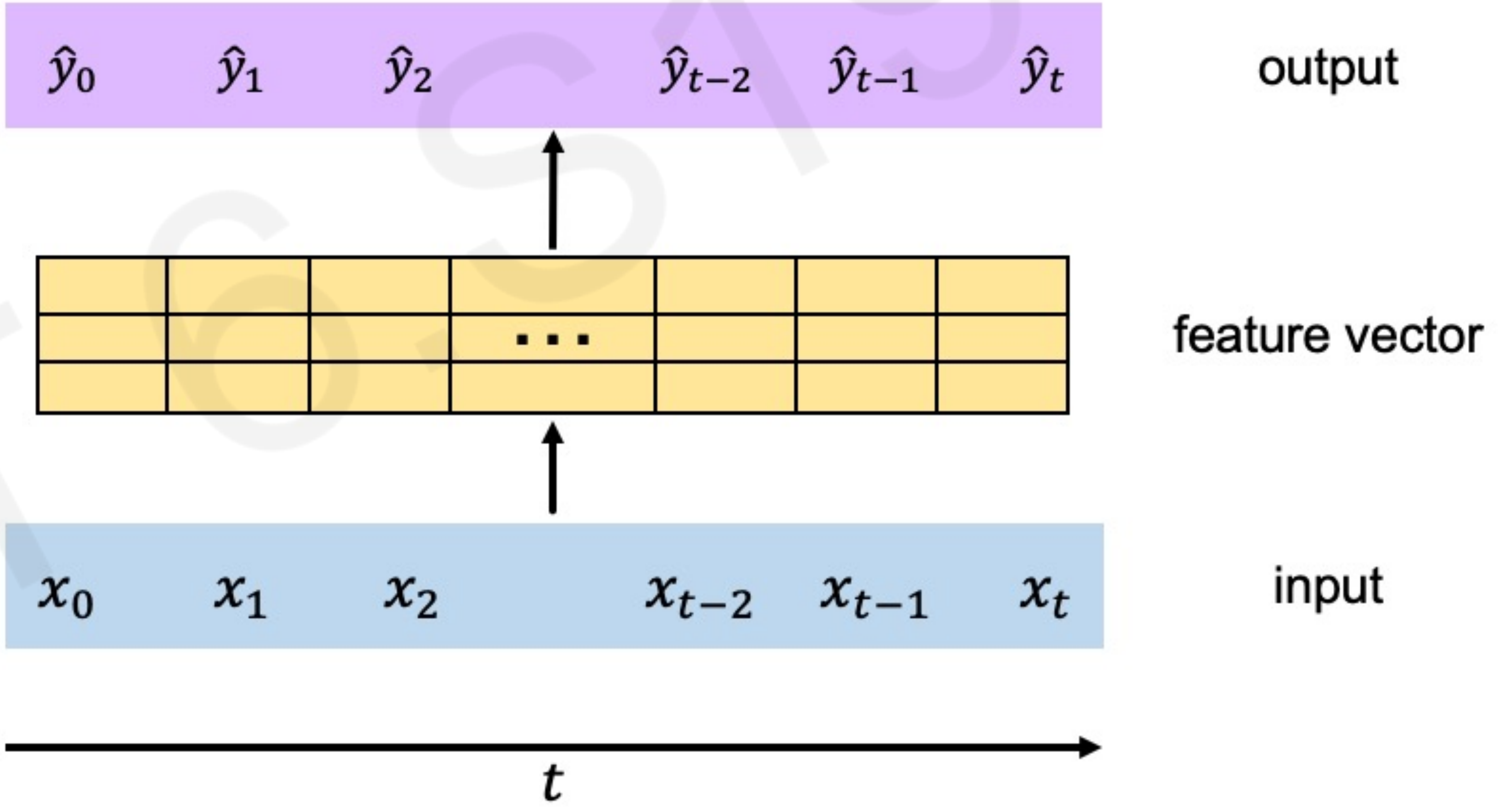


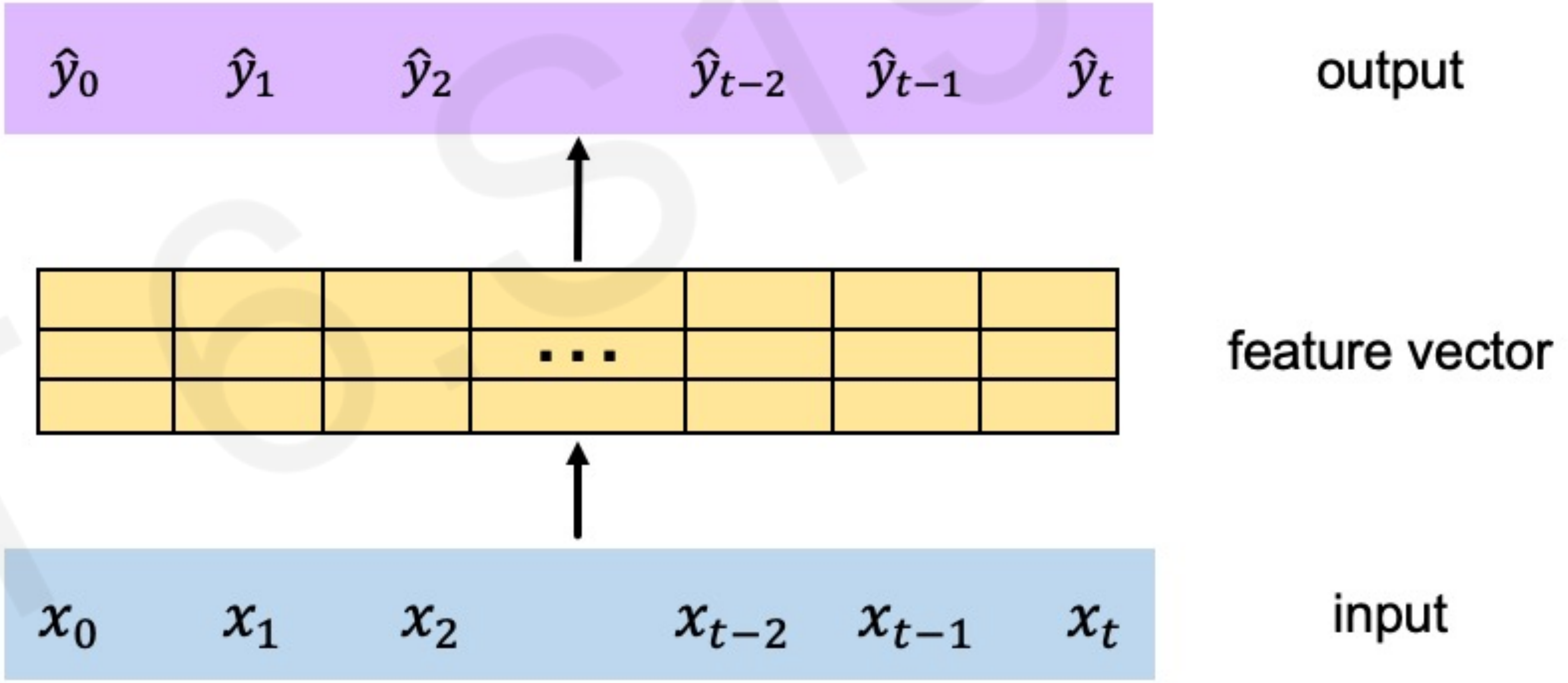
Goal of Sequence Modeling

Idea 1: Feed everything into dense network

- ✓ No recurrence
- ✗ Not scalable
- ✗ No order
- ✗ No long memory

Idea: Identify and attend to what's important

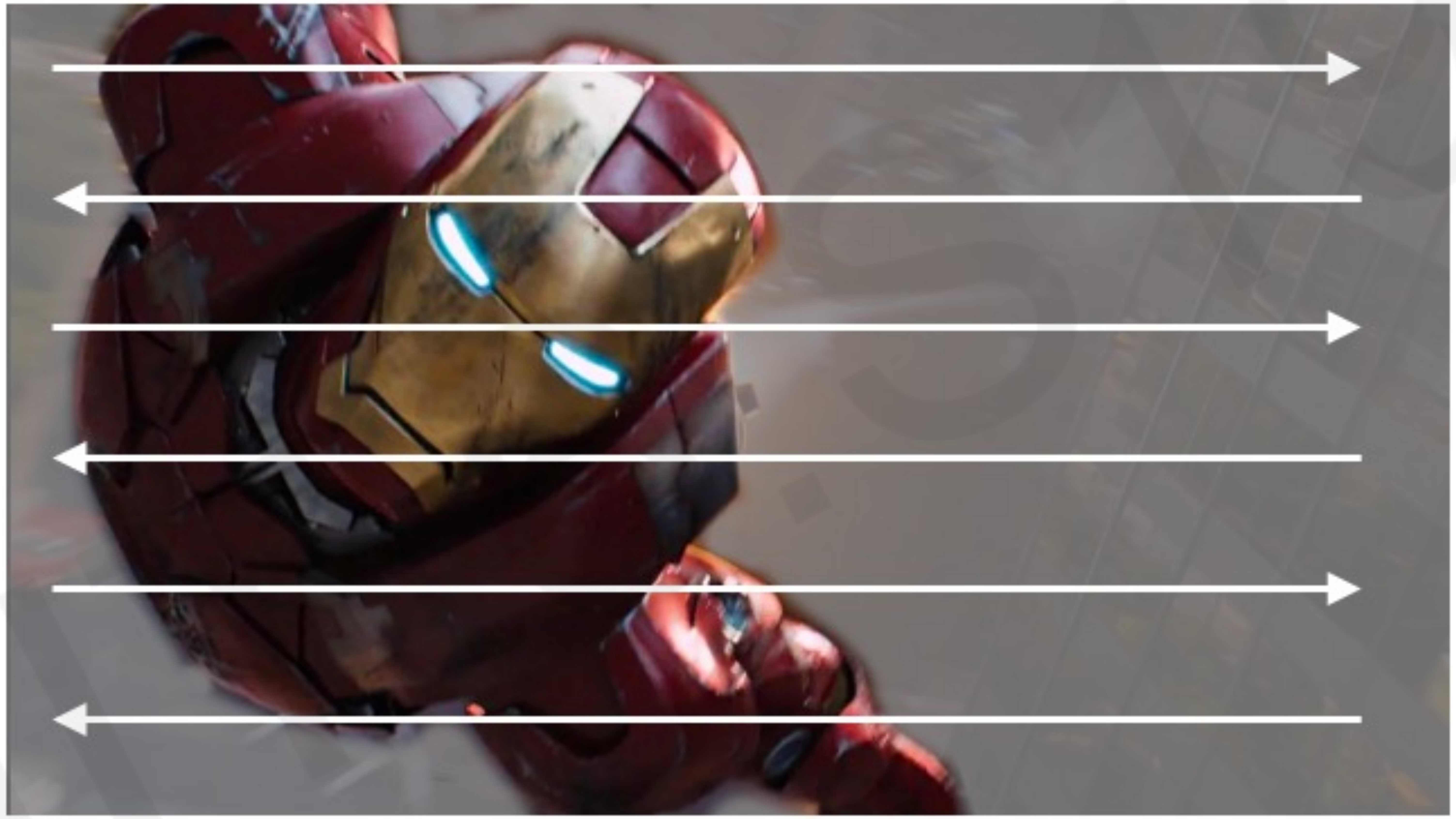
Can we eliminate the need for recurrence entirely?



Attention Is All You Need

Intuition Behind Self-Attention

Attending to the most important parts of an input.

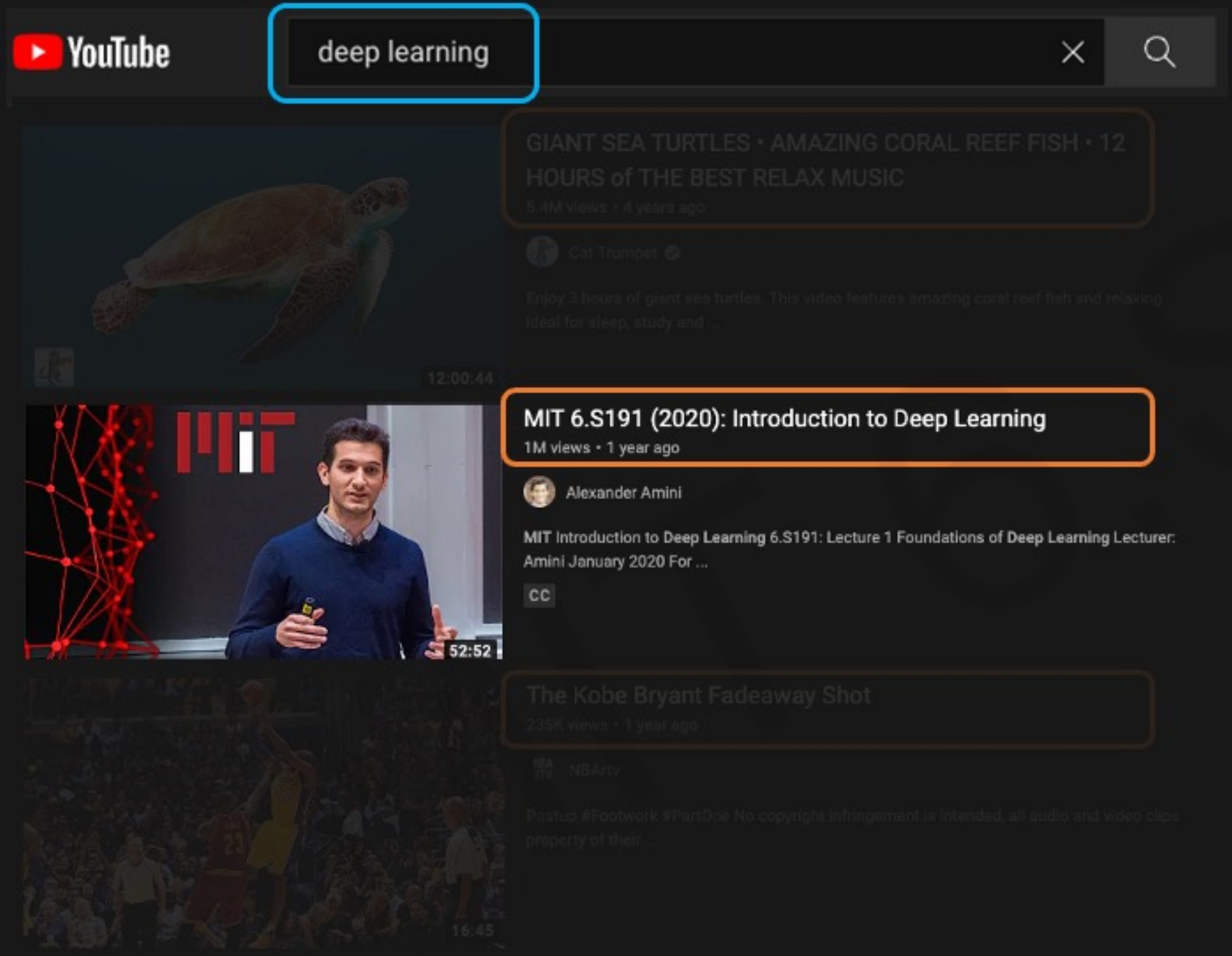


1. Identify which parts to attend to
2. Extract the features with high attention

Similar to a search problem!

A Simple Example: Search

Understanding Attention with Search



Query (Q)

Key (K_1)

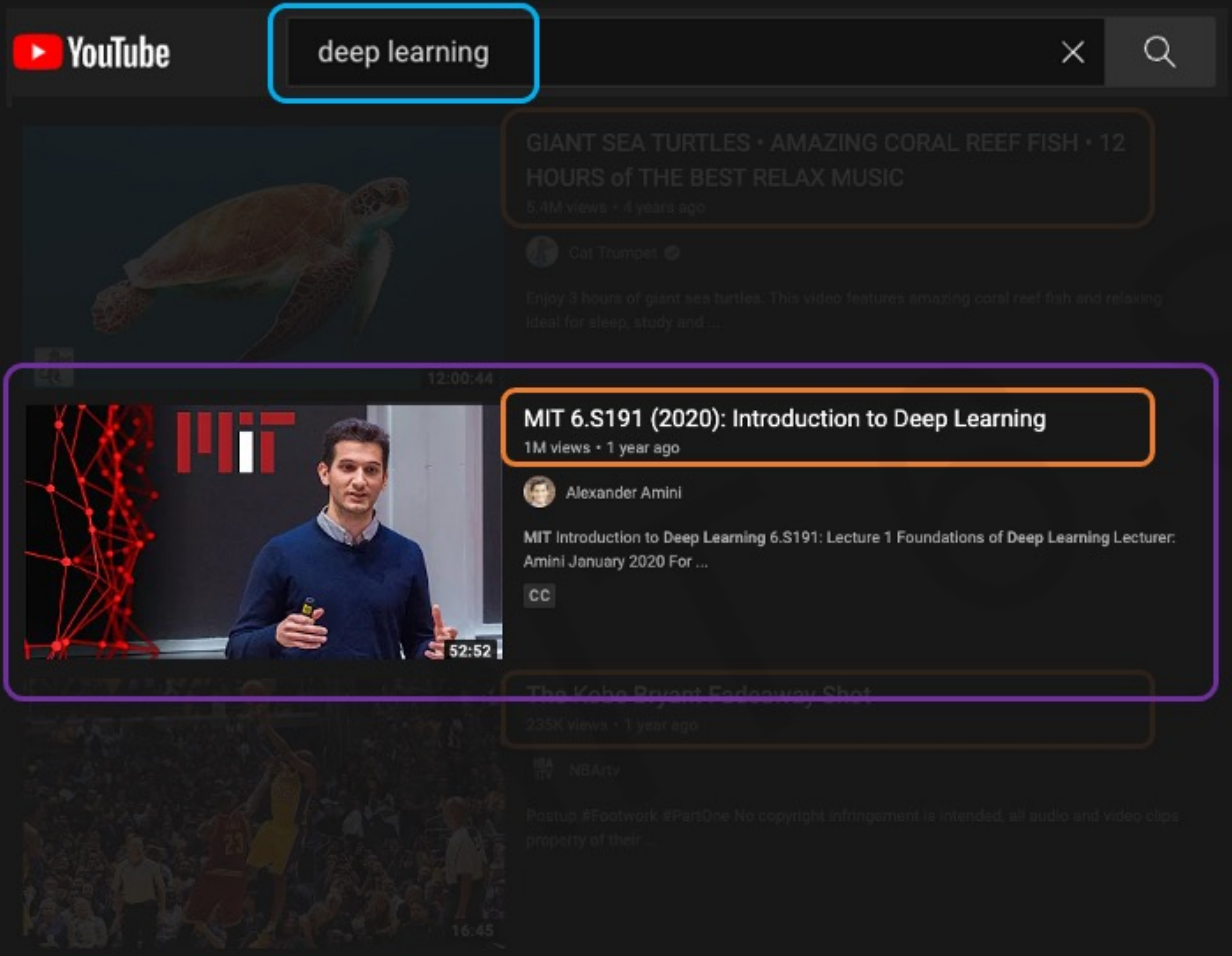
Key (K_2)

Key (K_3)

How similar is the key to the query?

1. **Compute attention mask:** how similar is each key to the desired query?

Understanding Attention with Search



Query (Q)

Key (K_1)

Key (K_2)

Value (V)

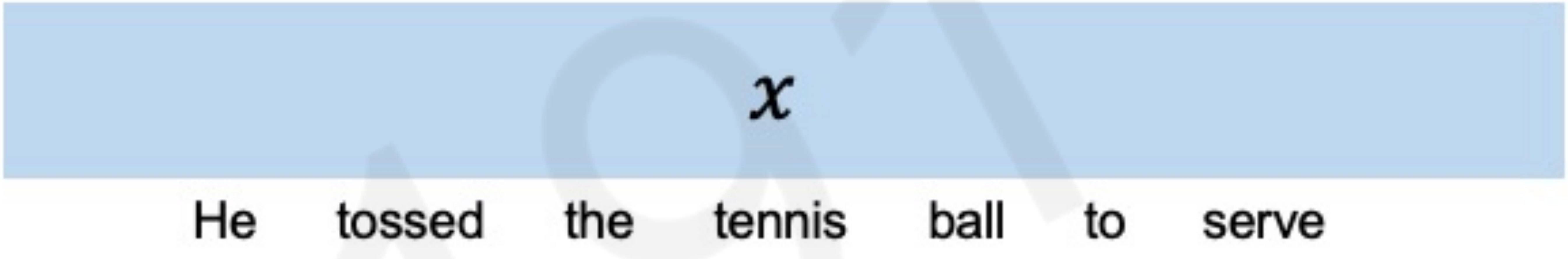
Key (K_3)

2. **Extract values based on attention:**
Return the values highest attention

Learning Self-Attention with Neural Networks

Goal: identify and attend to most important features in input.

1. Encode **position** information
2. Extract **query, key, value** for search
3. Compute **attention weighting**
4. Extract **features with high attention**



Data is fed in all at once! Need to encode position information to understand order.

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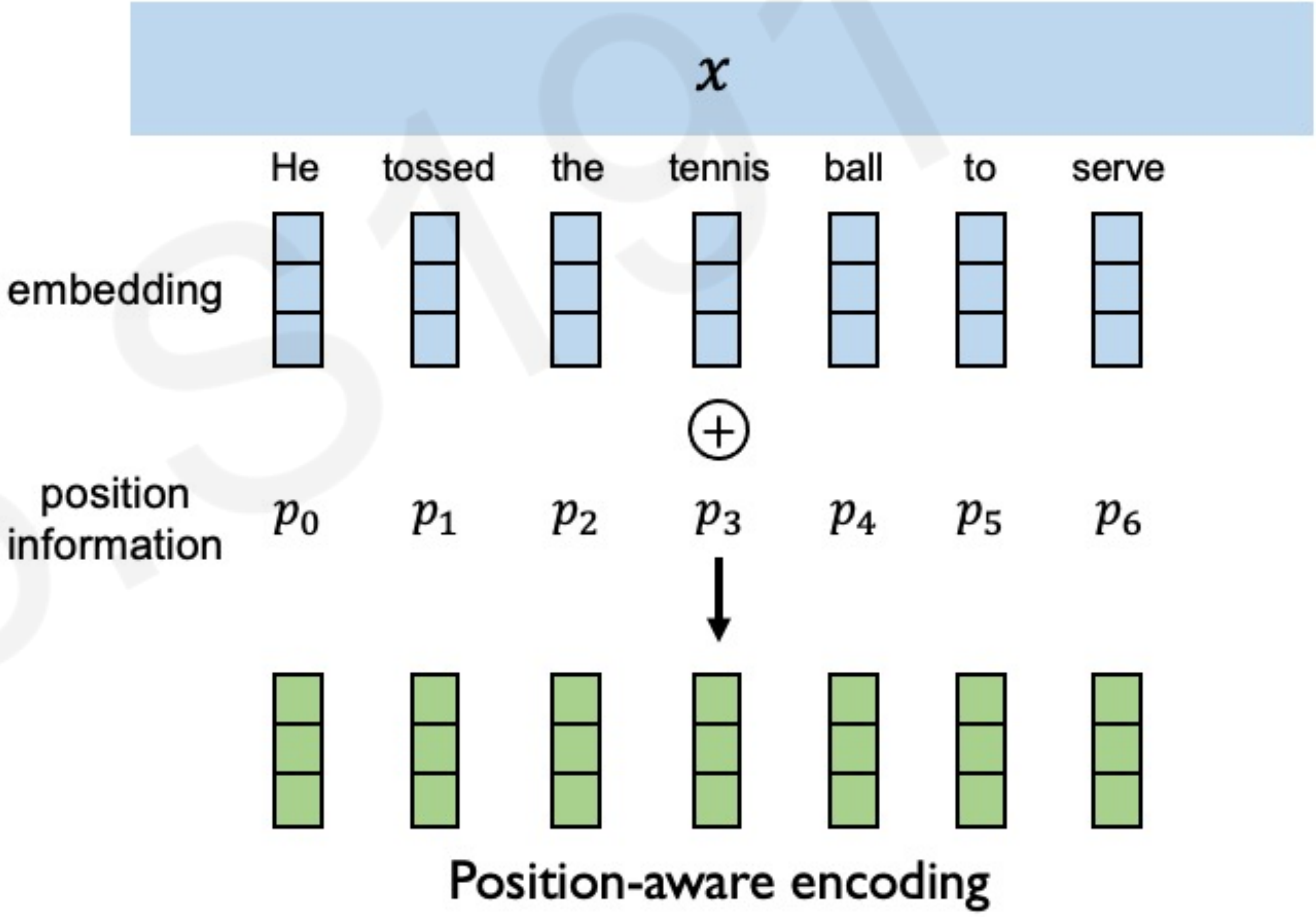

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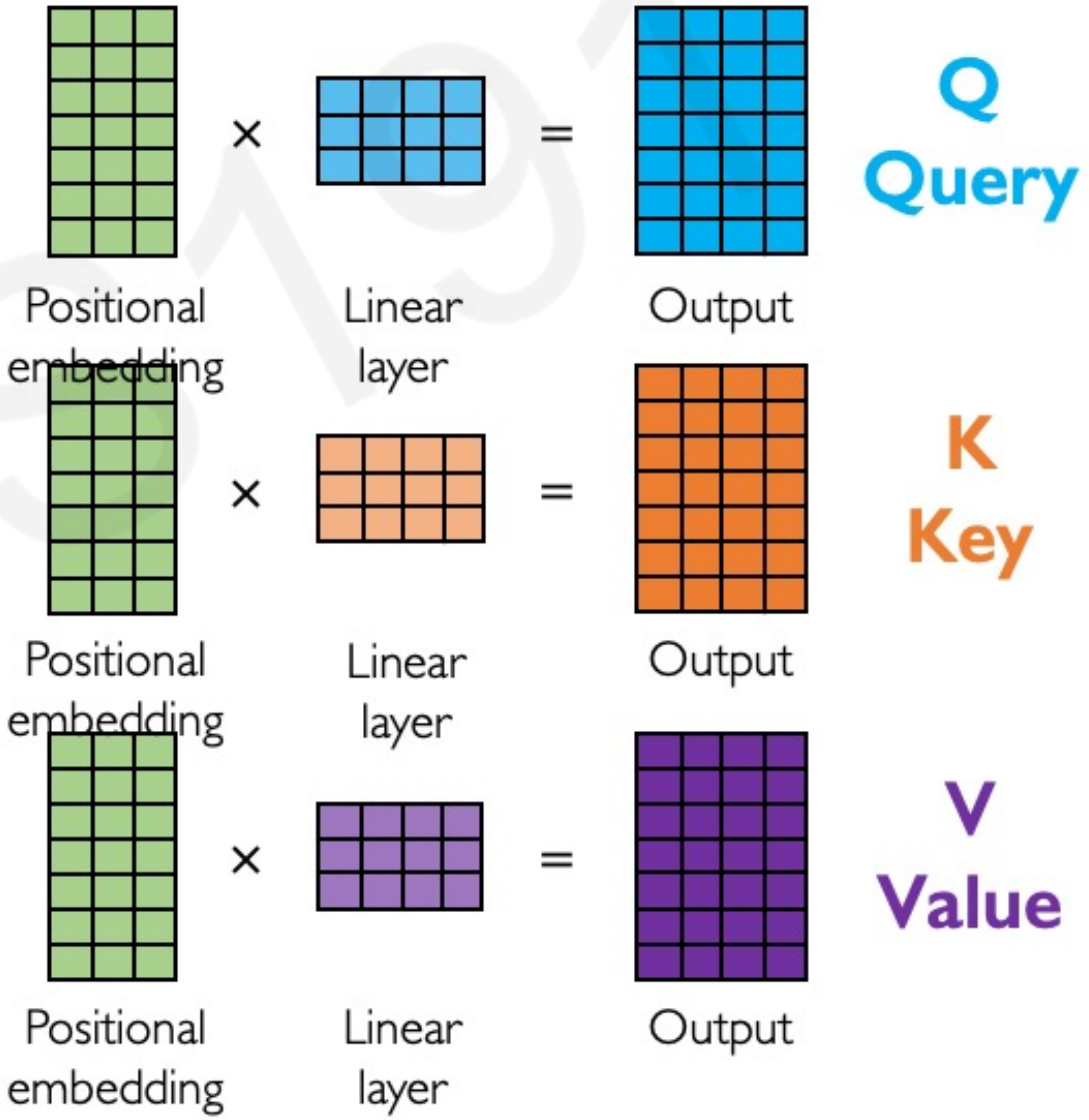

Learning Self-Attention with Neural Networks

Goal: identify and attend to most important features in input.

1. Encode **position** information
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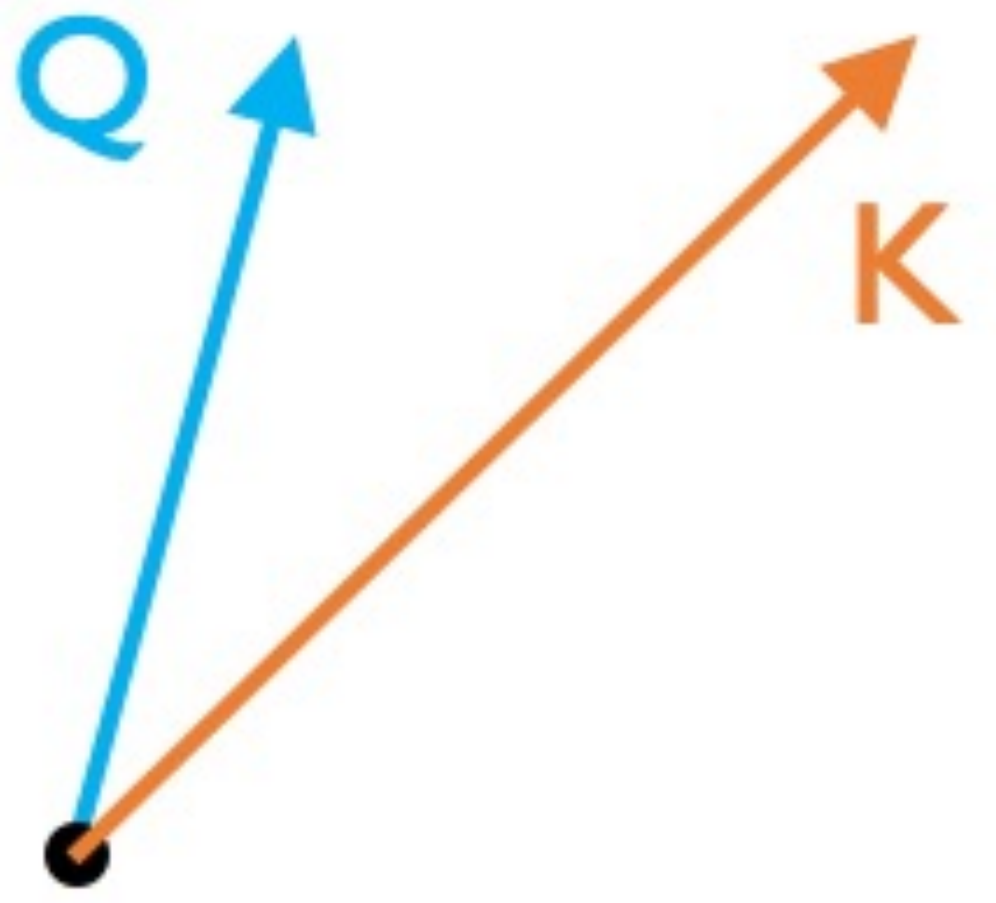
Attention score: compute pairwise similarity between each query and key

How to compute similarity between two sets of features?



Dot product

Scale

$$\frac{Q \cdot K^T}{\text{scaling}}$$

Similarity metric

Also known as the "cosine similarity"

Learning Self-Attention with Neural Networks

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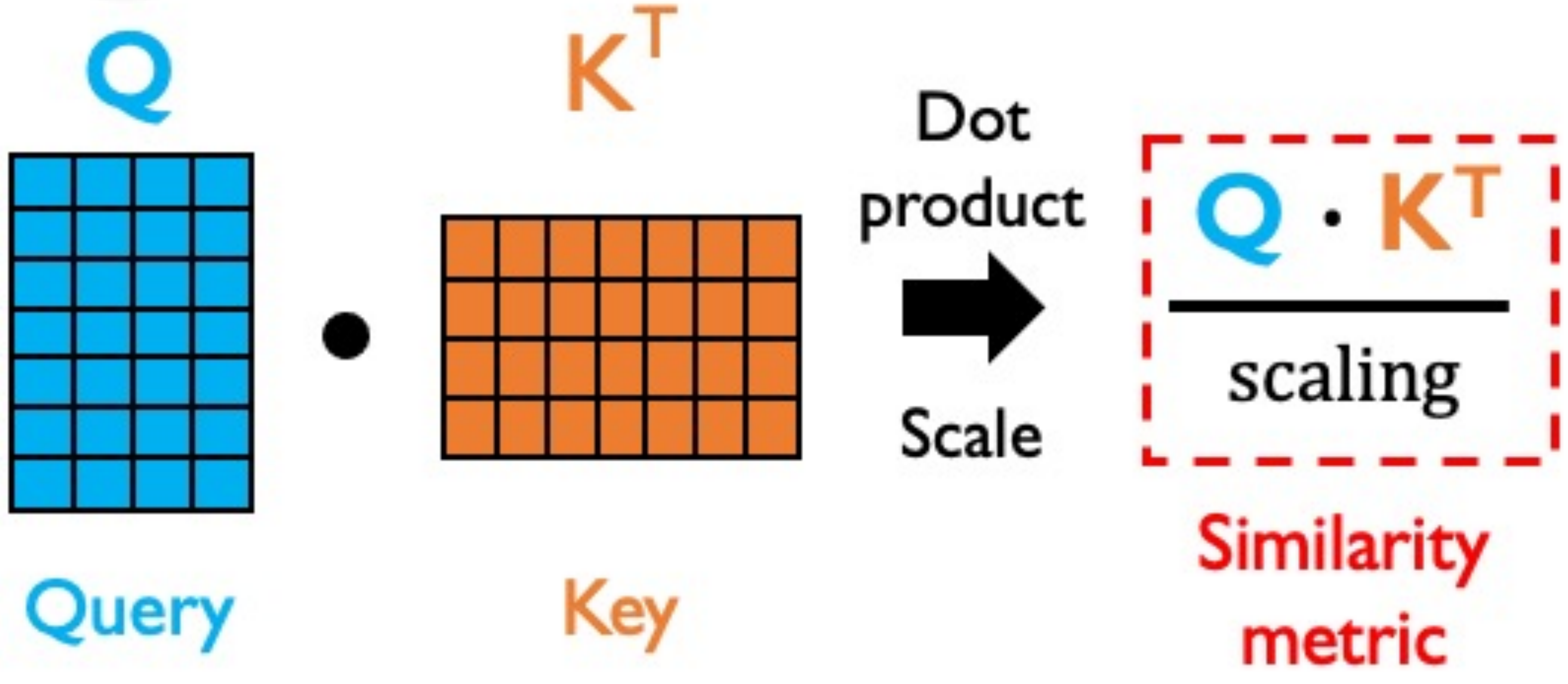

Also known as the "cosine similarity"

Learning Self-Attention with Neural Networks

Goal: identify and attend to most important features in input.

1. Encode **position** information
2. Extract **query, key, value** for search
3. Compute **attention weighting**
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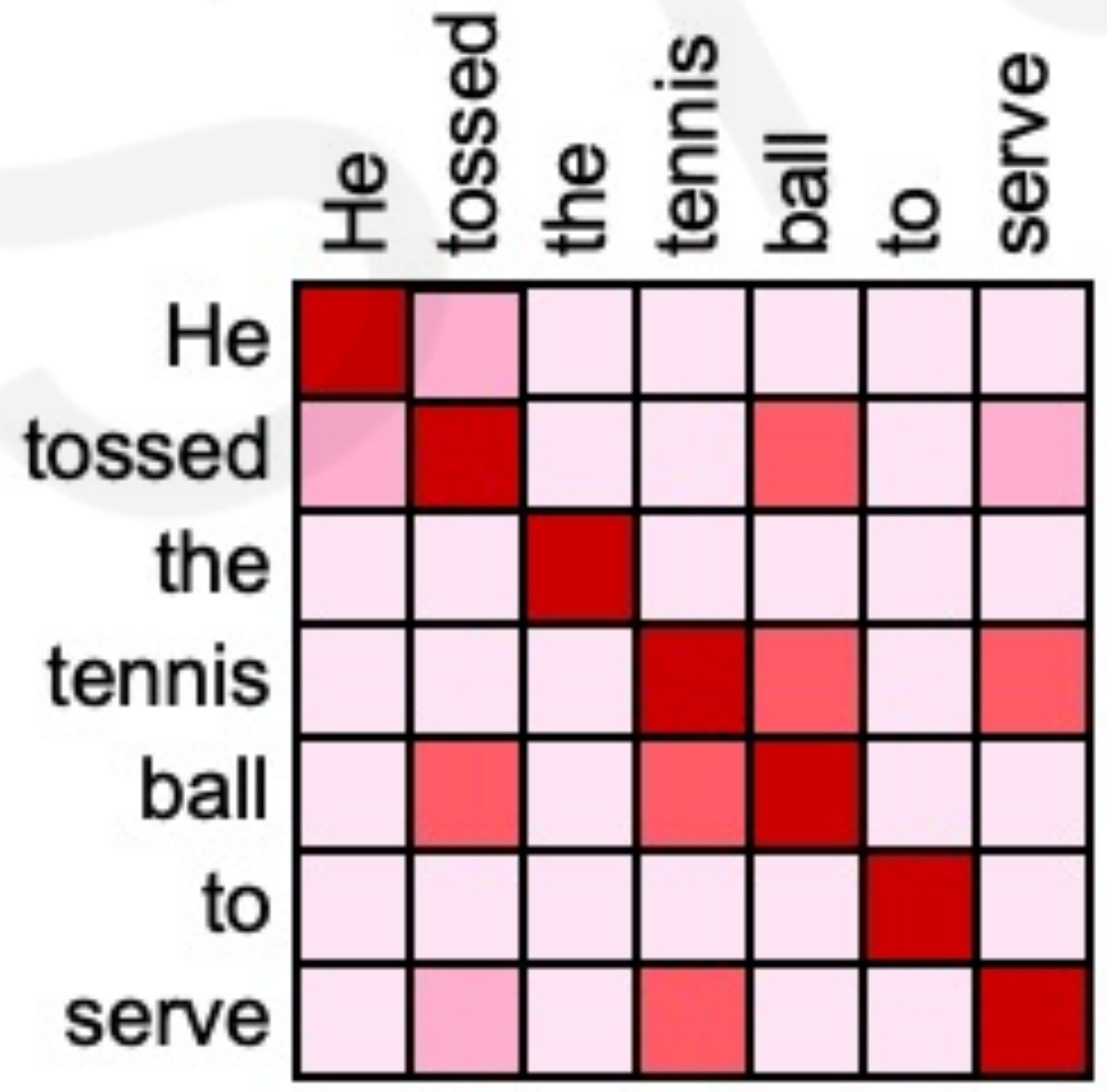
Attention weighting: where to attend to! How similar is the key to the query?



$$softmax\left(\frac{Q \cdot K^T}{scaling}\right)$$

Attention weighting

Learning Self-Attention with Neural Networks

Goal: identify and attend to most important features in input.

1. Encode **position** information
2. Extract **query, key, value** for search
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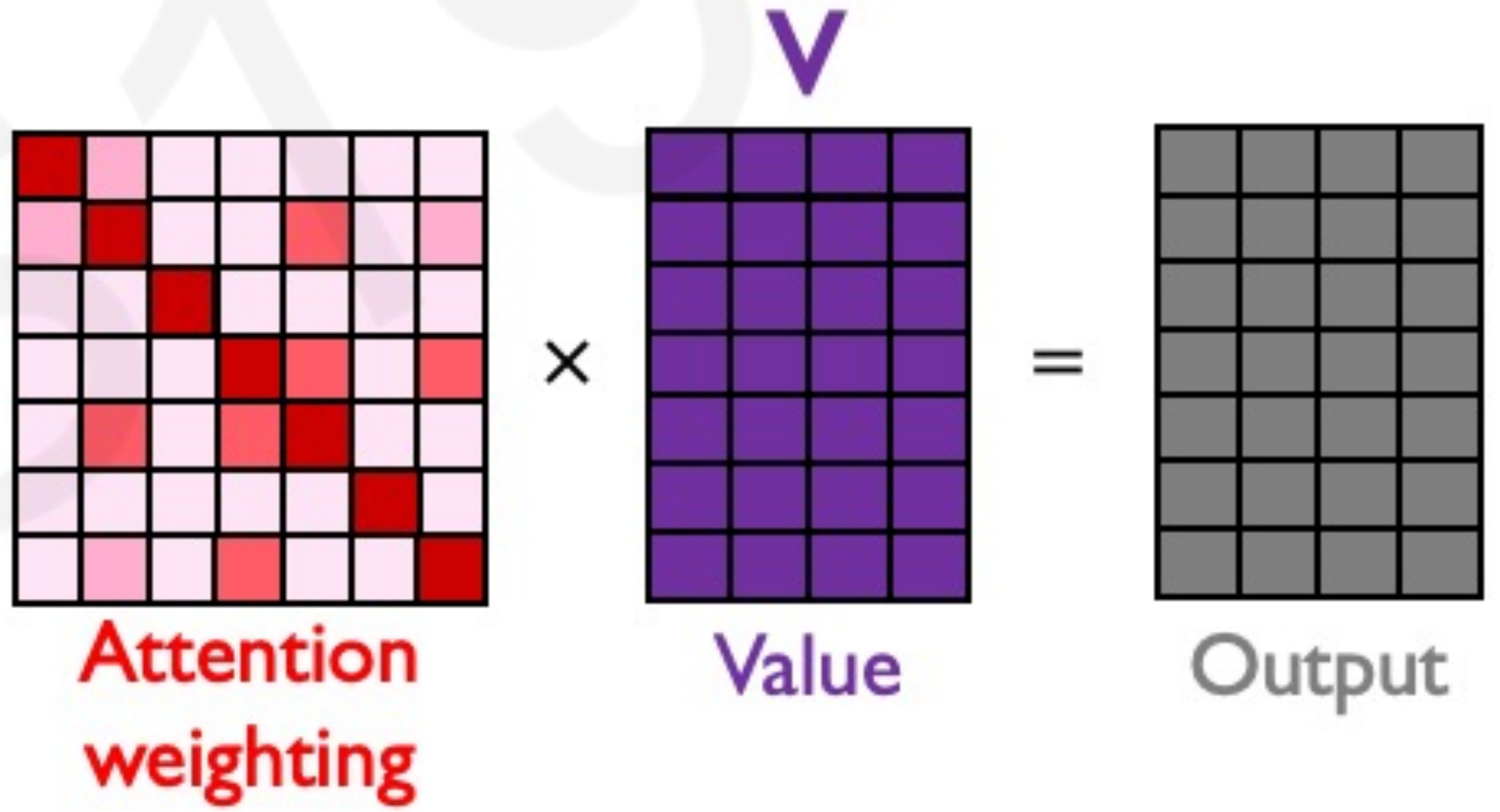
4. Extract **features with high attention**

Last step: self-attend to extract features



$$softmax\left(\frac{Q \cdot K^T}{scaling}\right) \cdot V = A(Q,K,V)$$

Learning Self-Attention with Neural Networks

Goal: identify and attend to most important features in input.

1. Encode **position** information
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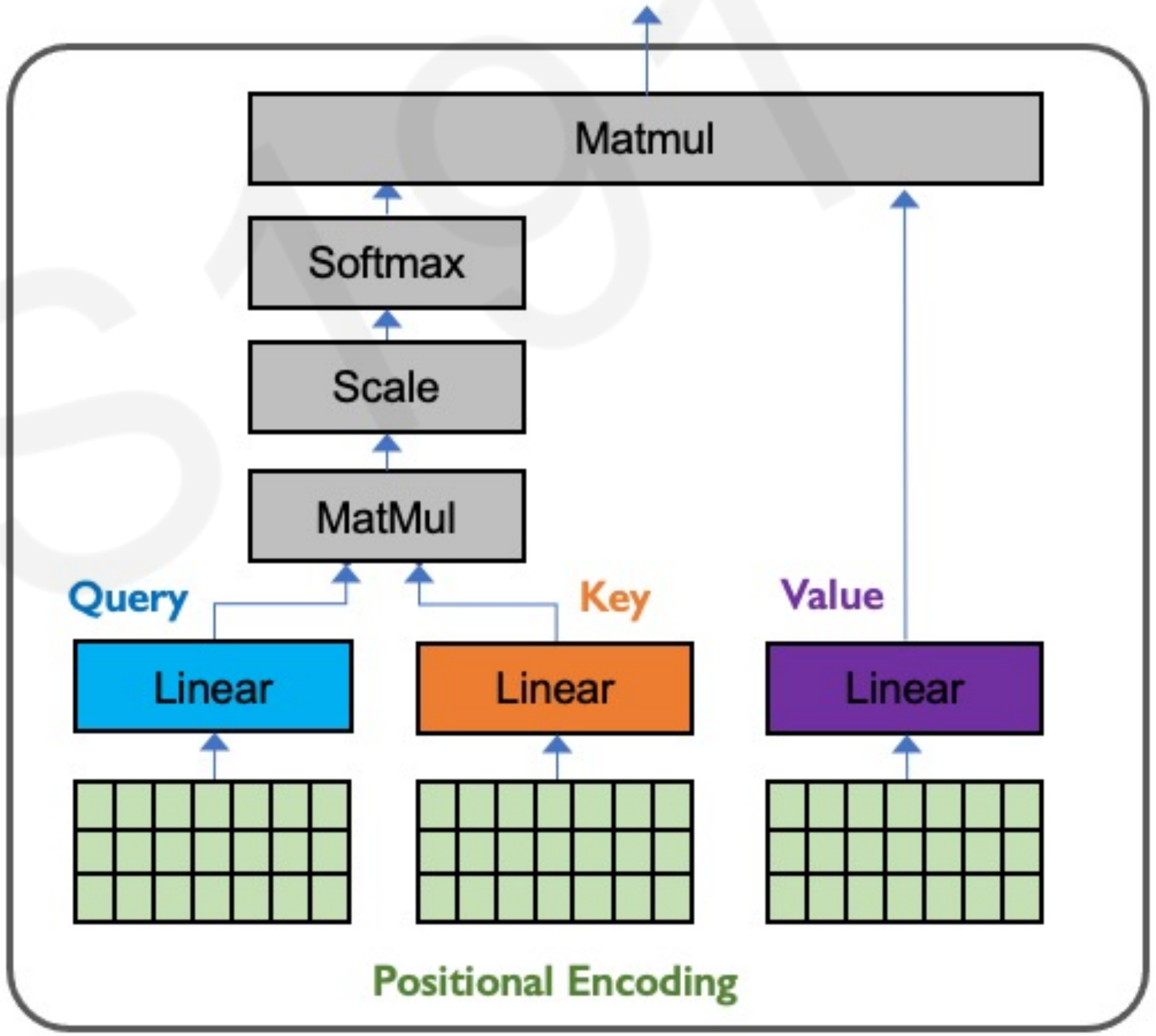
3. Compute **attention weighting**
4. Extract **features with high attention**

These operations form a self-attention head that can plug into a larger network. Each head attends to a different part of input.



$$softmax\left(\frac{\boxed{Q \cdot K^T}}{scaling}\right) \cdot V$$

Applying Multiple Self-Attention Heads

Attention weighting

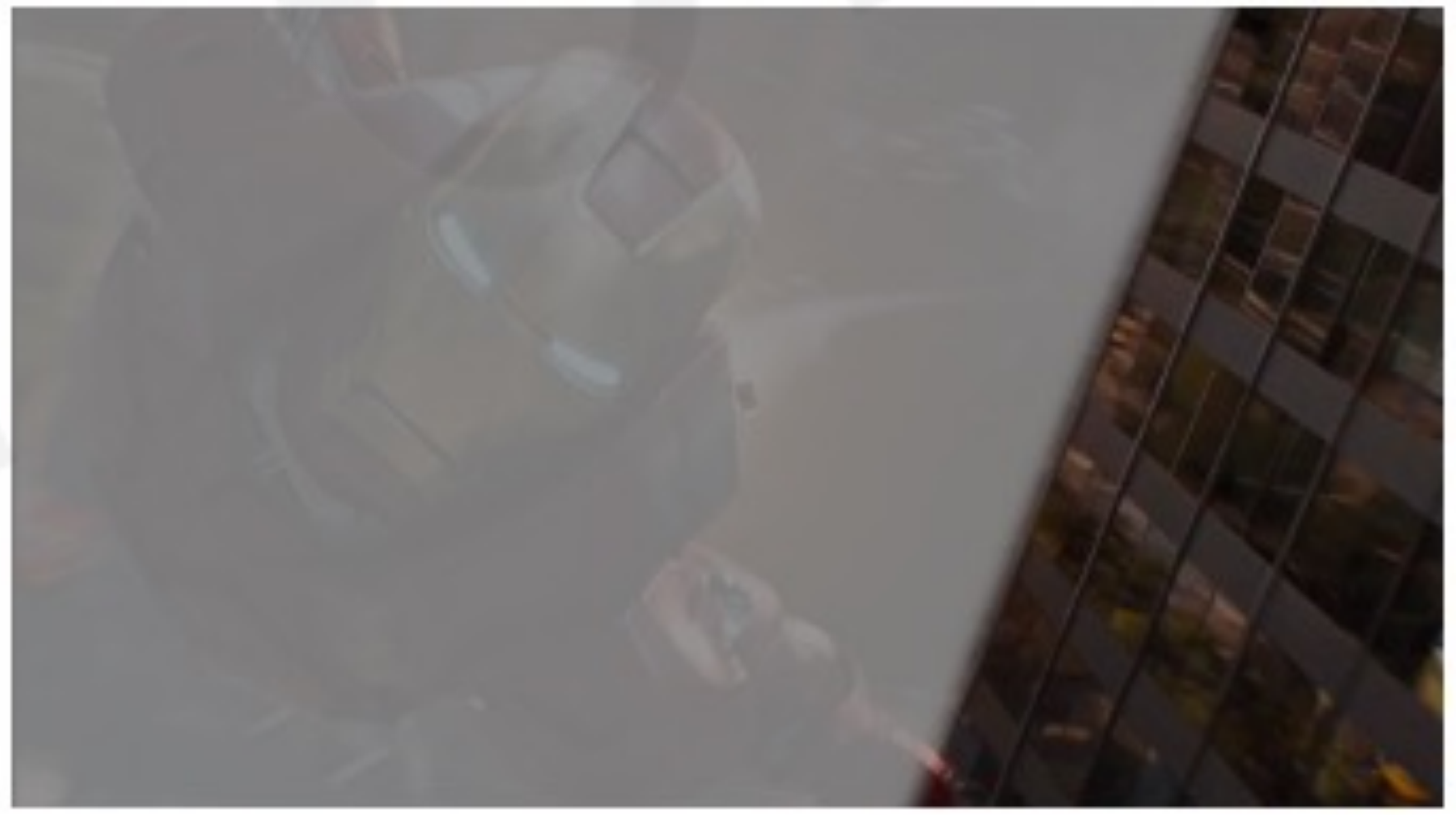
×

Value

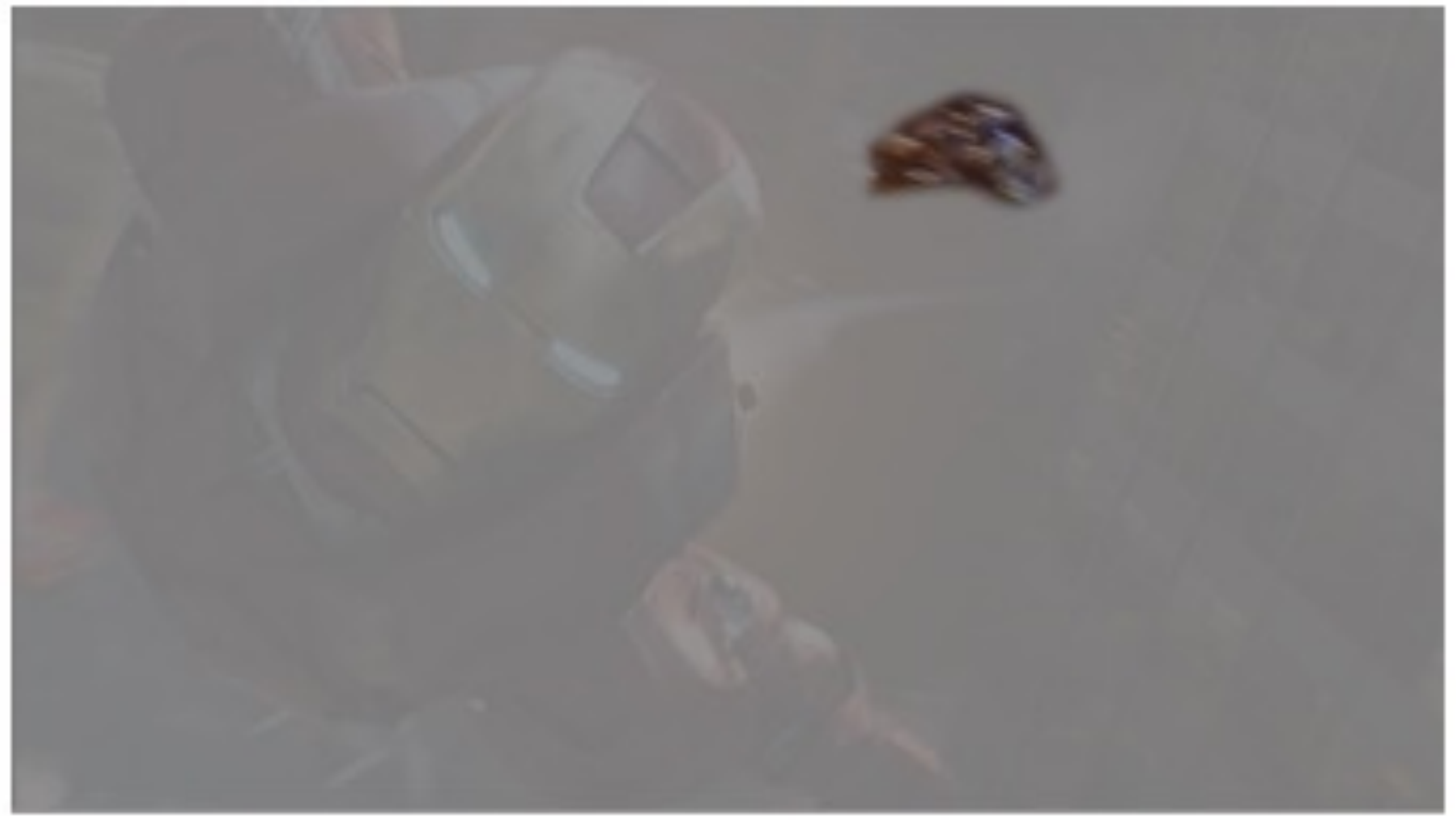
=

Output

Output of attention head 1



Output of attention head 2



Output of attention head 3

Self-Attention Applied

Language Processing

An armchair in the shape of an avocado

BERT, GPT-3

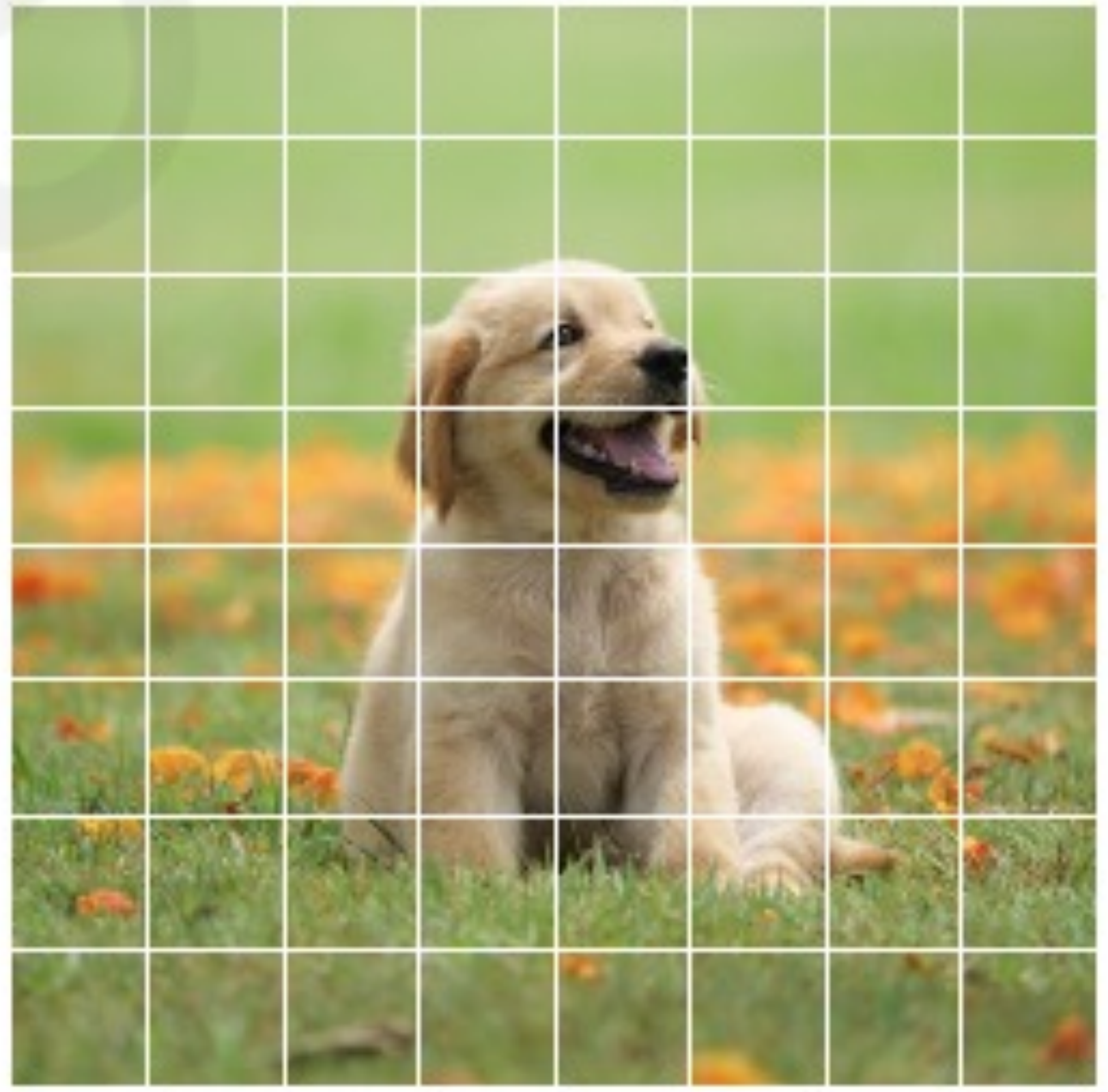
Devlin et al., *NAACL* 2019
Brown et al., *NeurIPS* 2020

Biological Sequences

AlphaFold2

Jumper et al., *Nature* 2021

Computer Vision



Vision Transformers

Dosovitskiy et al., *ICLR* 2020

Deep Learning for Sequence Modeling: Summary

1. RNNs are well suited for **sequence modeling** tasks
2. Model sequences via a **recurrence relation**
3. Training RNNs with **backpropagation through time**
4. Models for **music generation**, classification, machine translation, and more
5. Self-attention to model **sequences without recurrence**

MIT Introduction to Deep Learning

Lab 1: Introduction to TensorFlow and Music Generation with RNNs

Link to download labs:
http://introtodeeplearning.com#schedule

1. Open the lab in Google Colab
2. Start executing code blocks and filling in the #TODOs
3. Need help? Come to 32-123!