Recurrent neural network

Chapter 2

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

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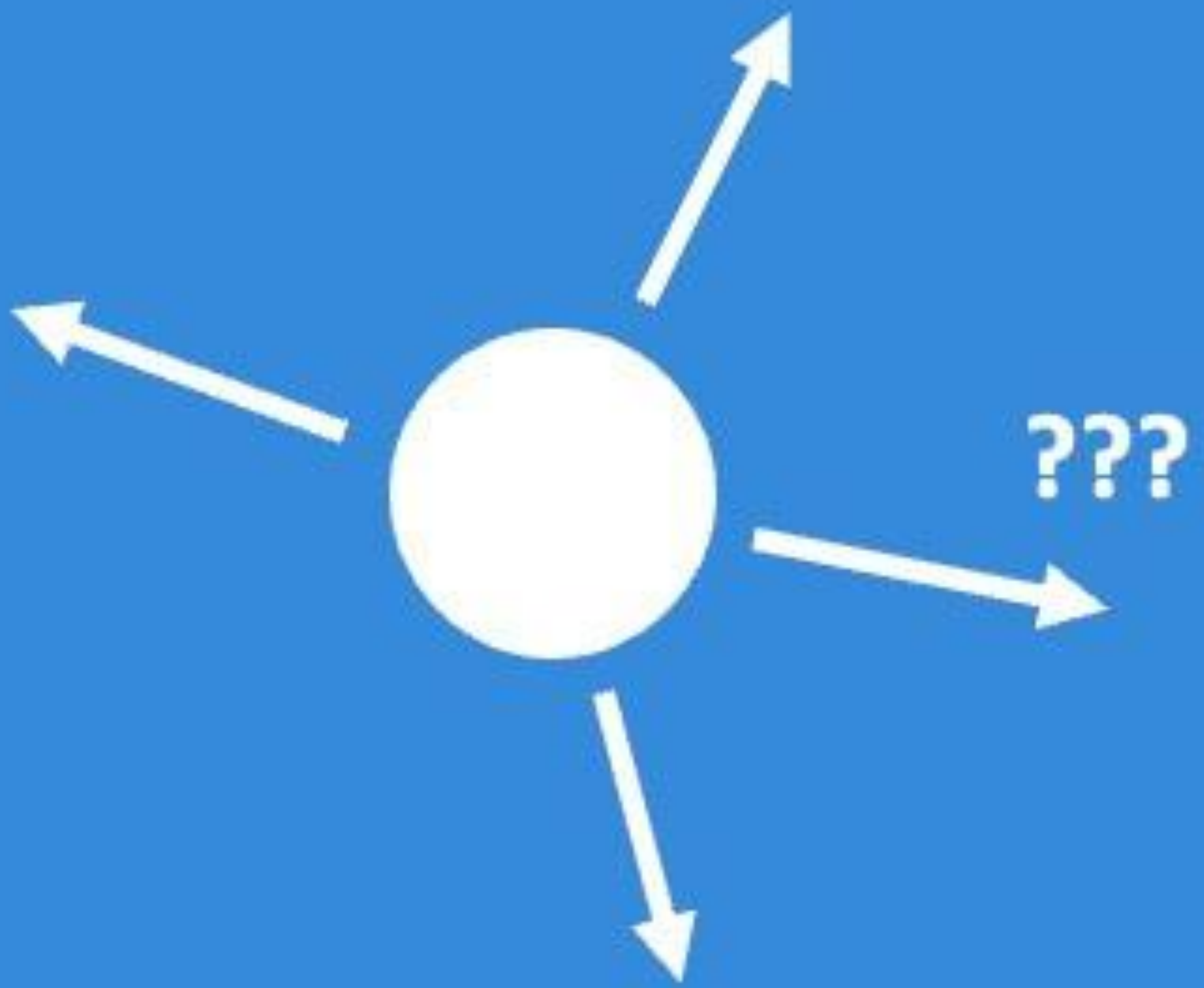

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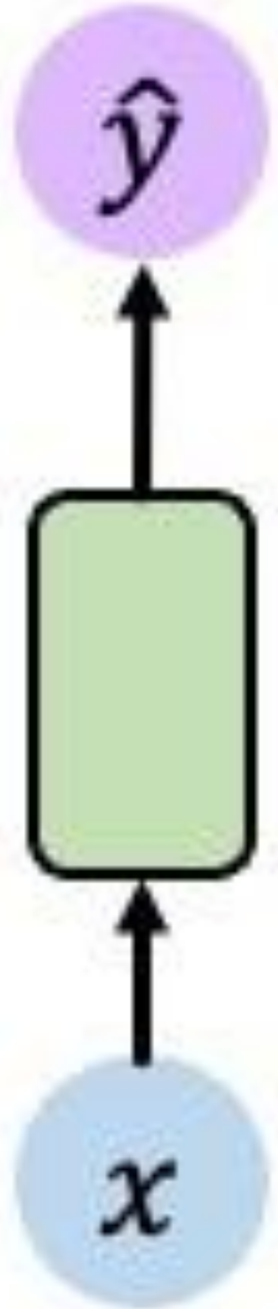
Sequences in the Wild

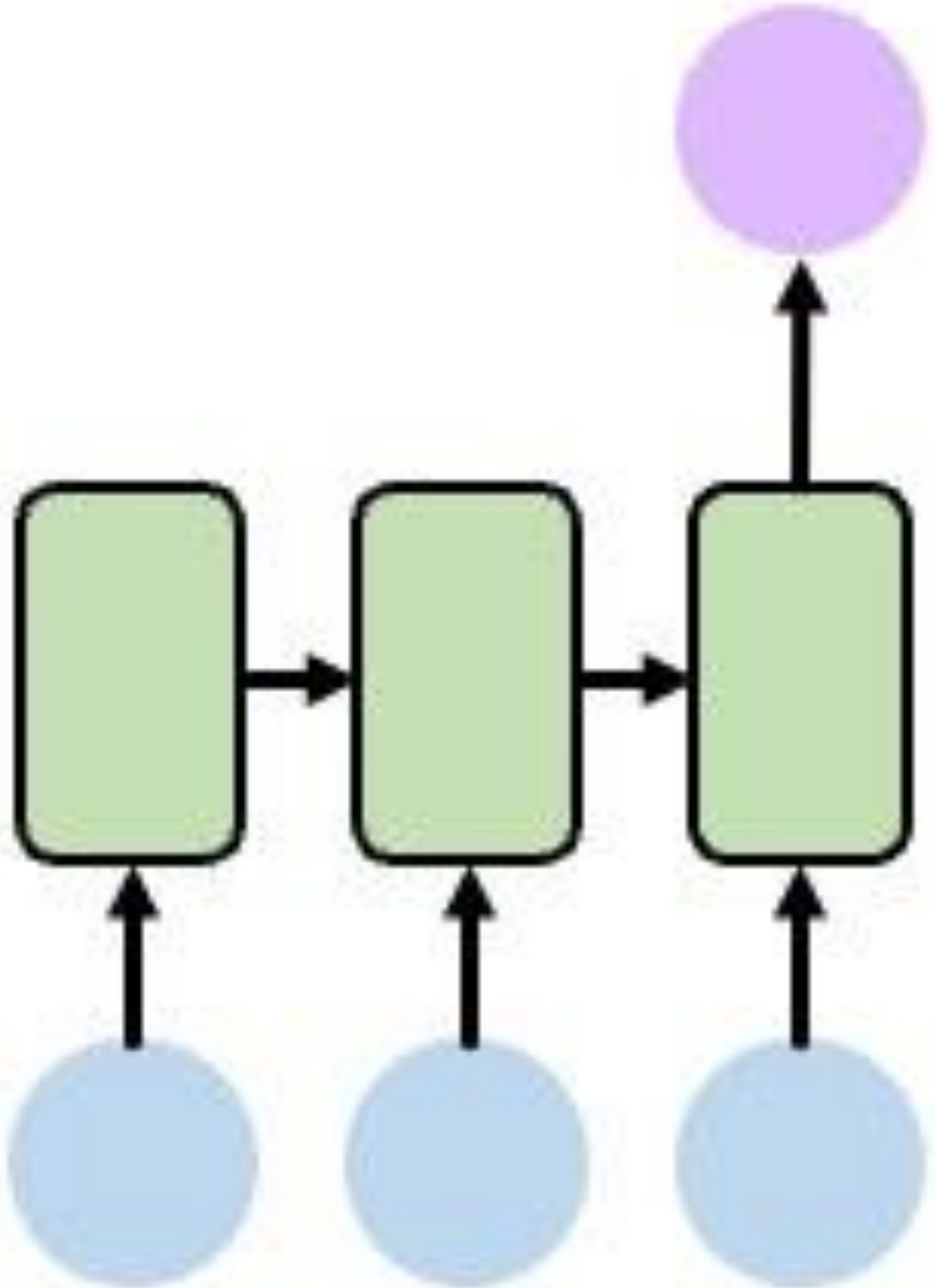
Audio

Sequence Modeling Applications

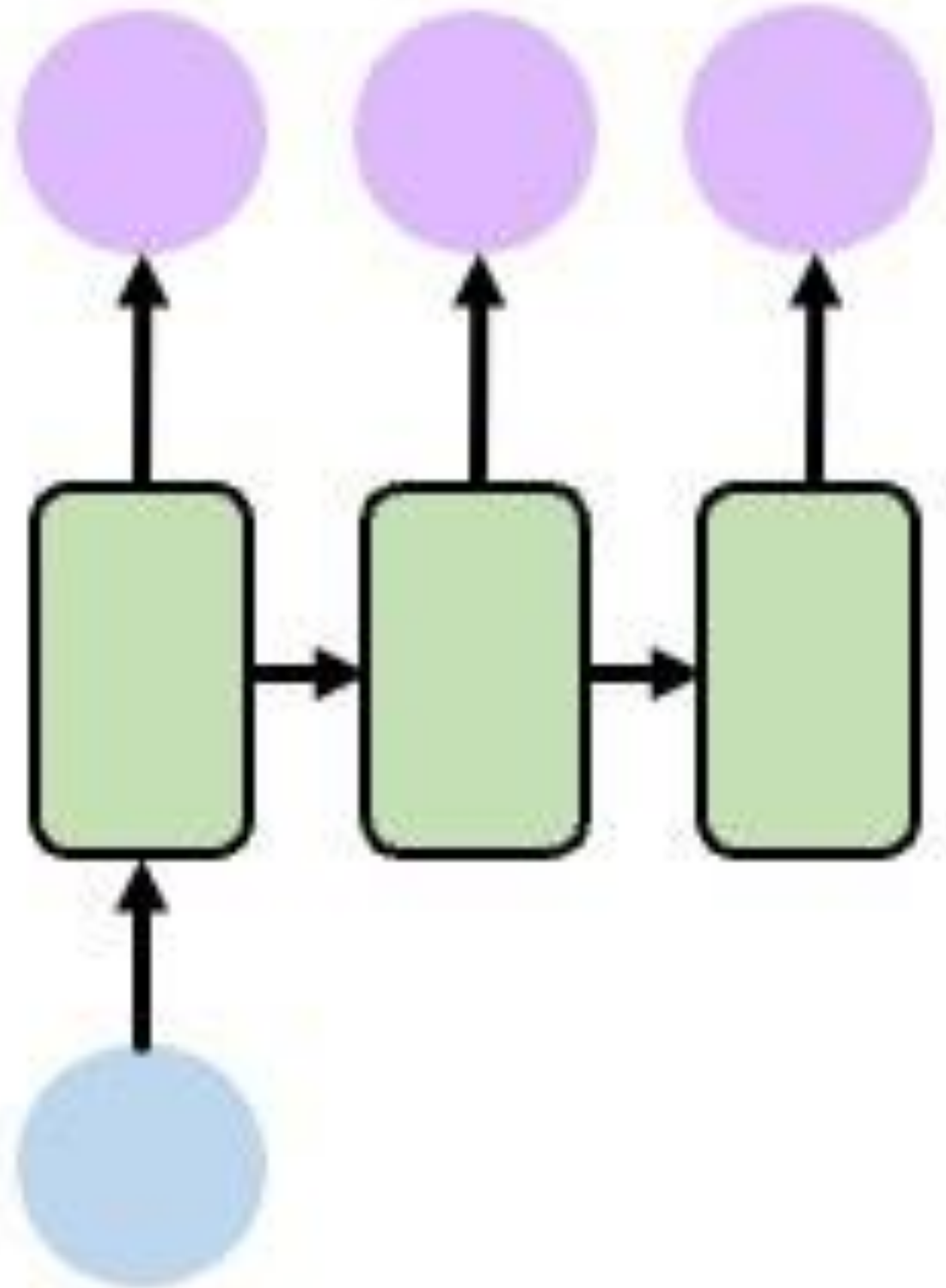


One to One
Binary Classification

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

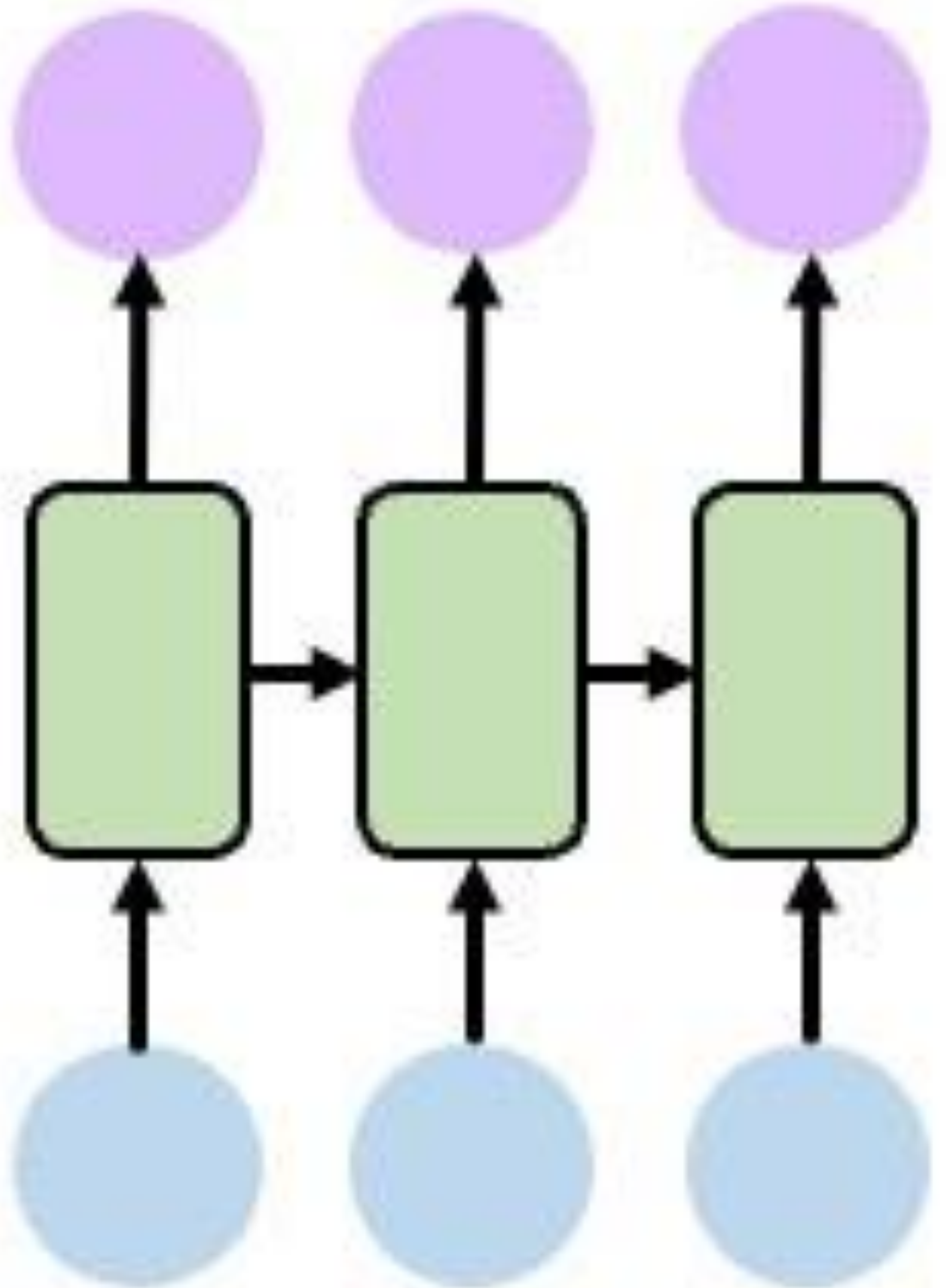


Many to One
Sentiment Classification



One to Many
Image Captioning

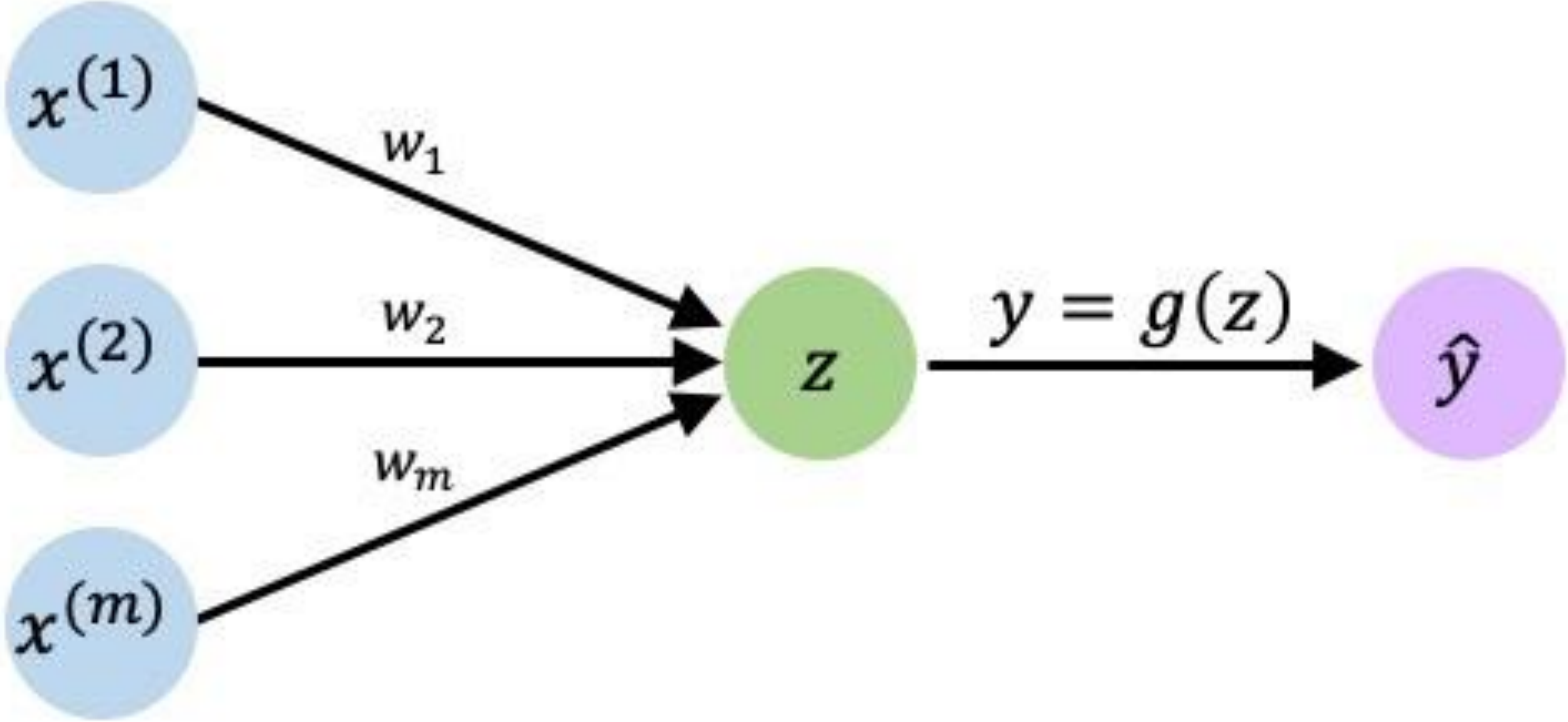
"A baseball player throws a ball."



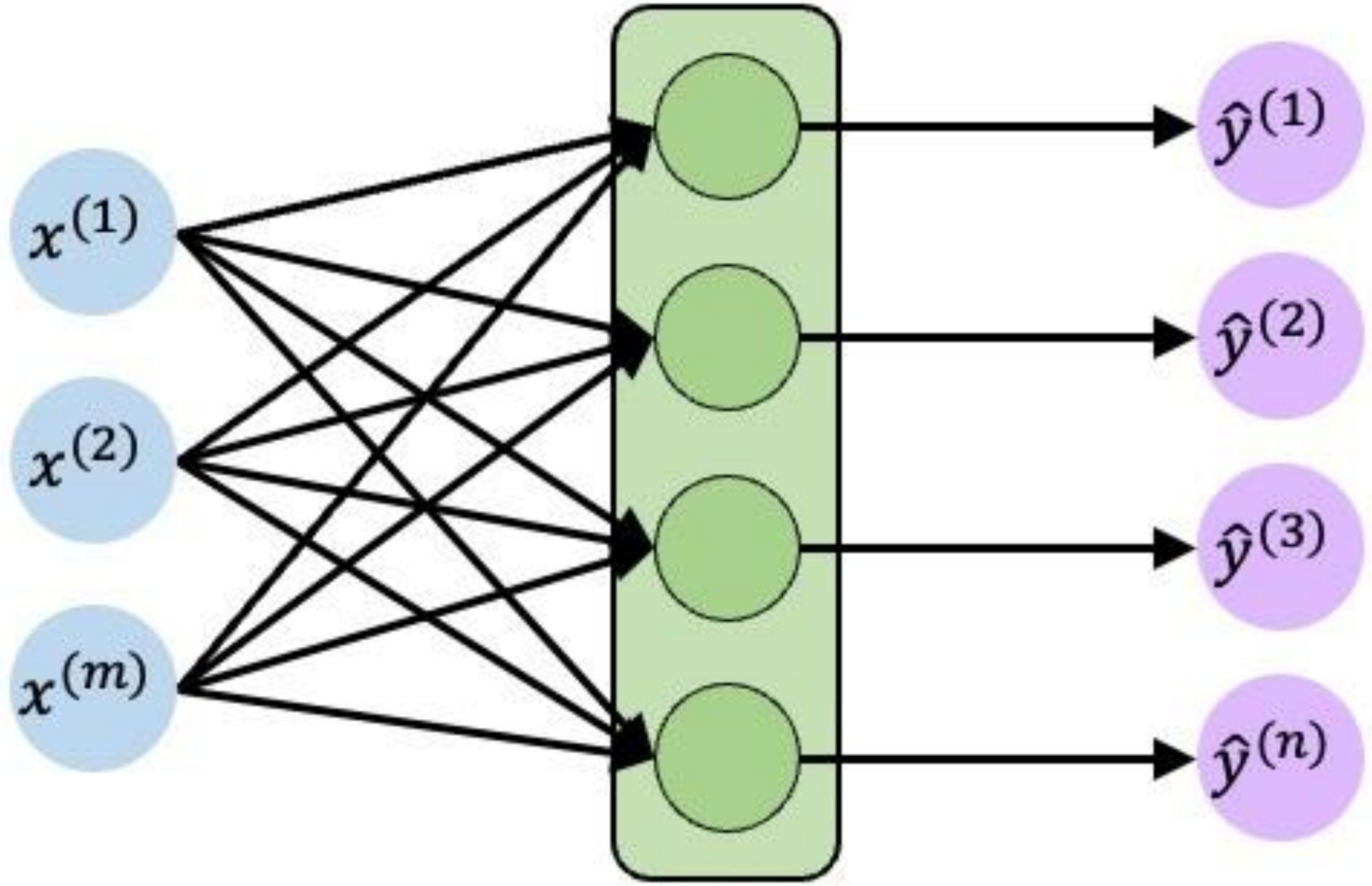
Many to Many
Machine Translation

Neurons with Recurrence

The Perceptron Revisited



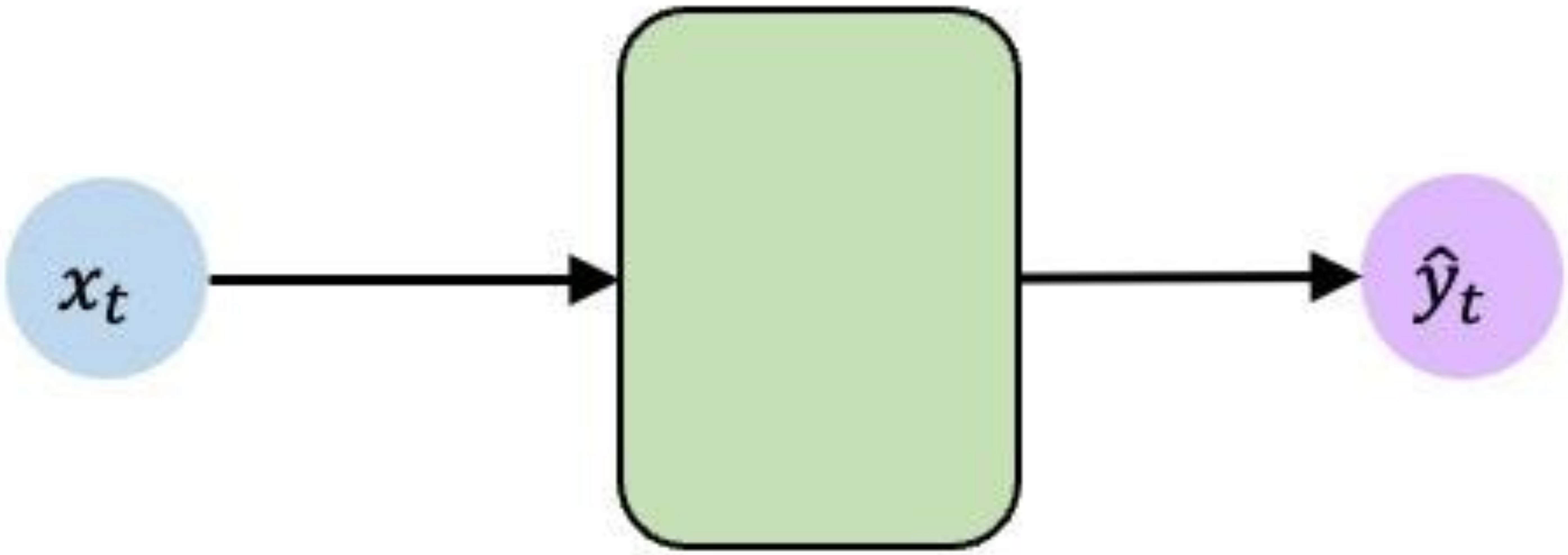
Feed-Forward Networks Revisited



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

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

Feed-Forward Networks Revisited



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

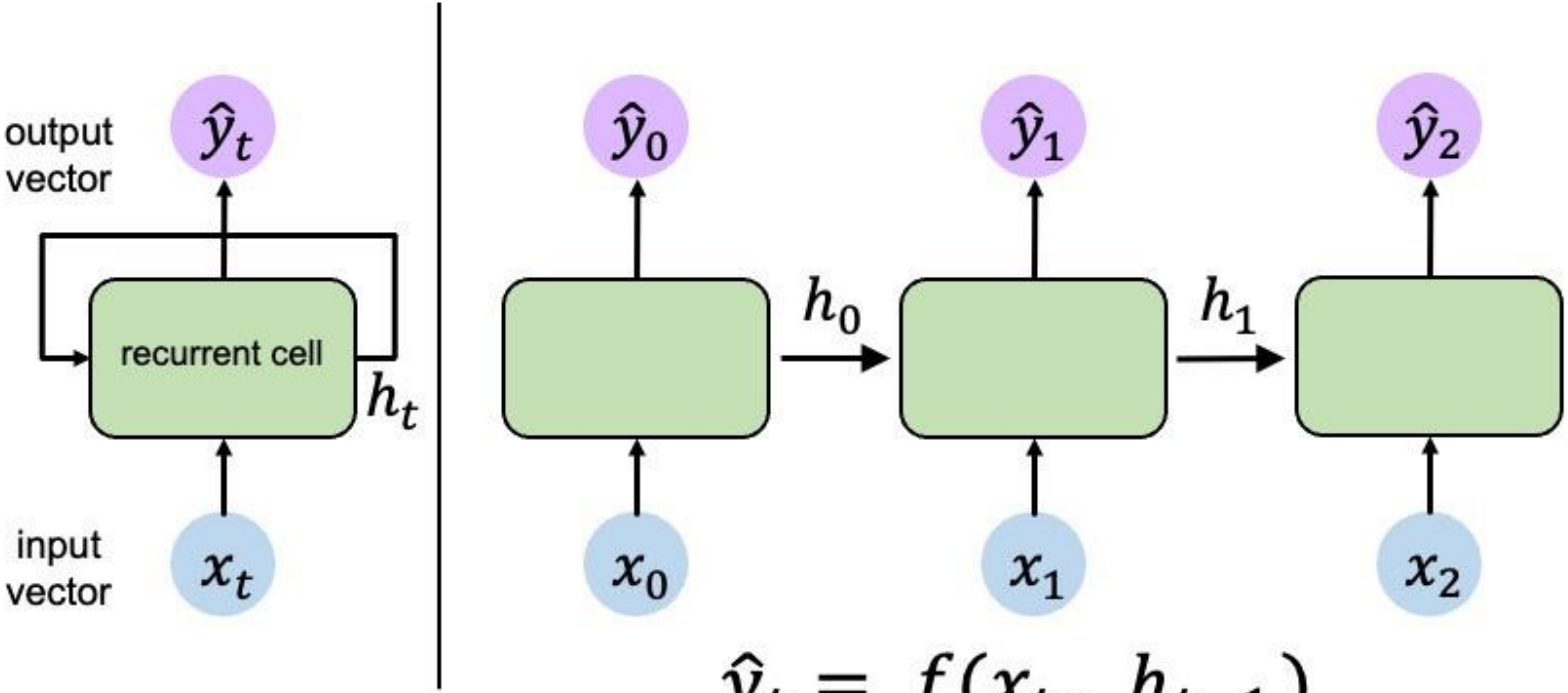
Handling Individual Time Steps

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

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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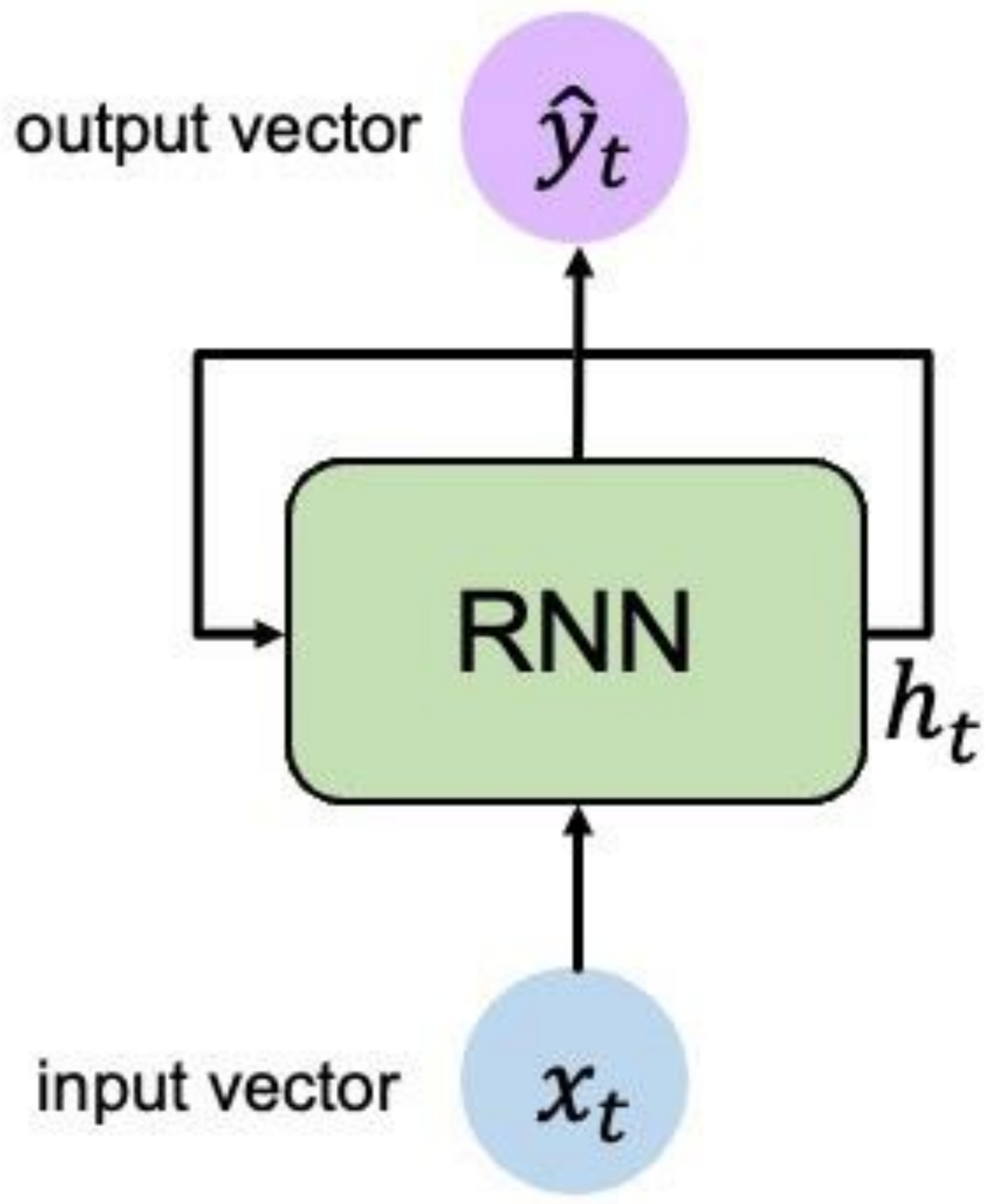


Apply a **recurrence relation** at every time step to process a sequence:

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

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

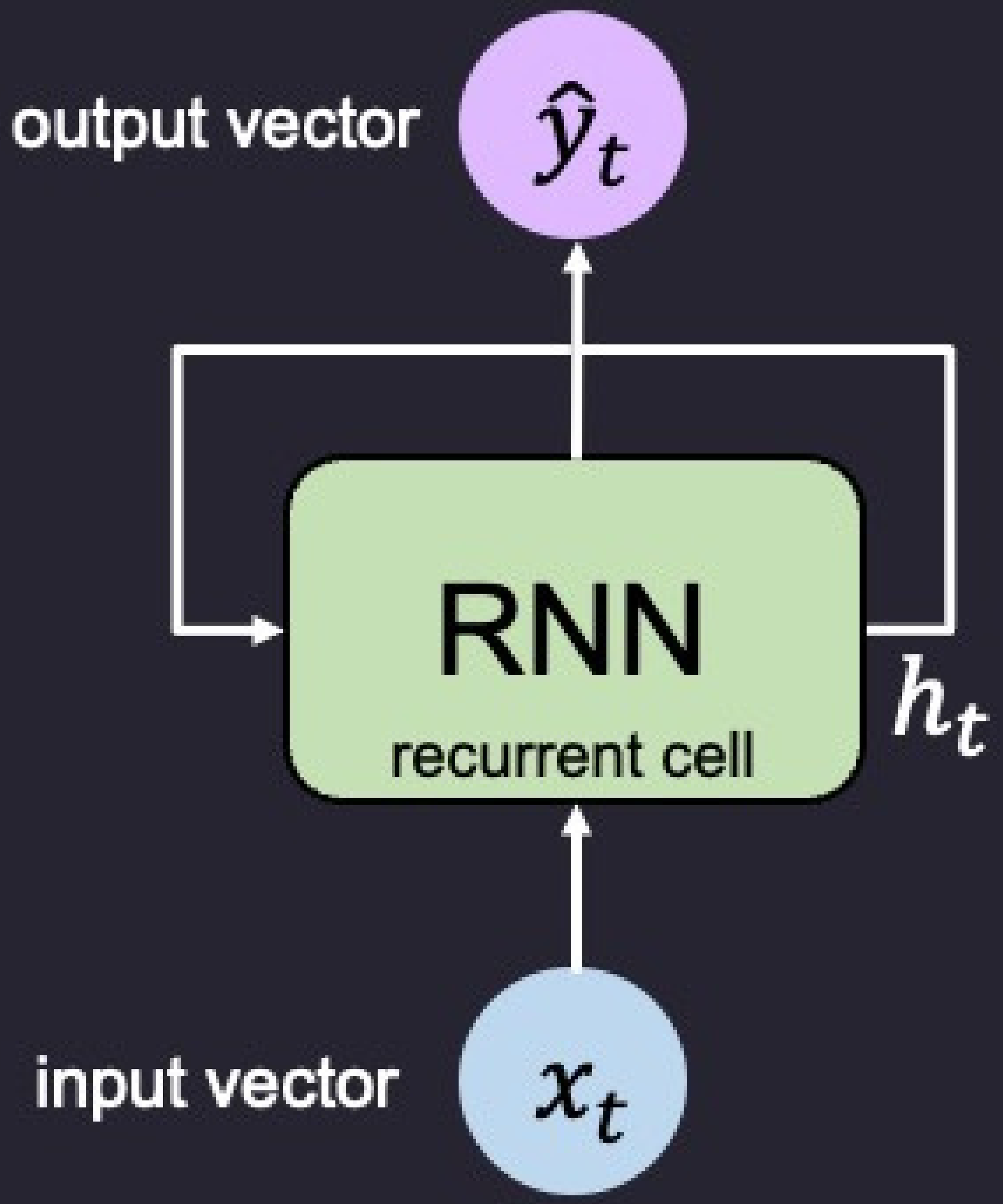
RNN Intuition

```
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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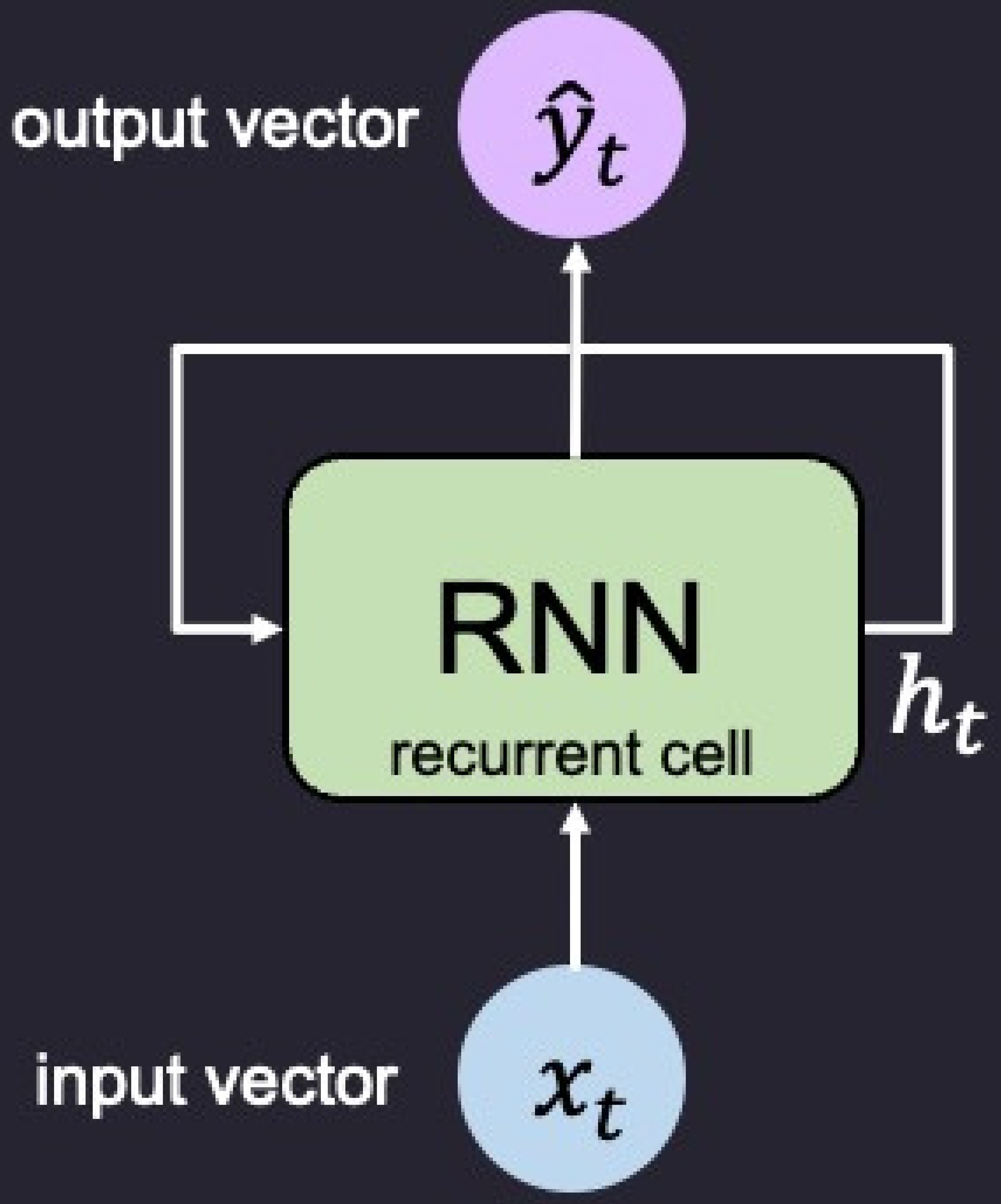

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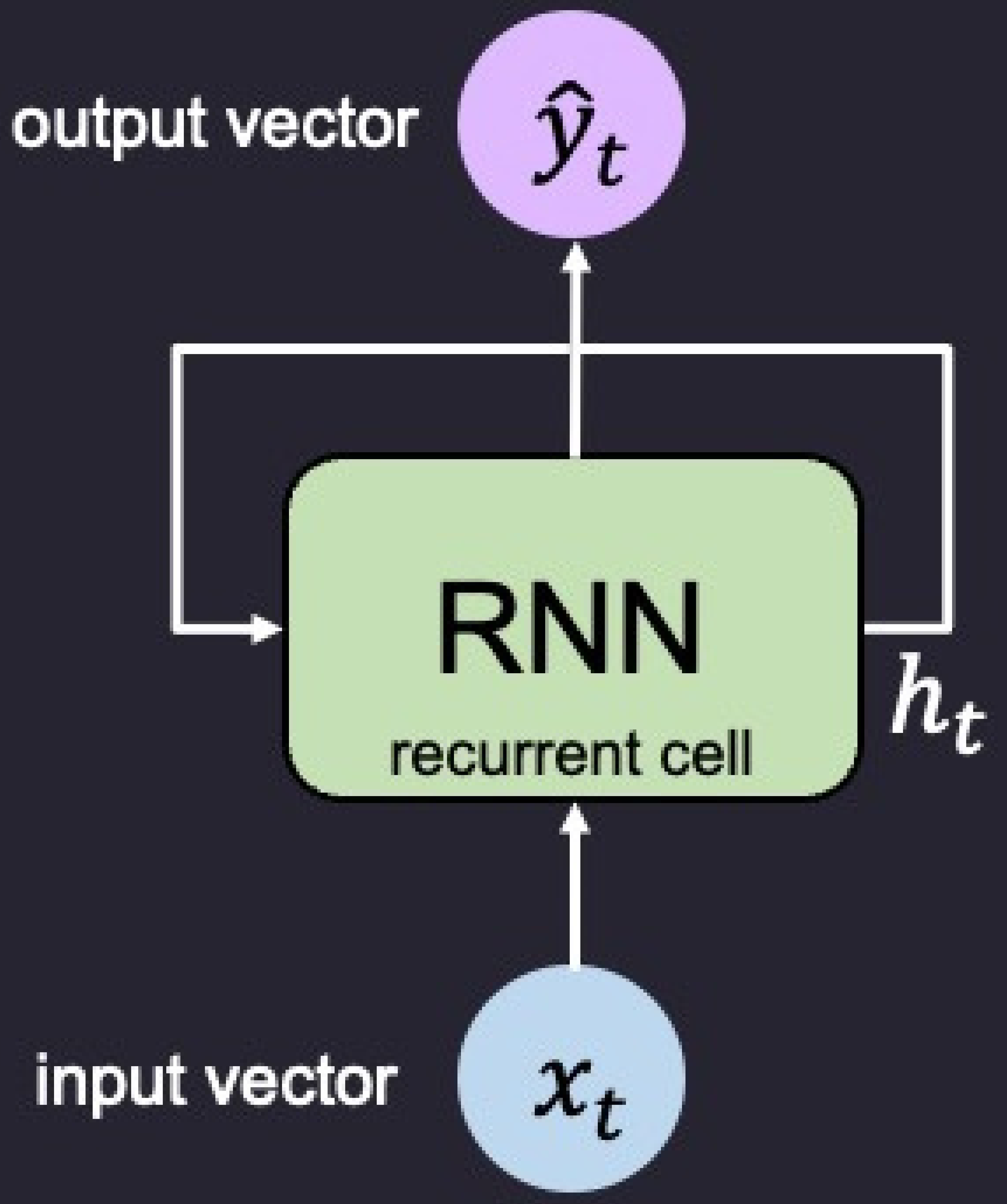
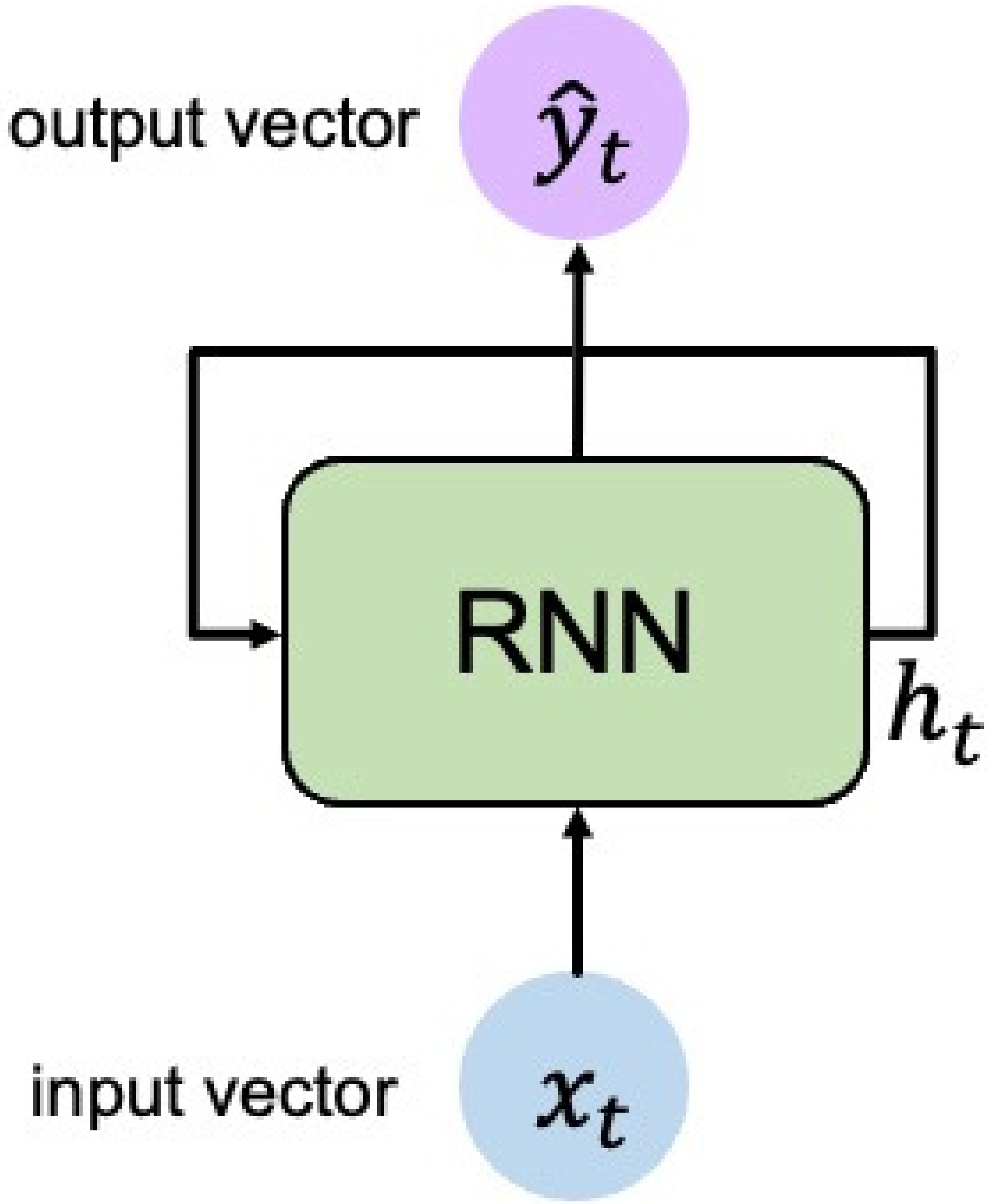


RNN State Update and Output



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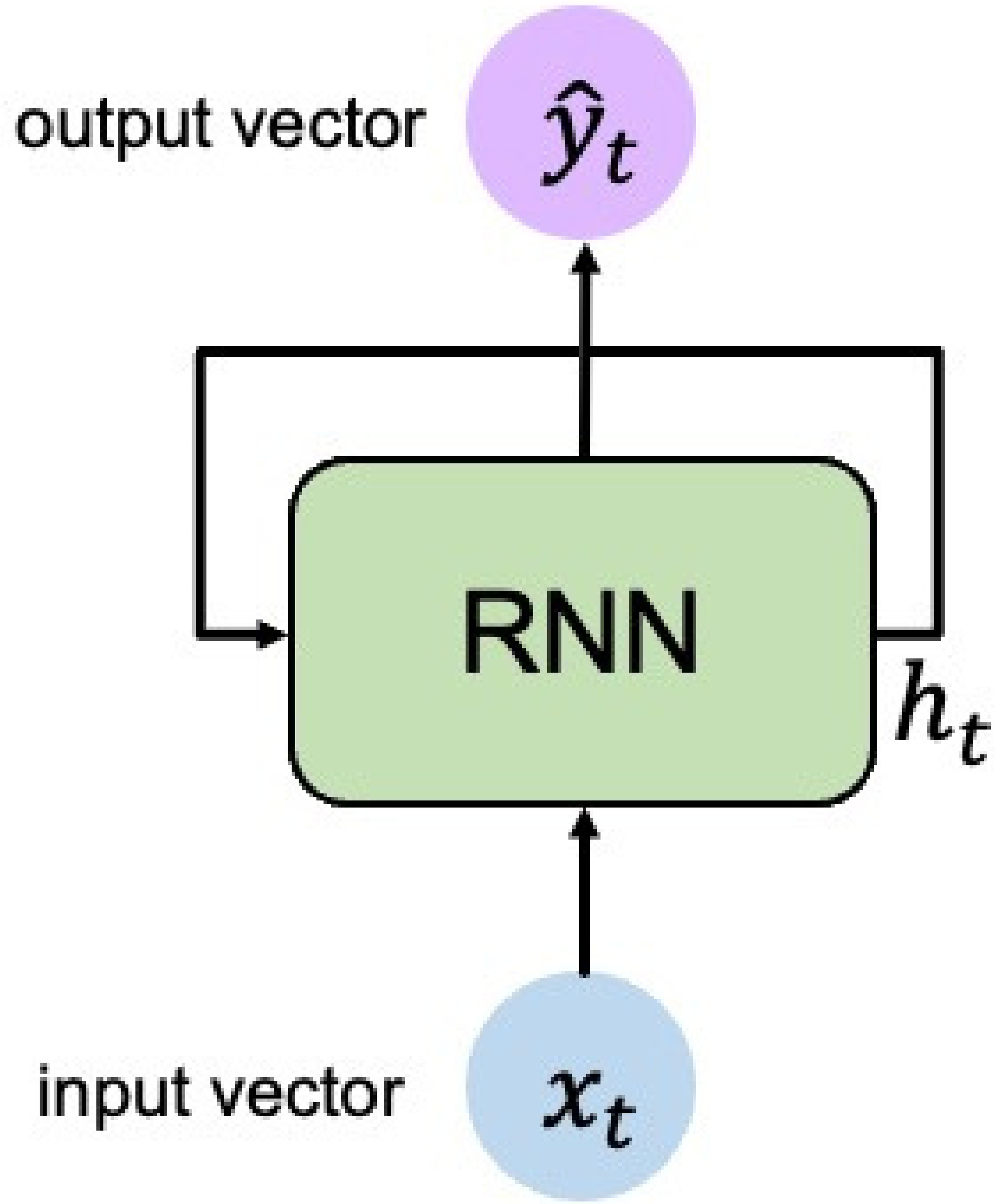
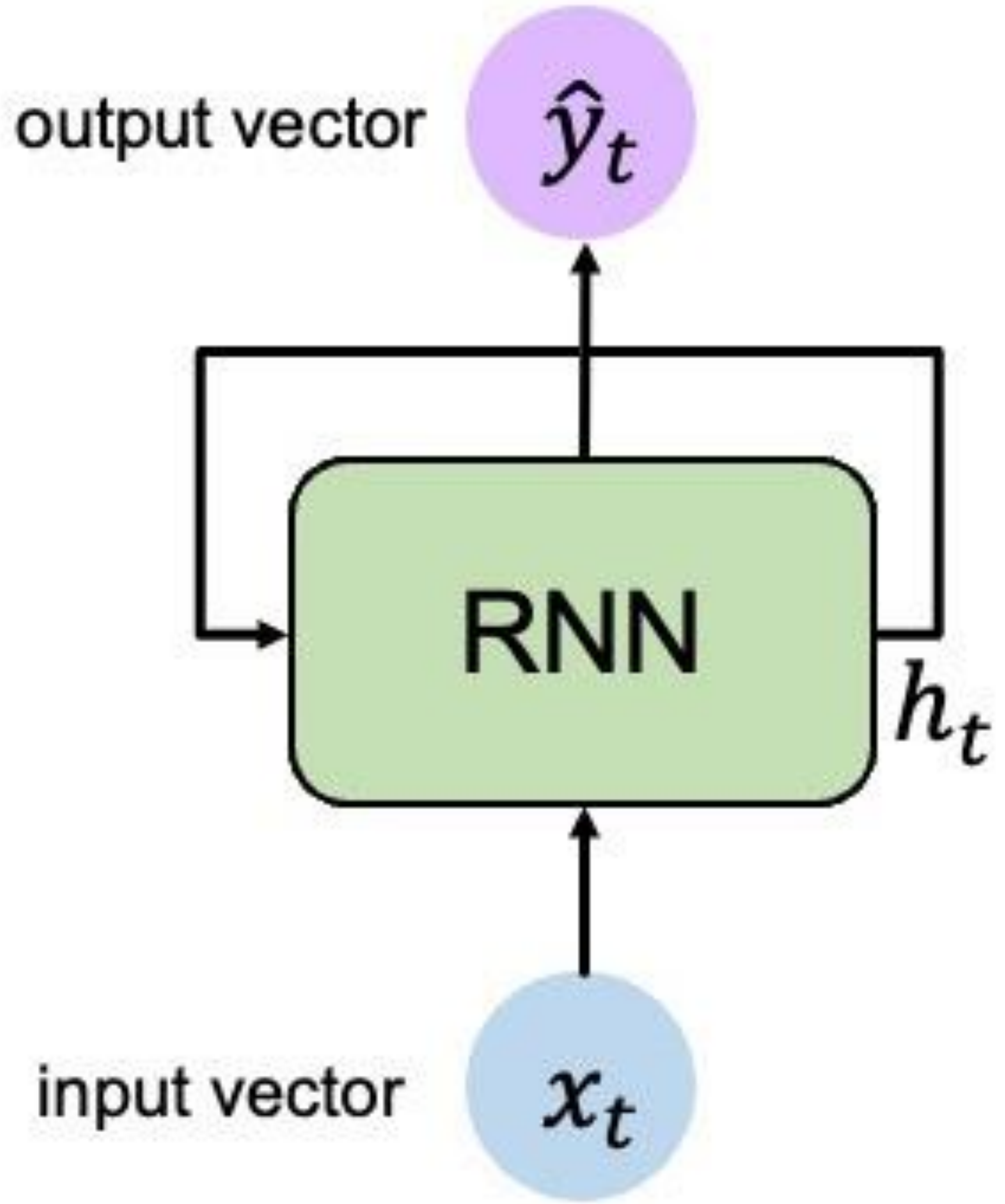


Input Vector

x_t

RNN State Update and Output



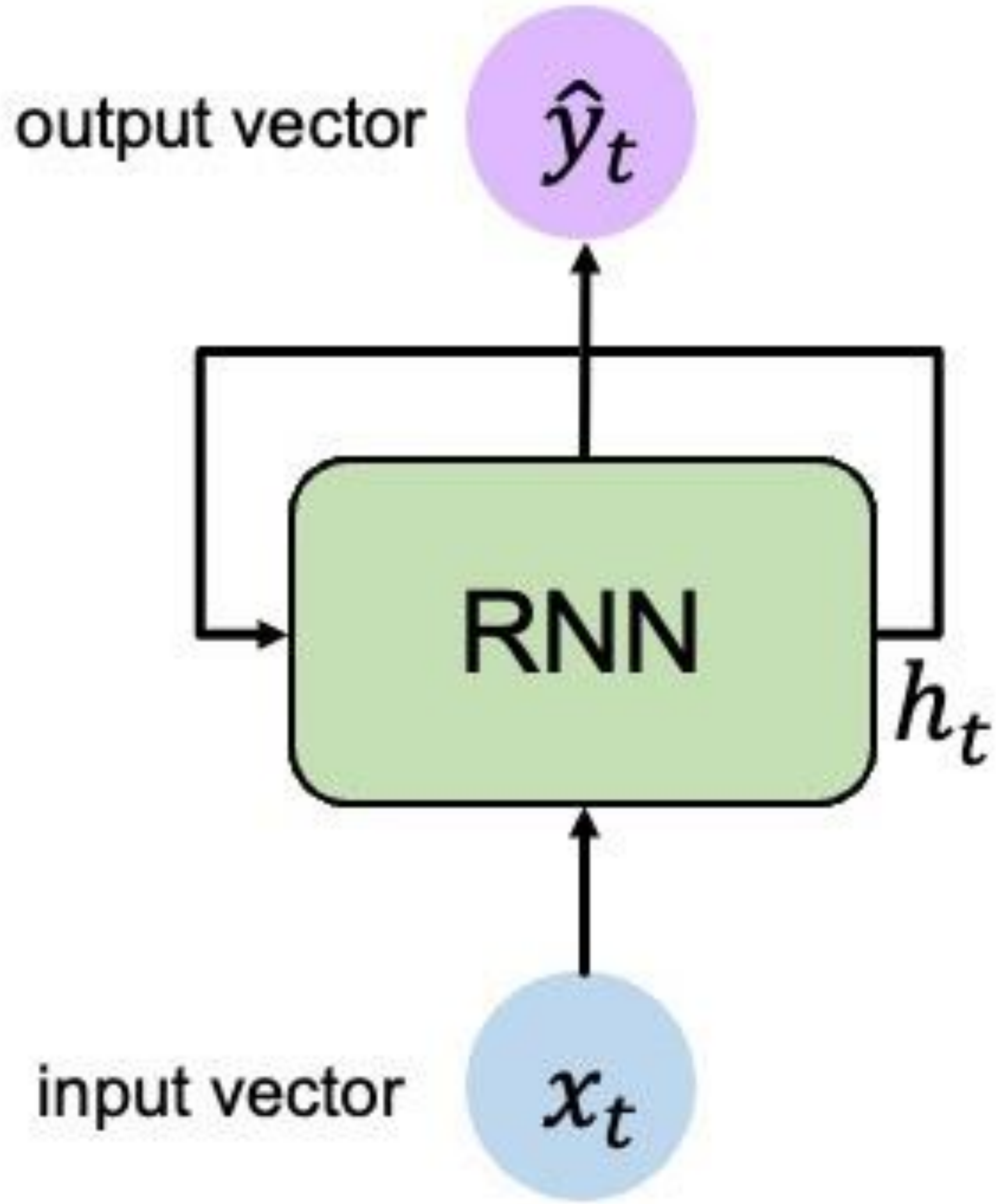
Update Hidden State

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

Input Vector

$$x_t$$

RNN State Update and Output



Output Vector

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

Update Hidden State

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

Input Vector

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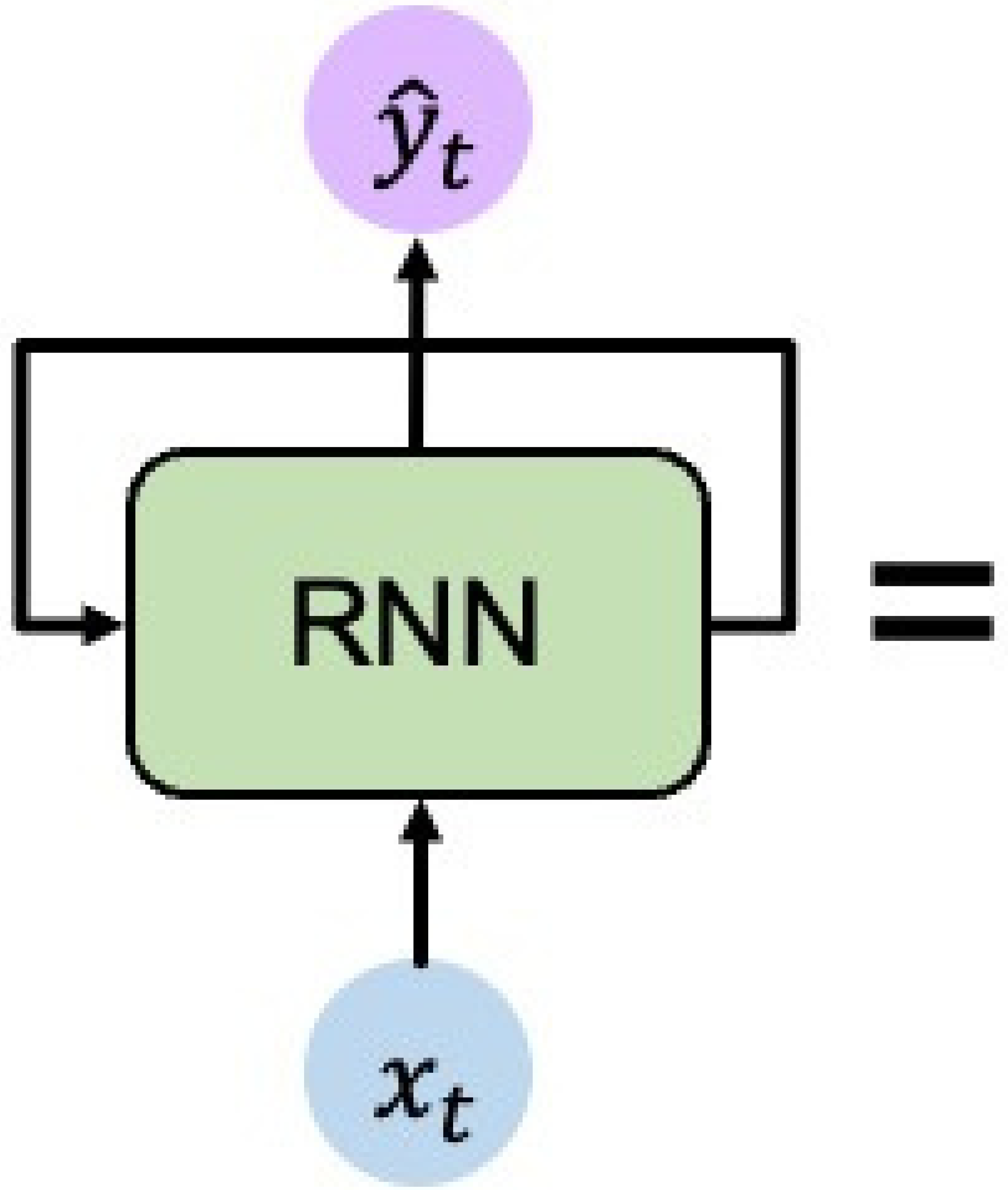
RNNs: Computational Graph Across Time

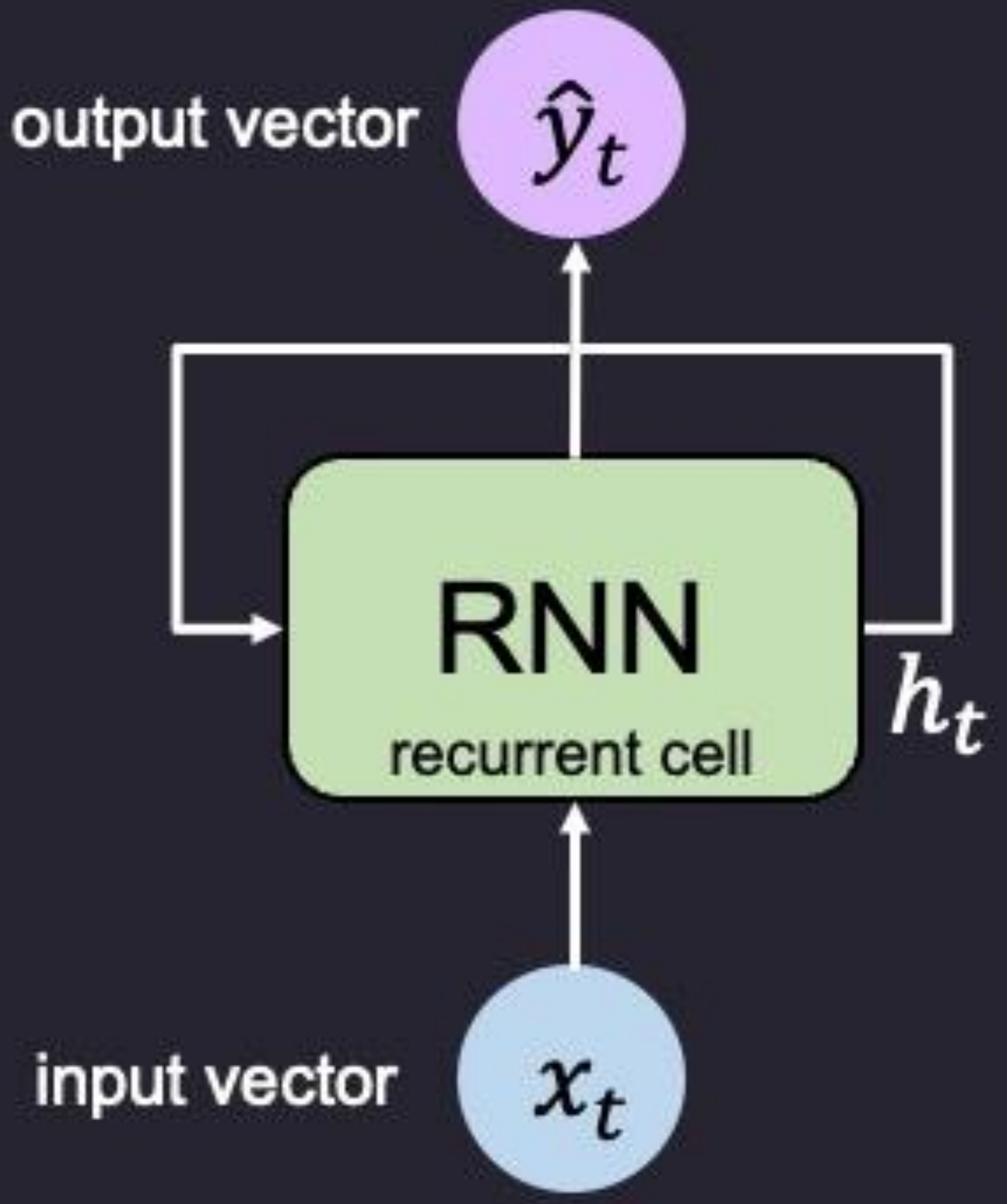


Represent as computational graph unrolled across time

RNNs: Computational Graph Across Time

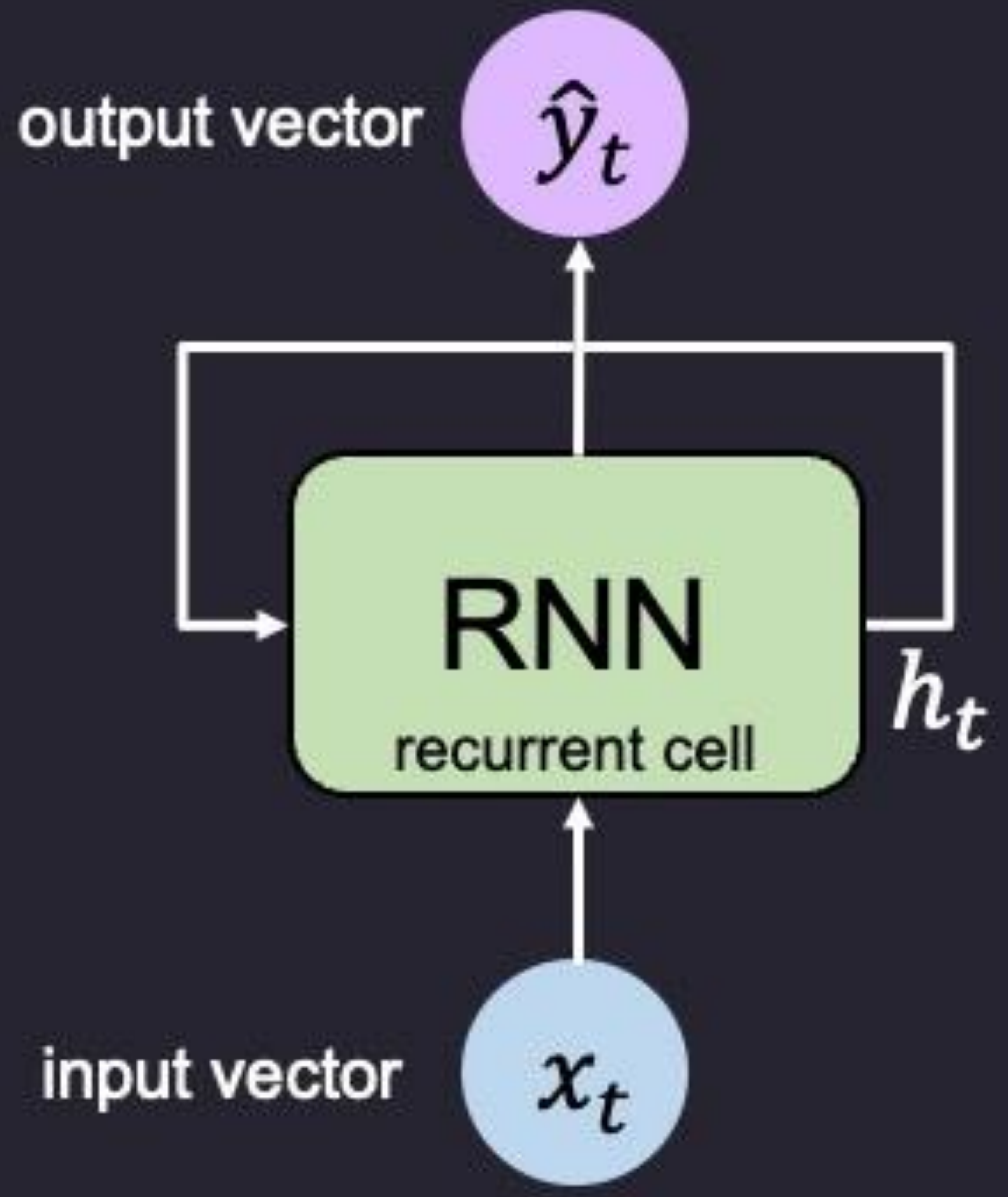
RNNs from Scratch

```
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

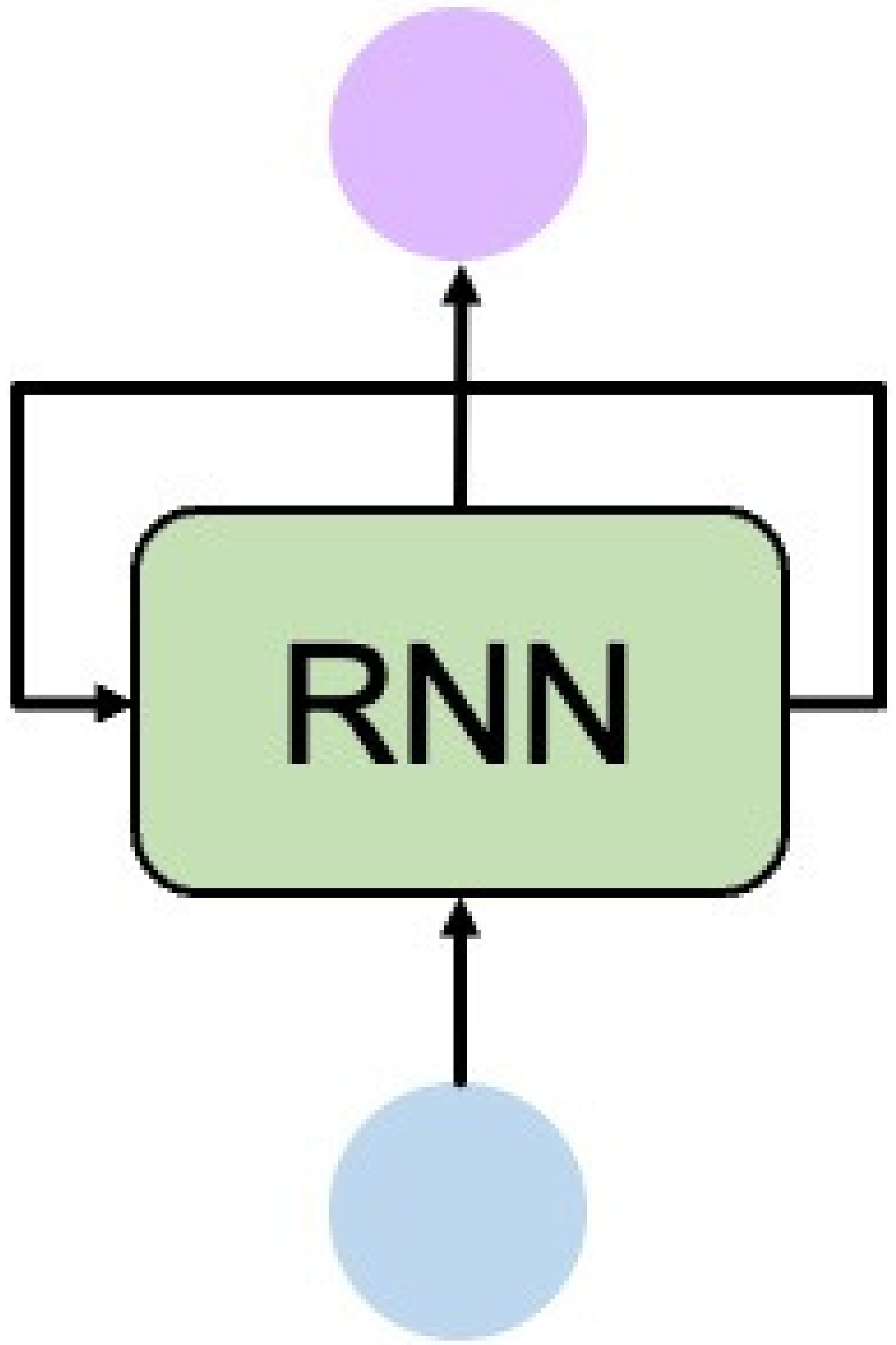
... and many other architectures and applications

6.S191 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

A Sequence Modeling Problem: Predict the Next Word

"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

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predict the next word

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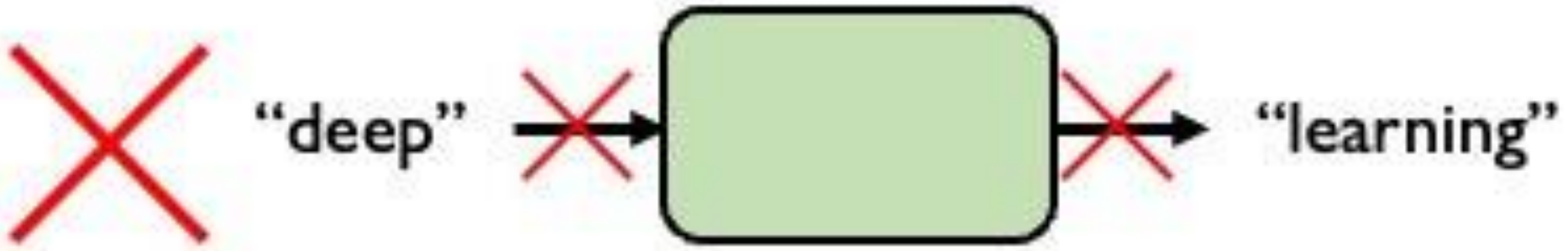
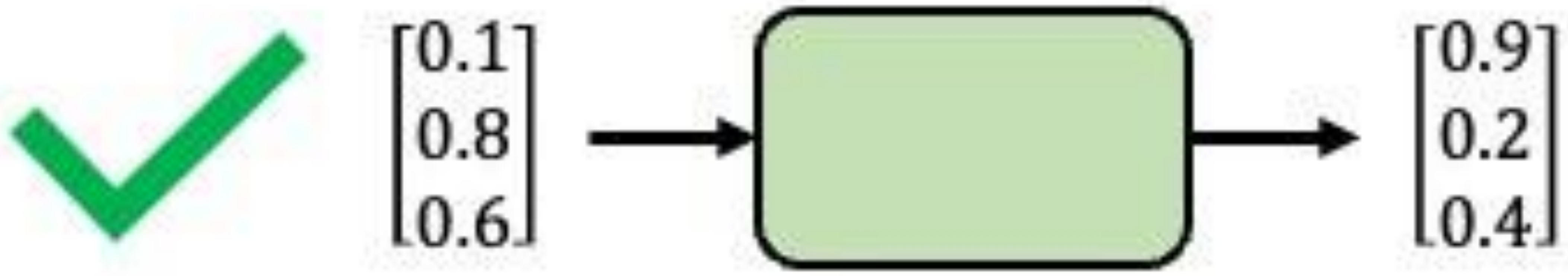
Representing Language to a Neural Network

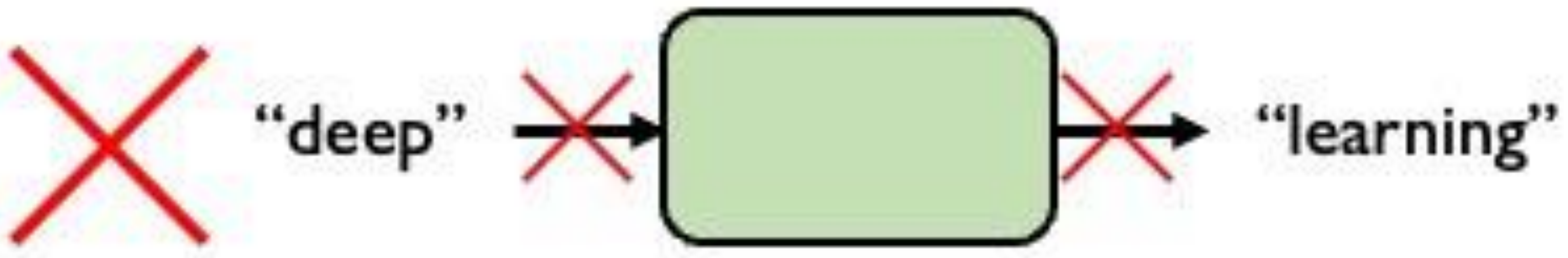


Neural networks cannot interpret words



Neural networks require numerical inputs

Encoding Language for a Neural Network



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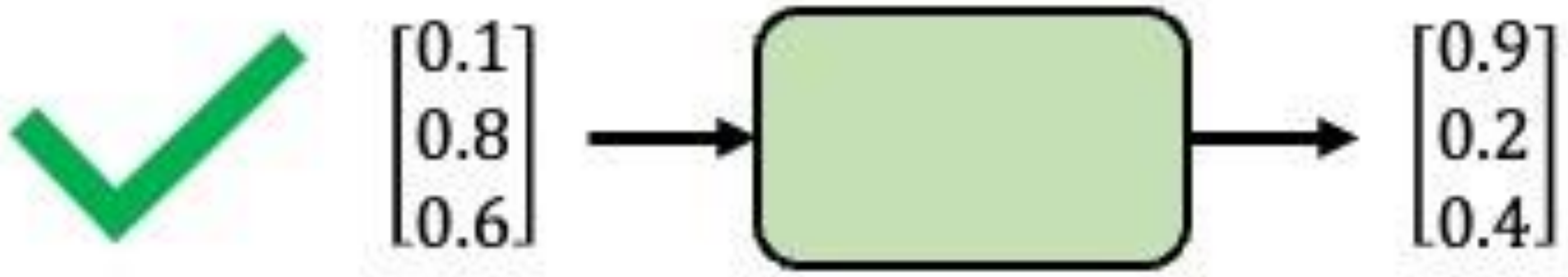
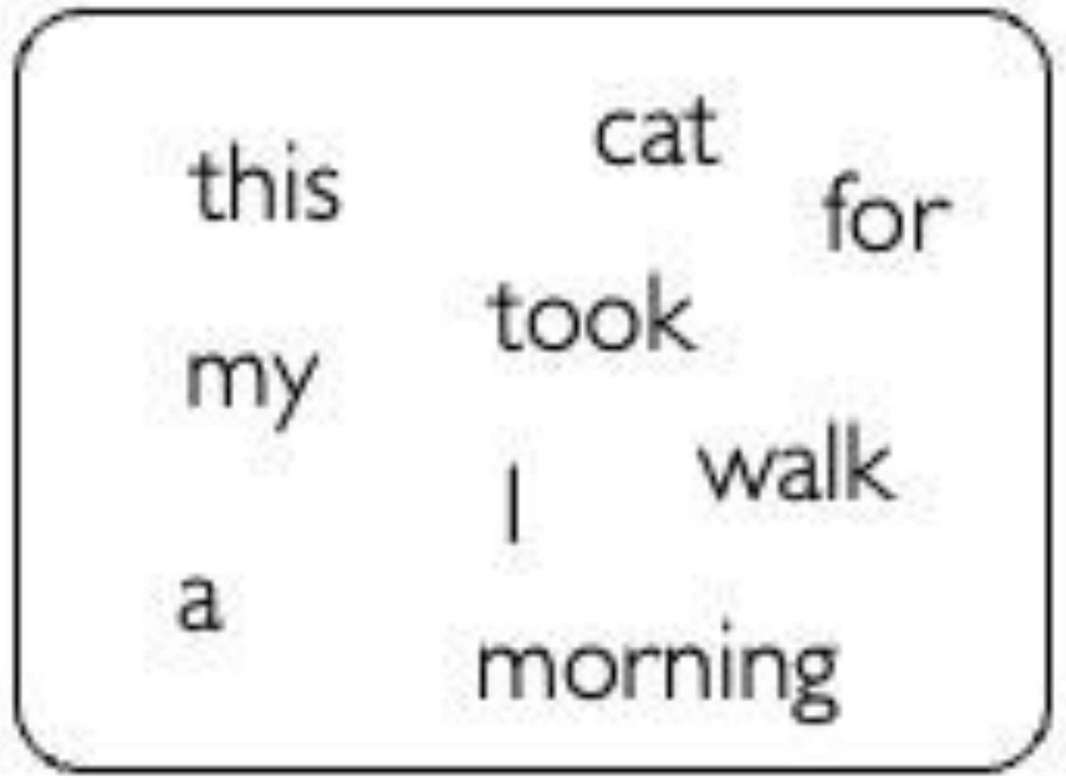
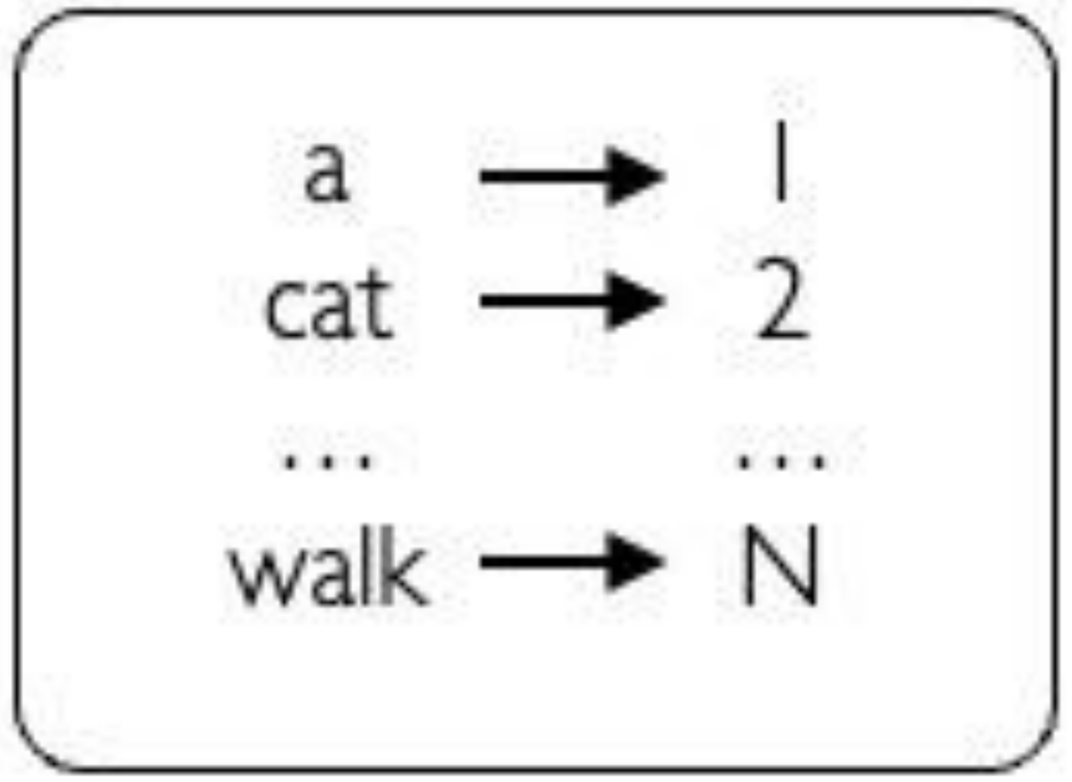


Neural networks require numerical inputs

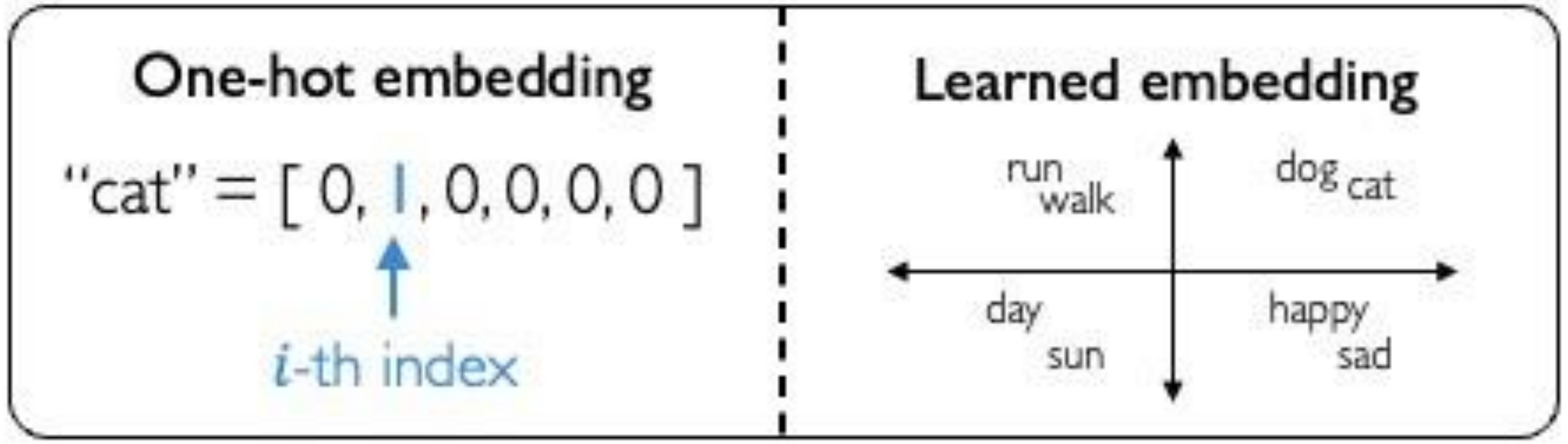
Embedding: transform indexes into a vector of fixed size.



1. Vocabulary:
Corpus of words



2. Indexing:
Word to index



3. Embedding:
Index to fixed-sized vector

Handle Variable Sequence Lengths

The food was <u>great</u>

vs.

We visited a restaurant for <u>lunch</u>

vs.

We were hungry but cleaned the house before <u>eating</u>

Model Long-Term Dependencies

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

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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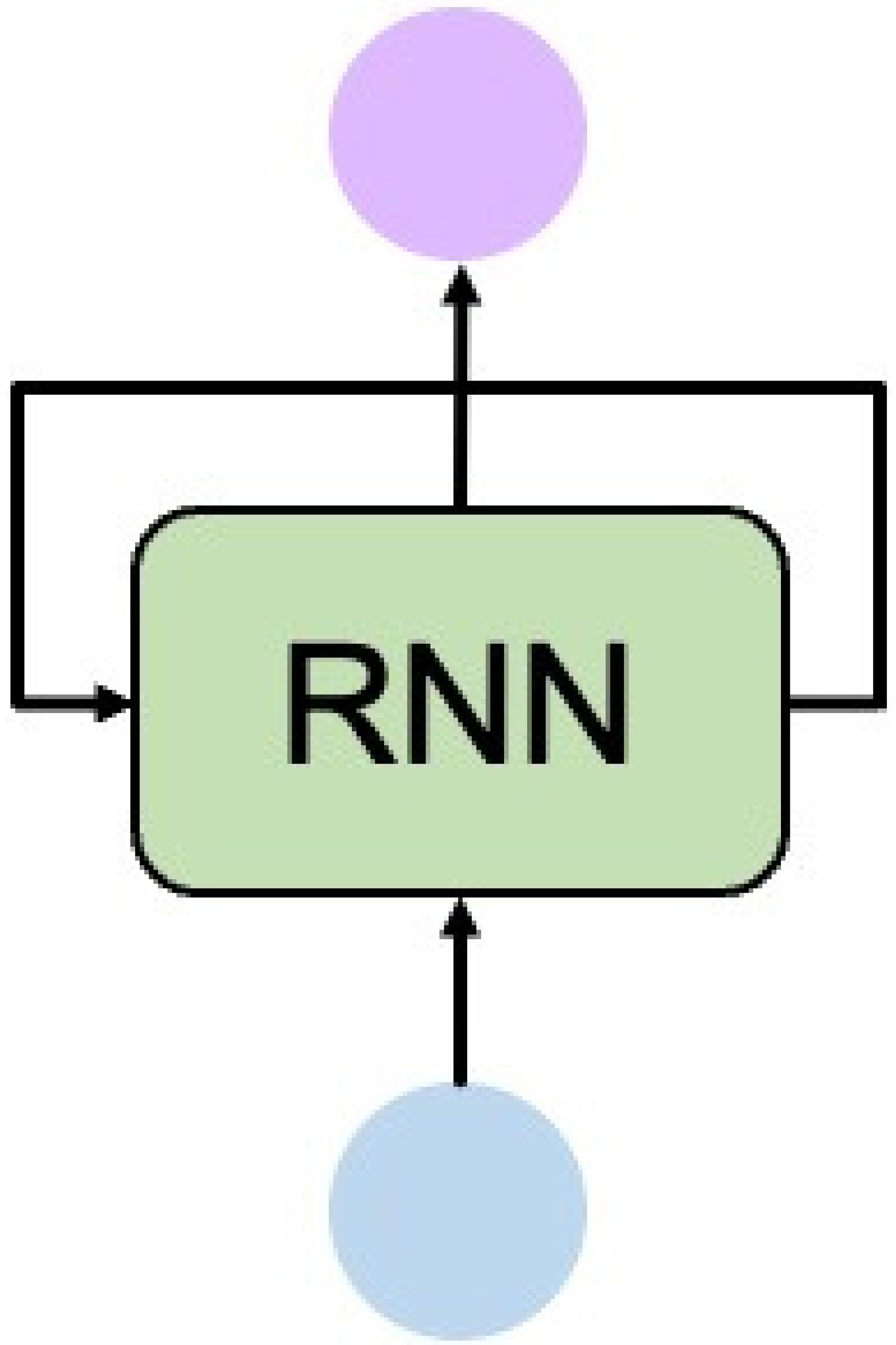
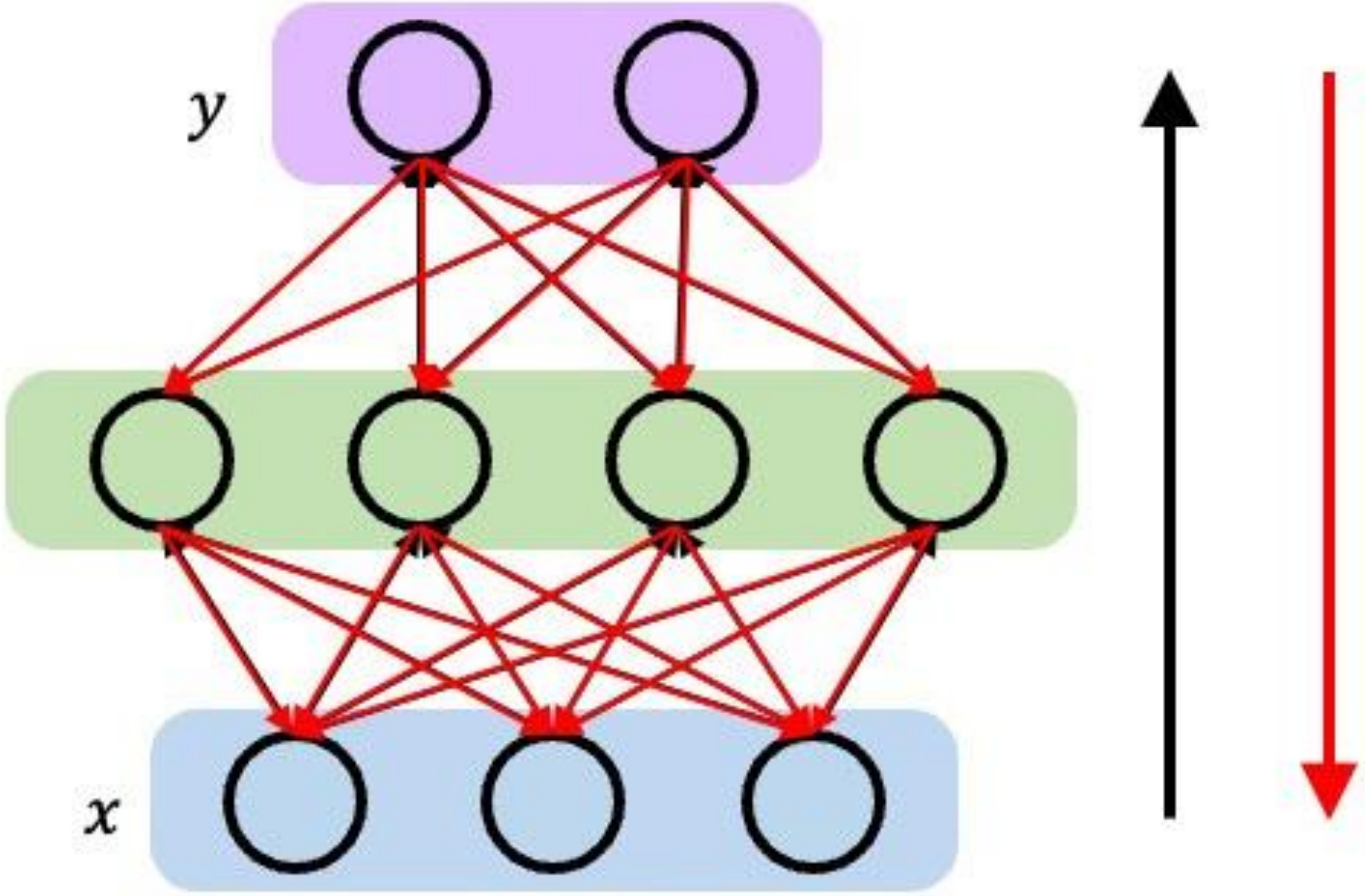


Recurrent Neural Networks (RNNs) meet these sequence modeling design criteria

Backpropagation Through Time (BPTT)

Recall: Backpropagation in Feed Forward Models



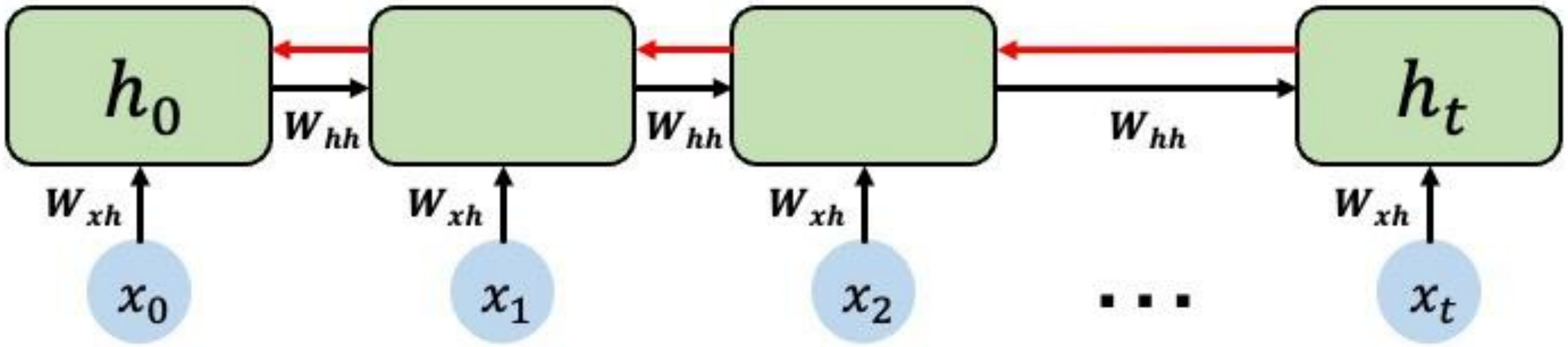
Backpropagation algorithm:

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

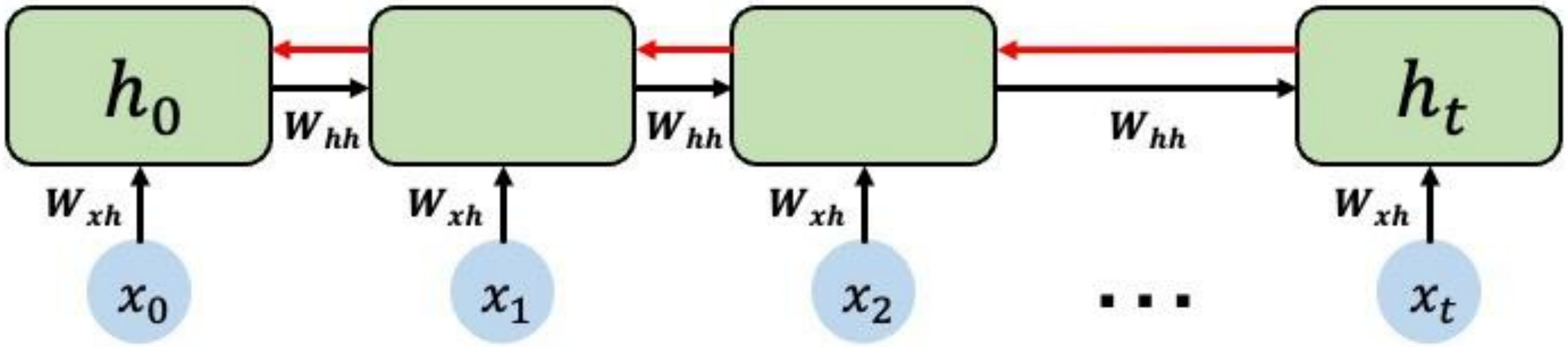
RNNs: Backpropagation Through Time

RNNs: Backpropagation Through Time

Standard RNN Gradient Flow

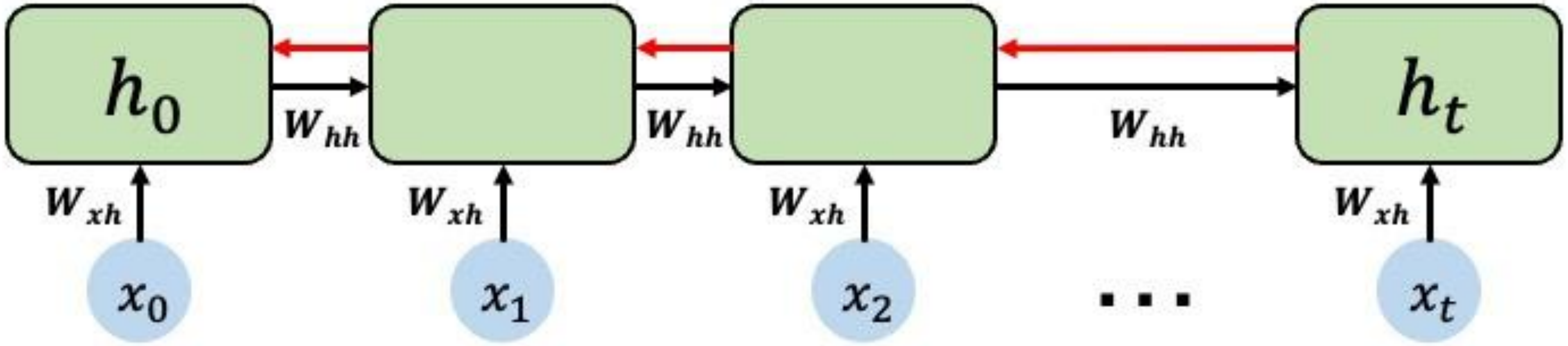


Standard RNN Gradient Flow



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

Standard RNN Gradient Flow: Exploding Gradients

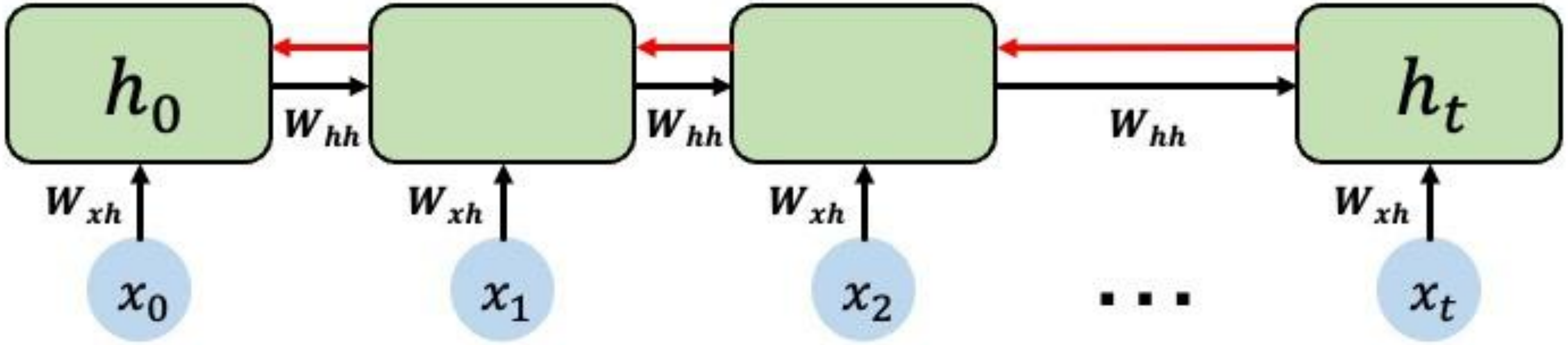


Computing the gradient wrt h_0 involves **many factors of** W_{hh} + **repeated gradient computation**!

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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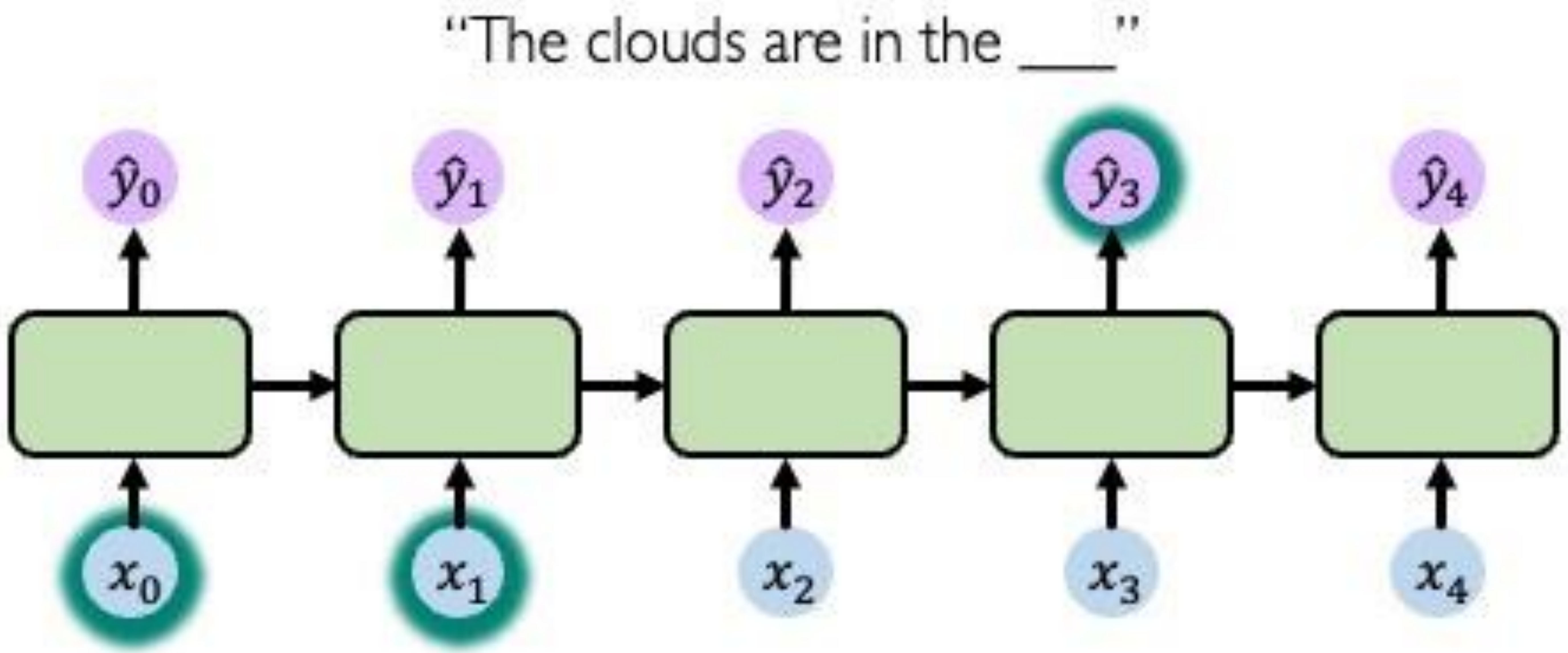

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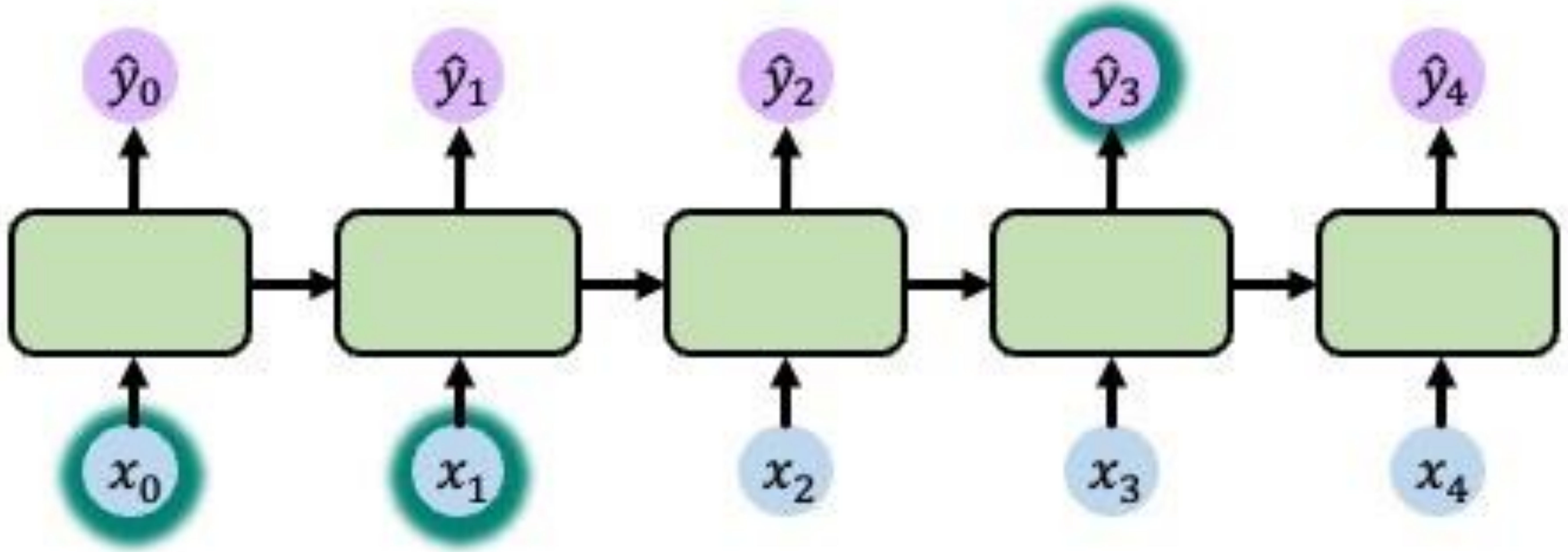

"I grew up in France, … and I speak fluent___ "

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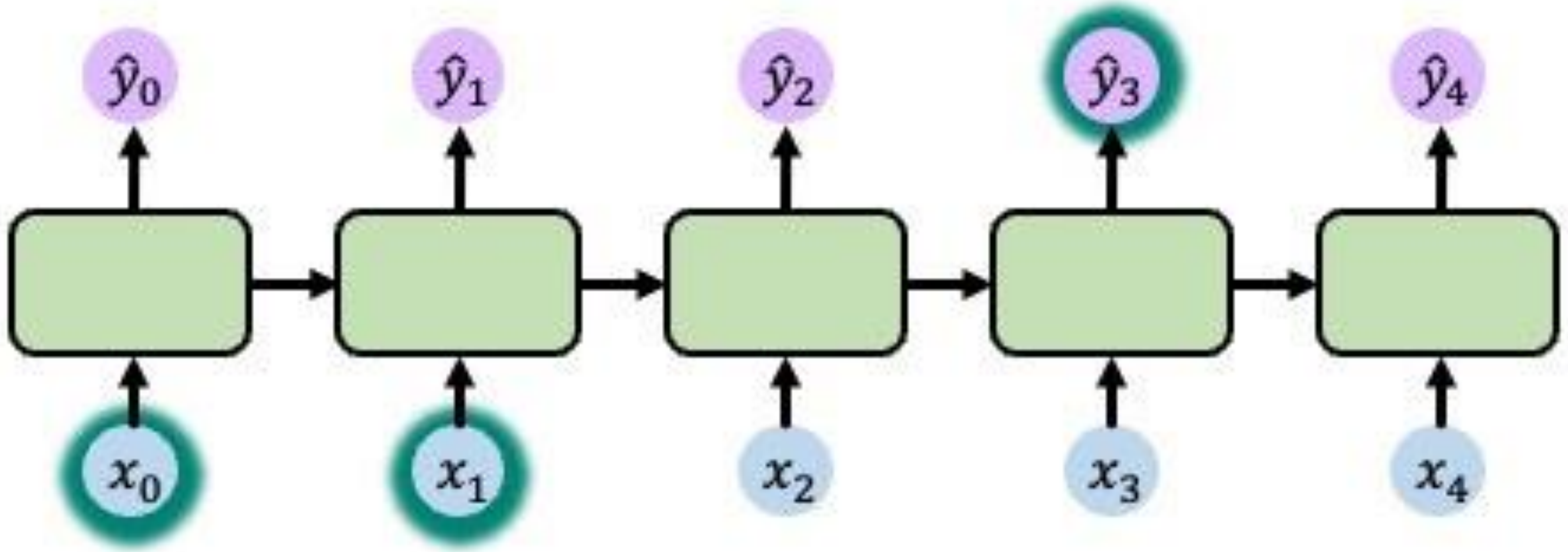

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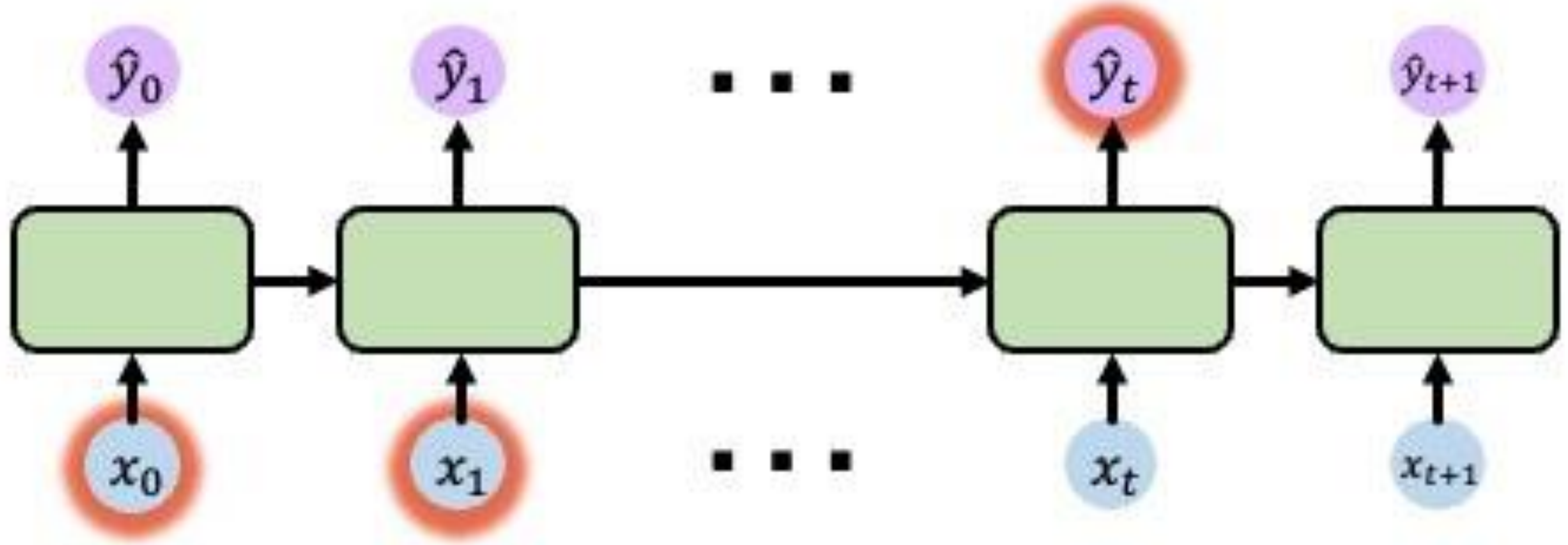
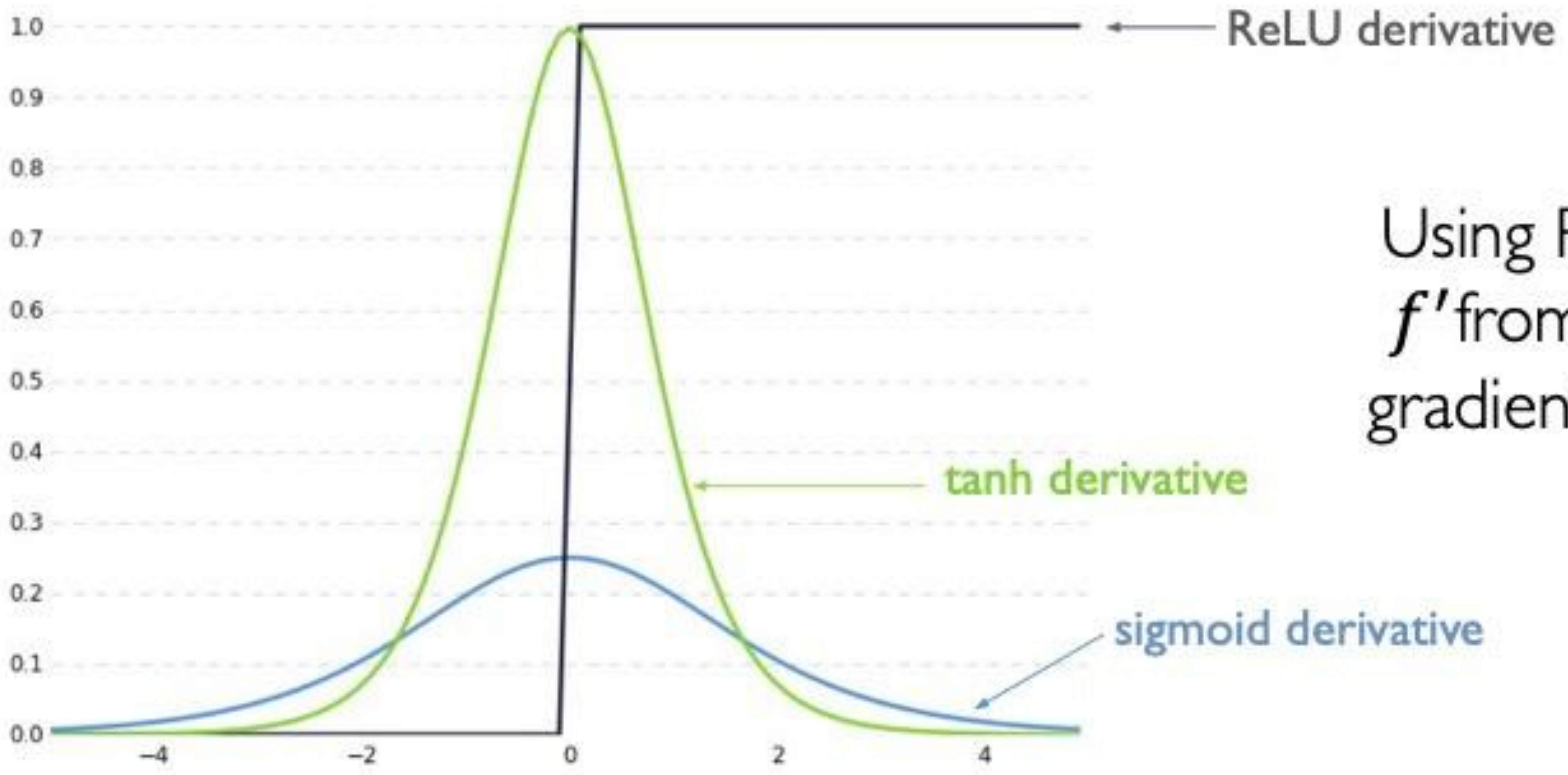


Trick #1: Activation Functions



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

Trick #2: Parameter Initialization

Initialize **weights** to identity matrix

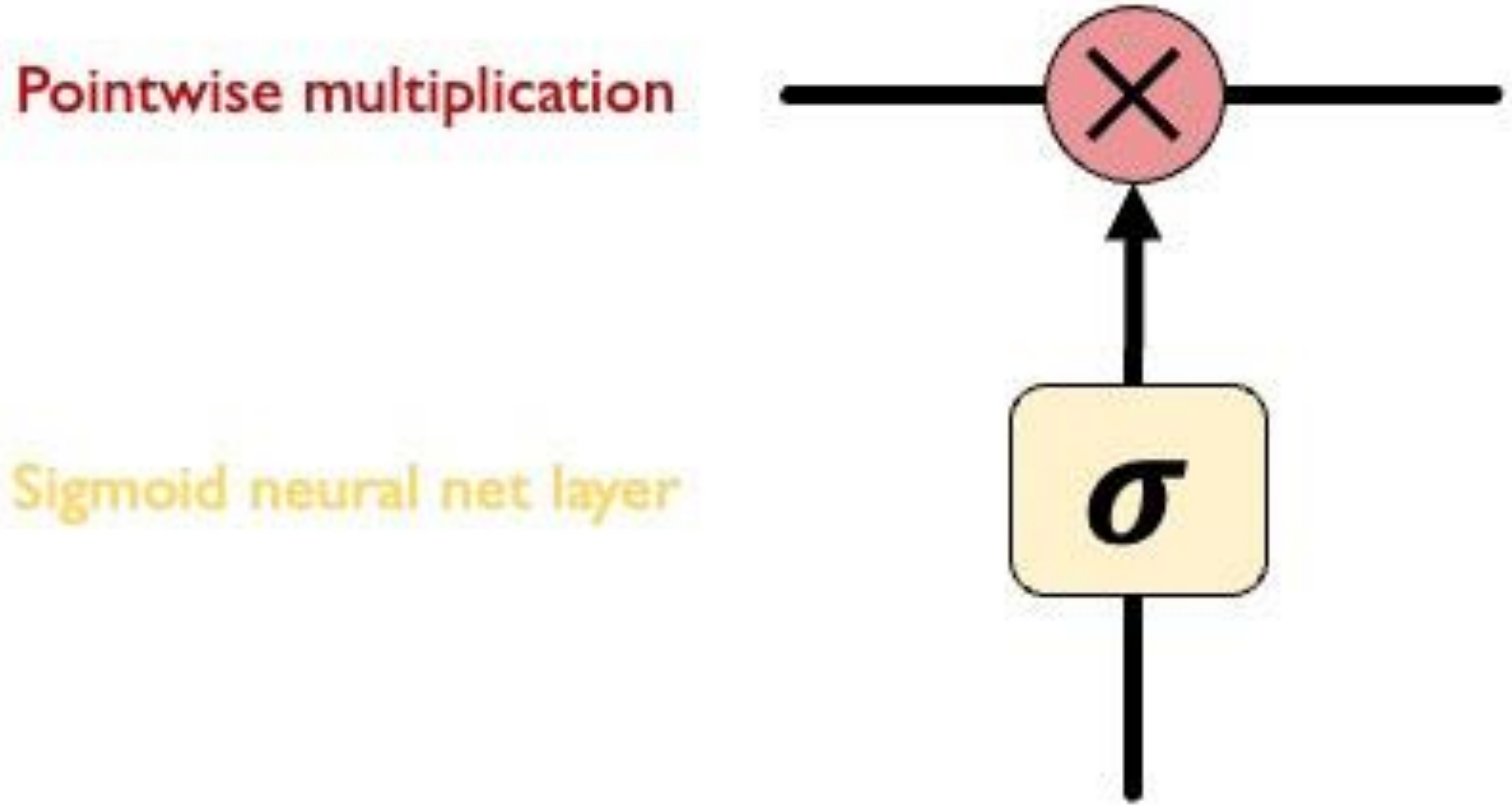
Initialize **biases** to zero

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

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**



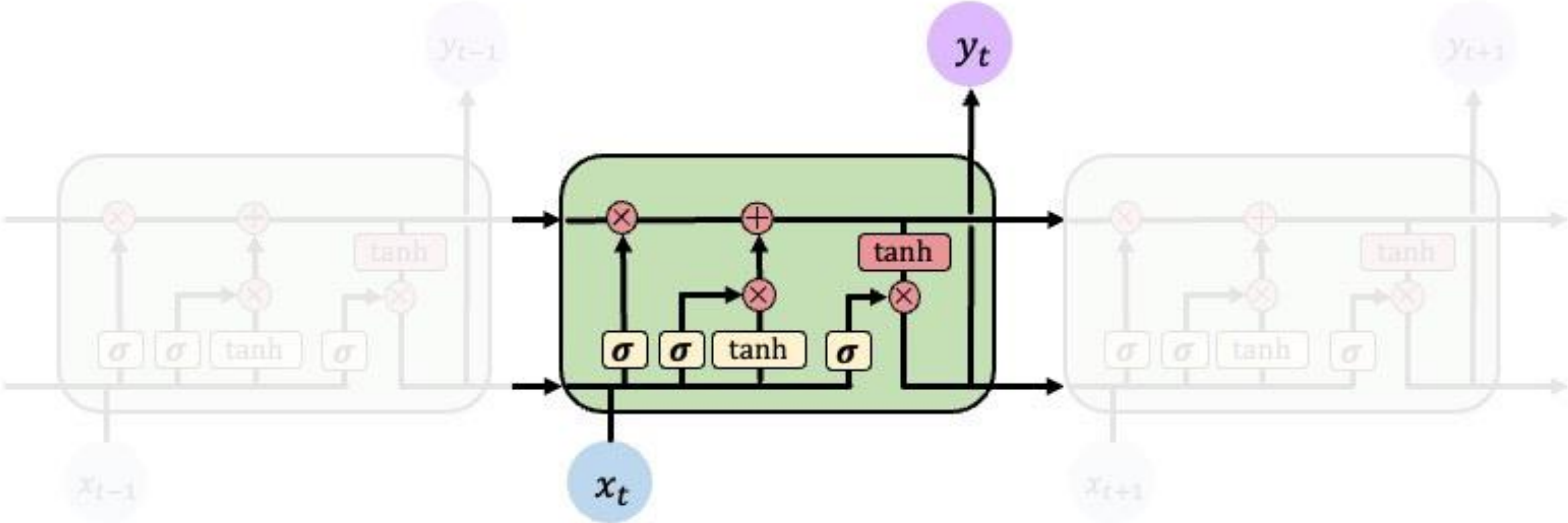
Gates optionally let information through the cell

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

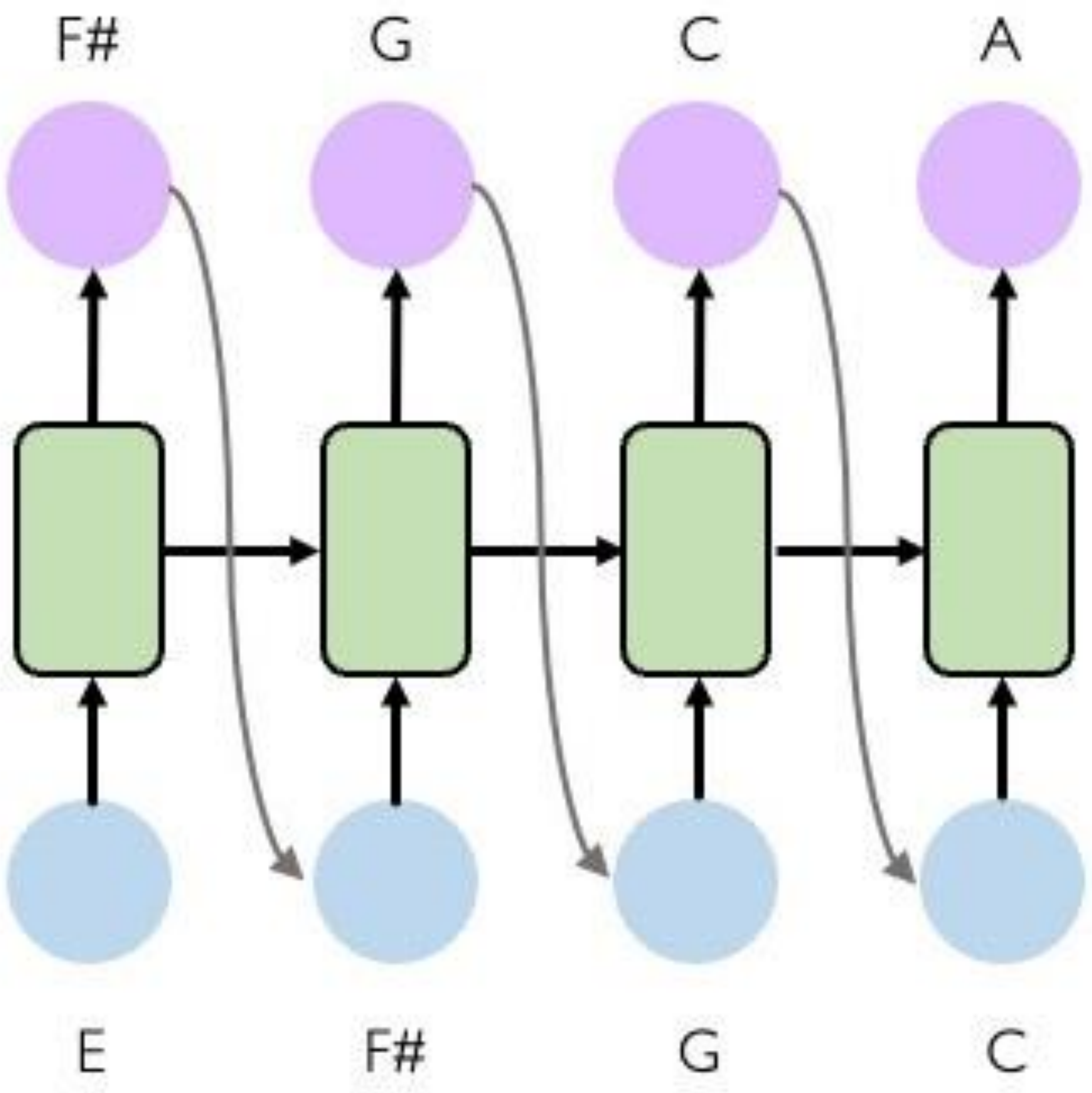
```
tf.keras.layers.LSTM(num_units)
```

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

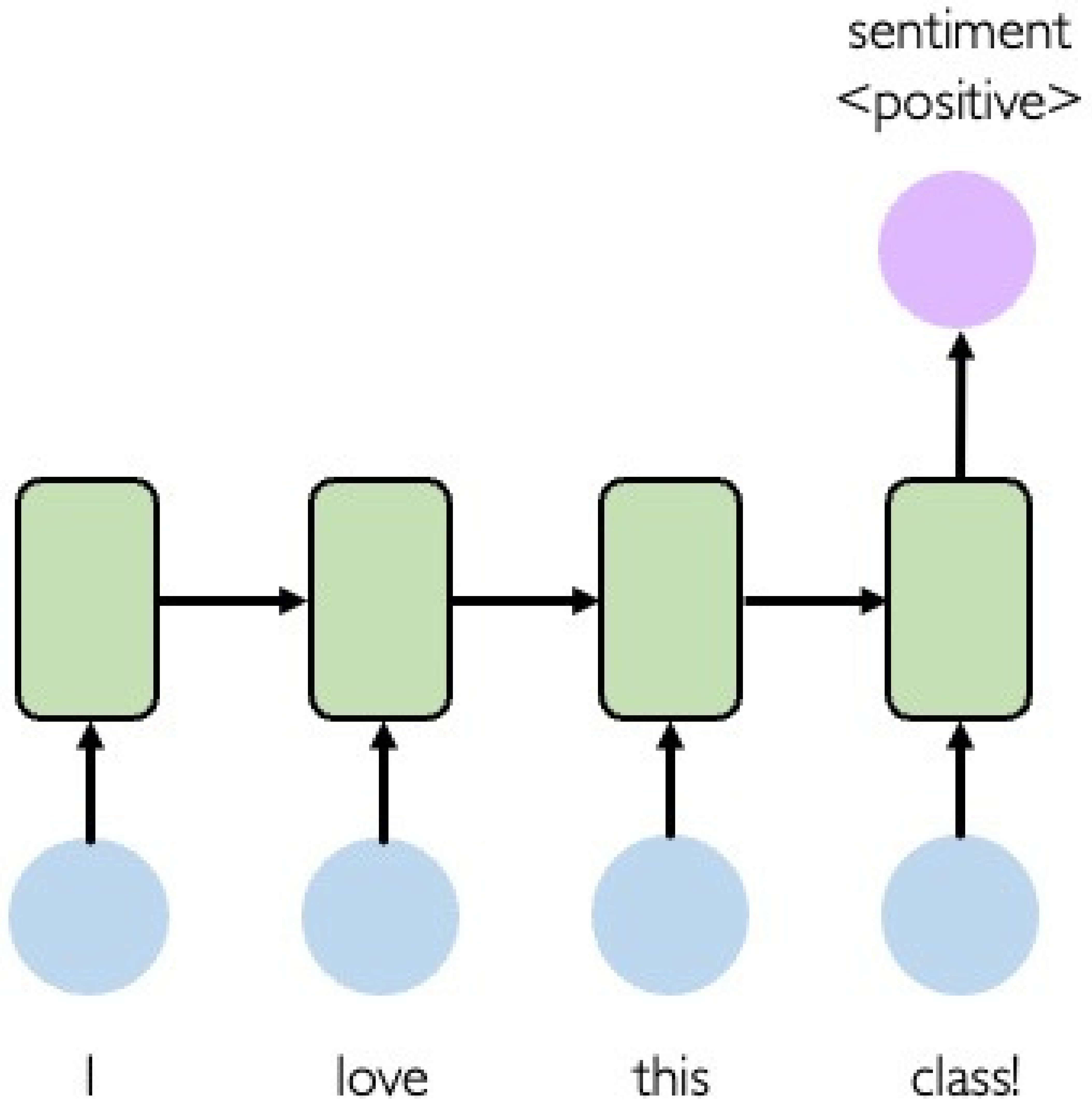
Example Task: Music Generation



Input: sheet music

Output: next character in sheet music

Example Task: Sentiment Classification

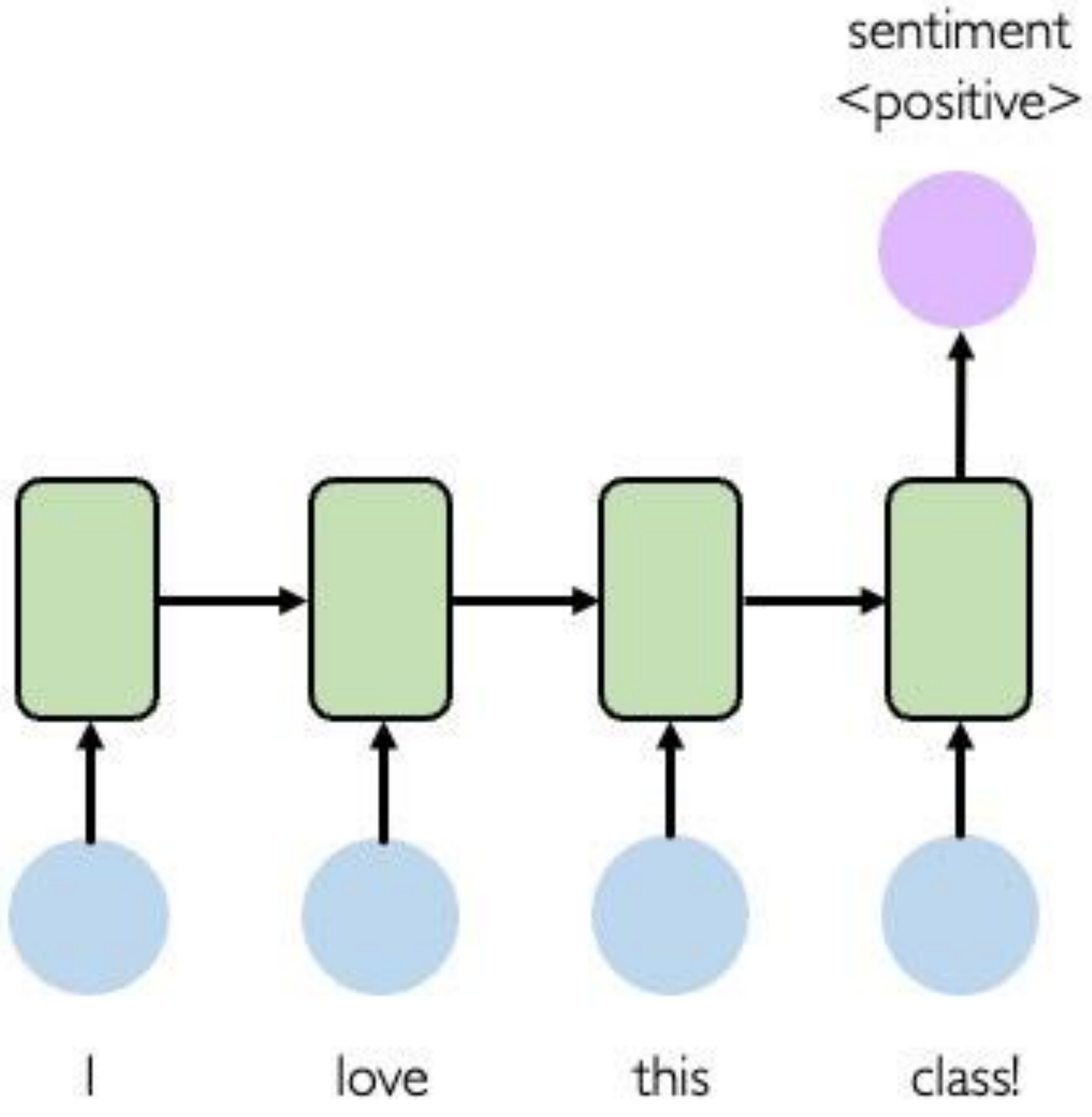


Input: sequence of words

Output: probability of having positive sentiment

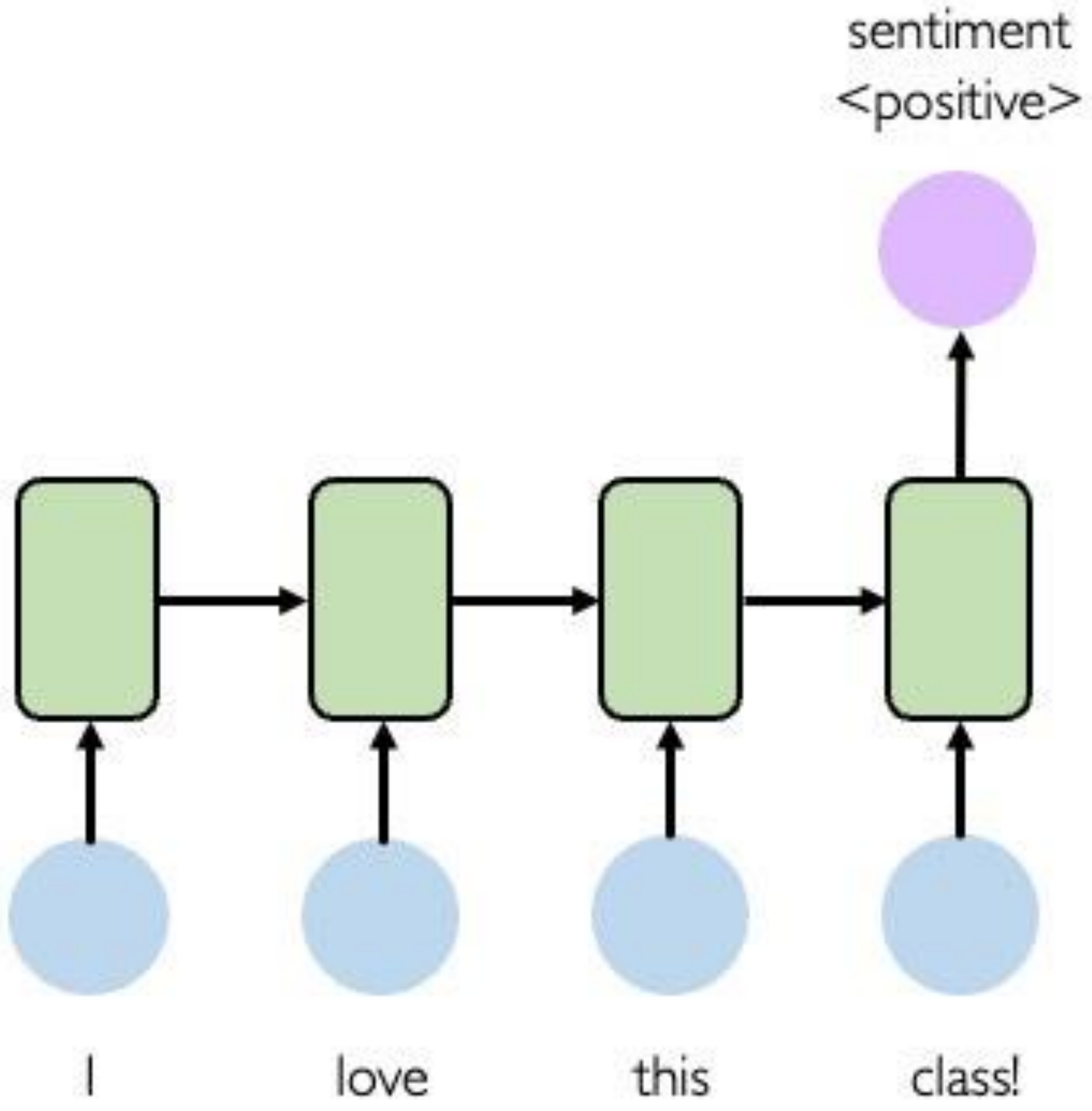
```
loss = tf.nn.softmax_cross_entropy_with_logits(y, predicted)
```

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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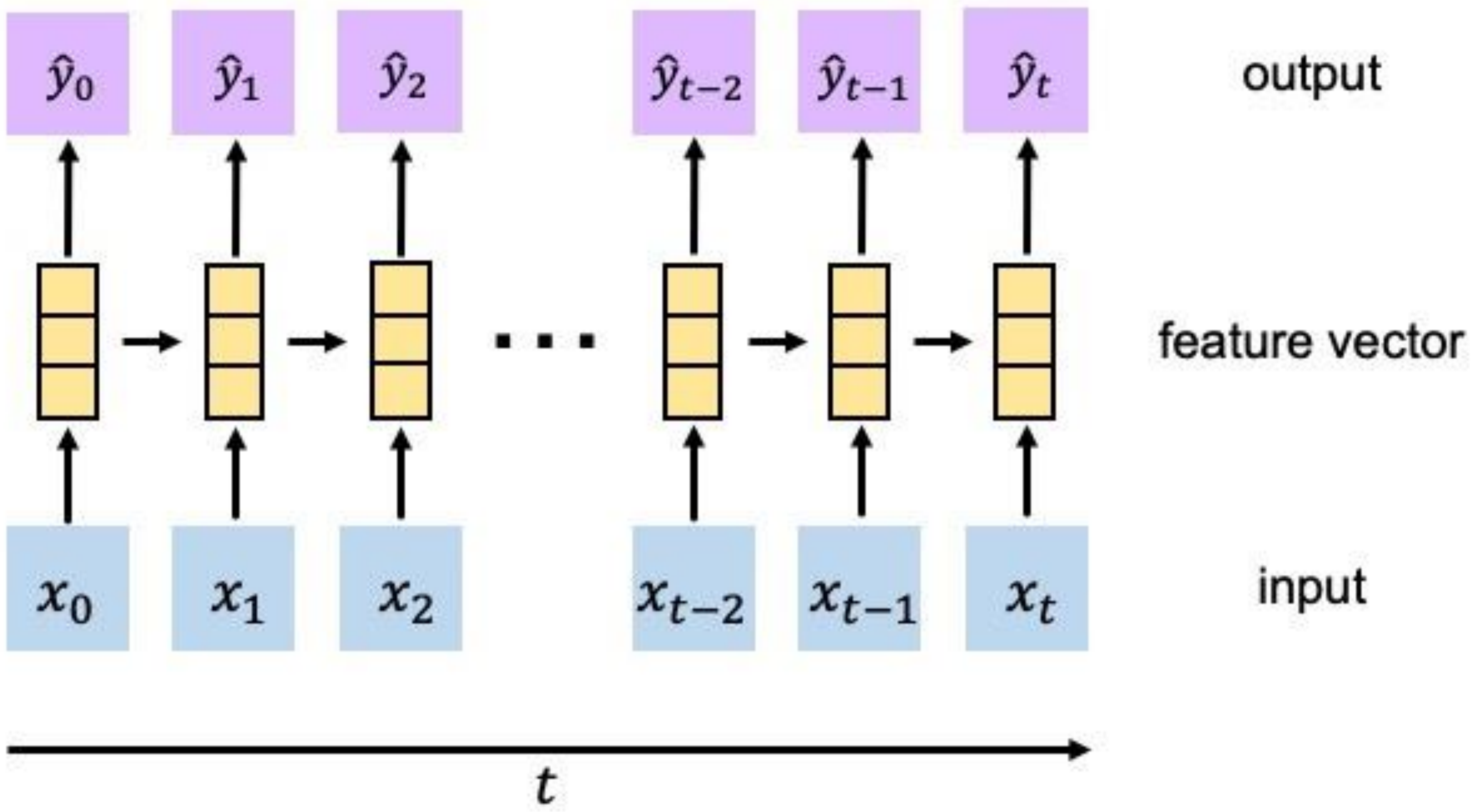


Goal of Sequence Modeling

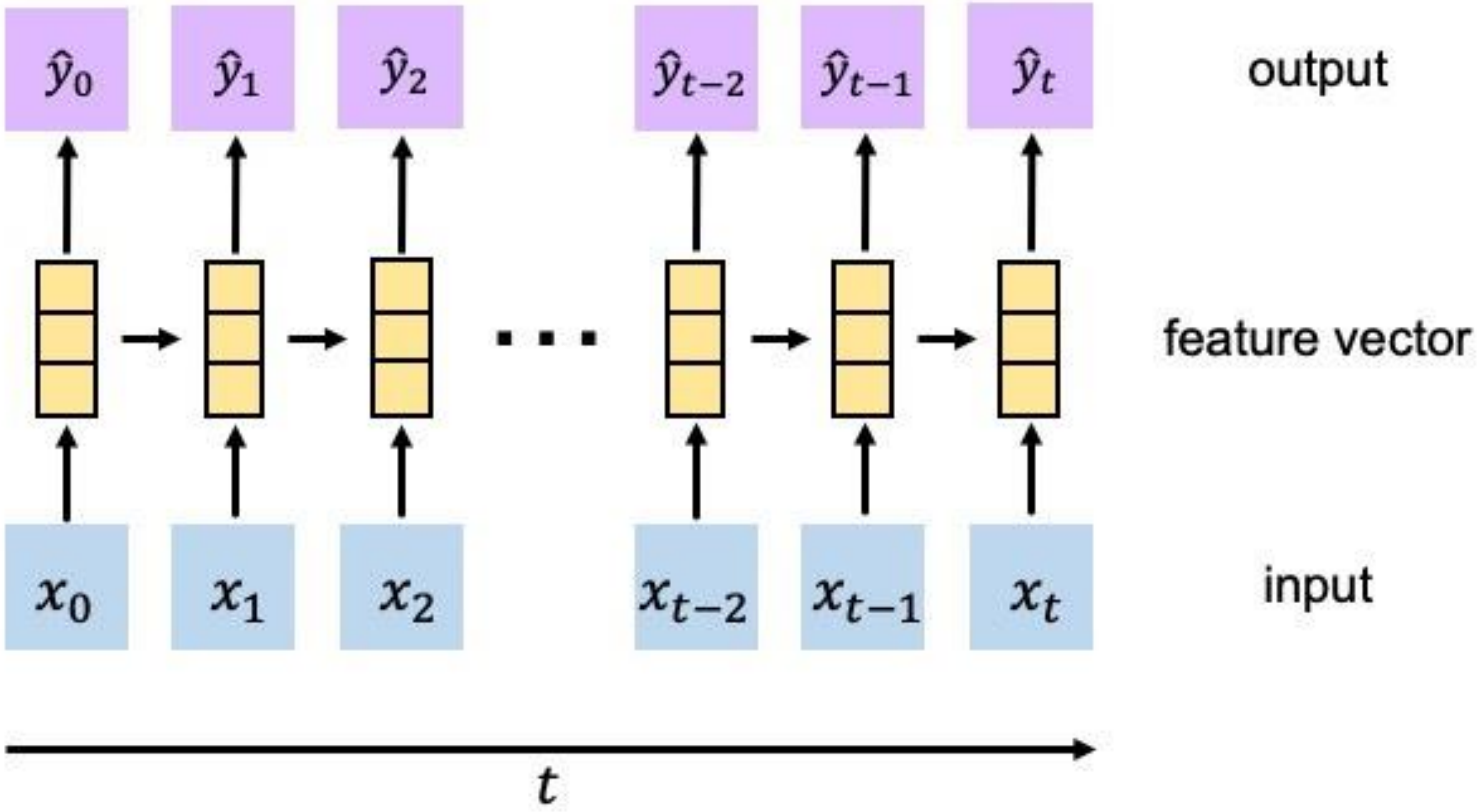
Can we eliminate the need for recurrence entirely?

Desired Capabilities


Continuous stream


Parallelization


Long memory



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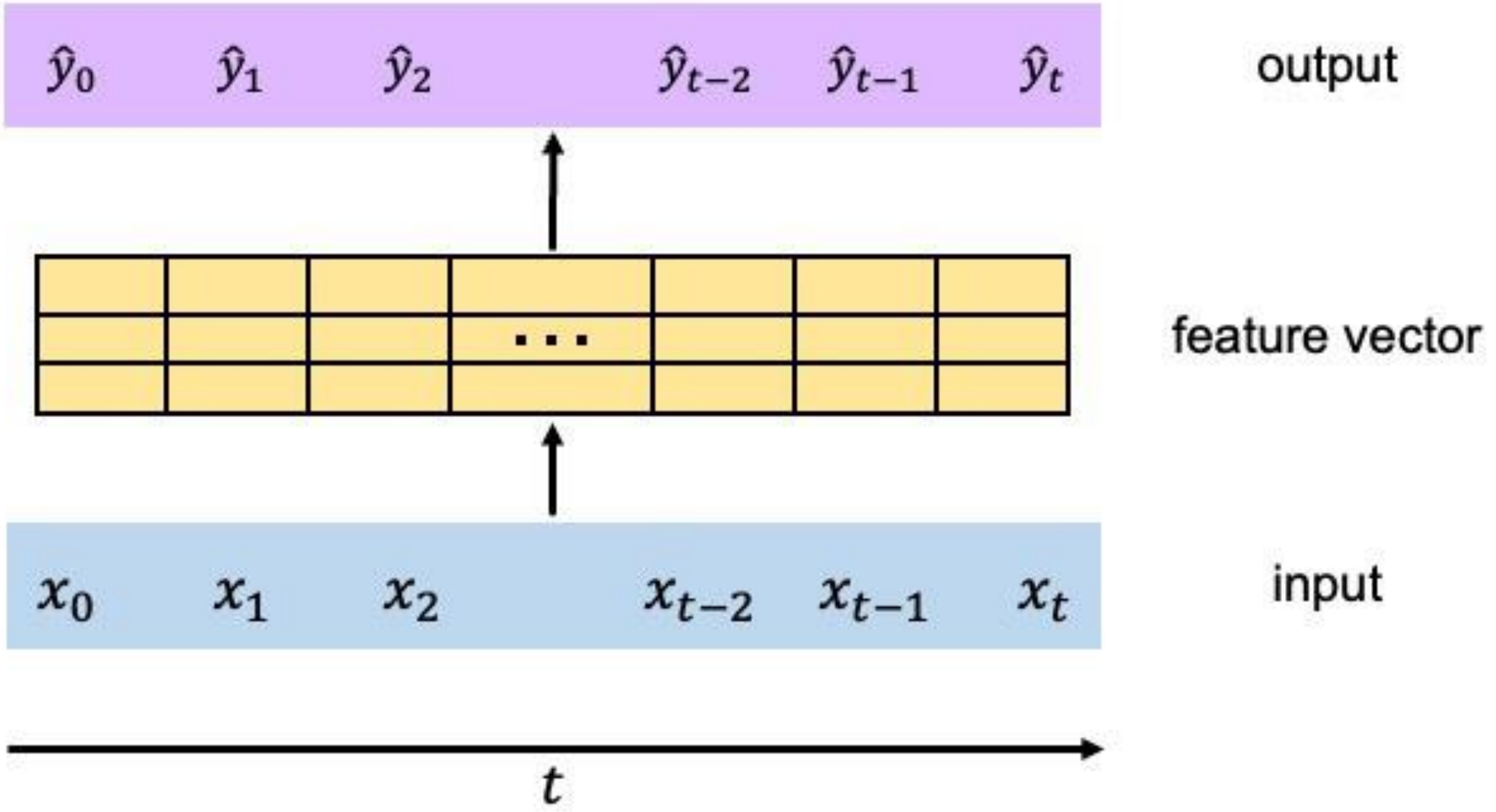
- Continuous stream
- Parallelization
- Long memory



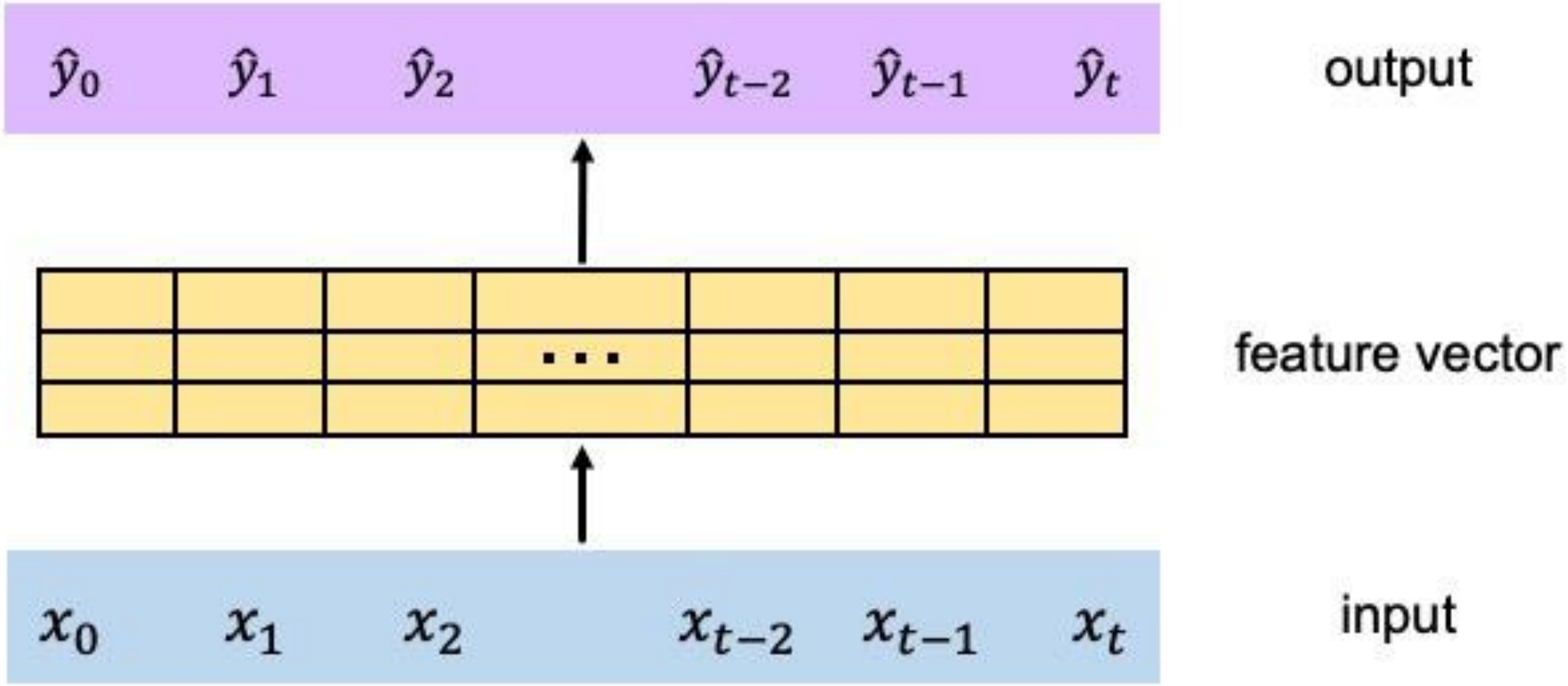
Goal of Sequence Modeling

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

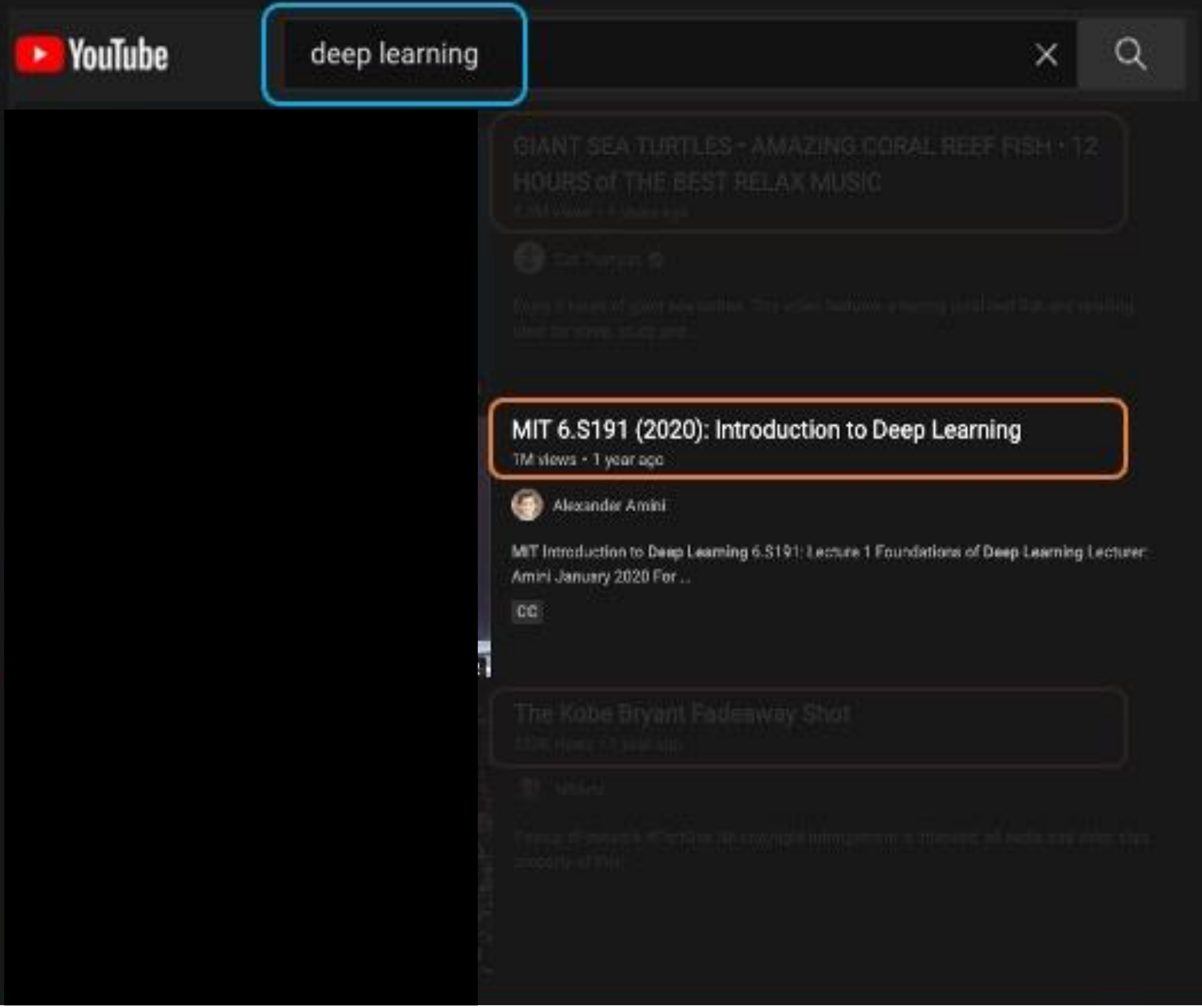
Attending to the most important parts of an input.

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)

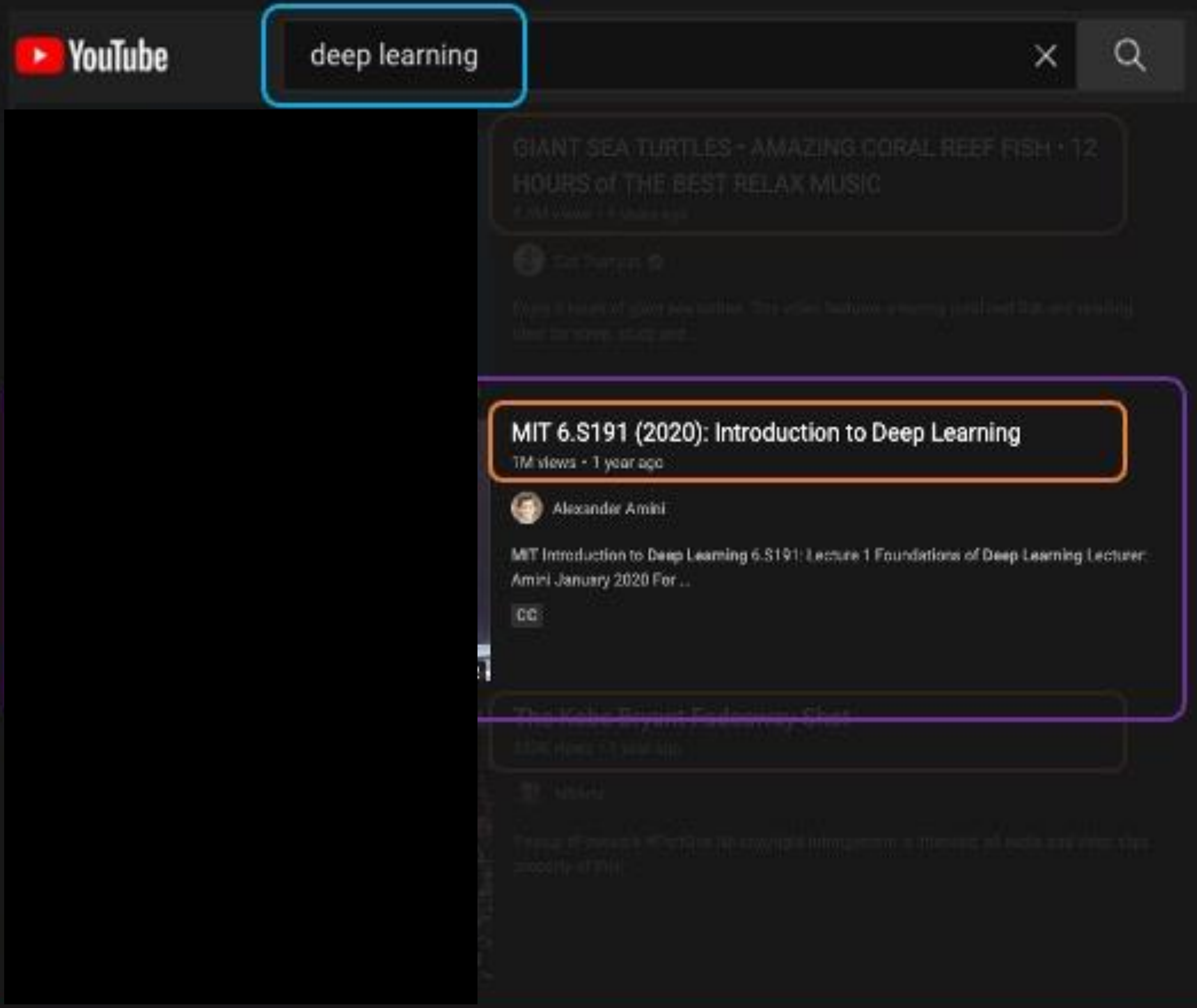
Key (K_2)

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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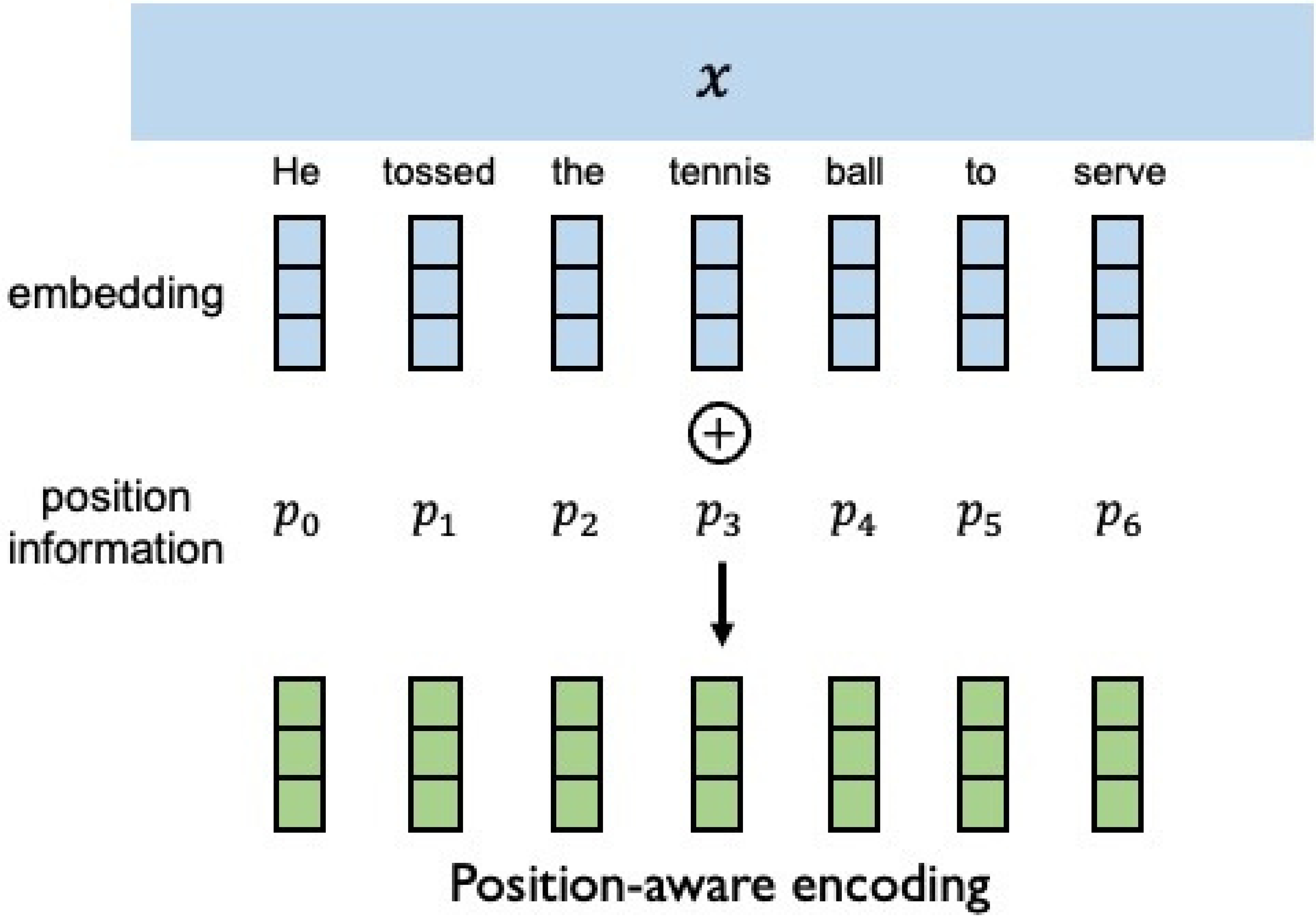

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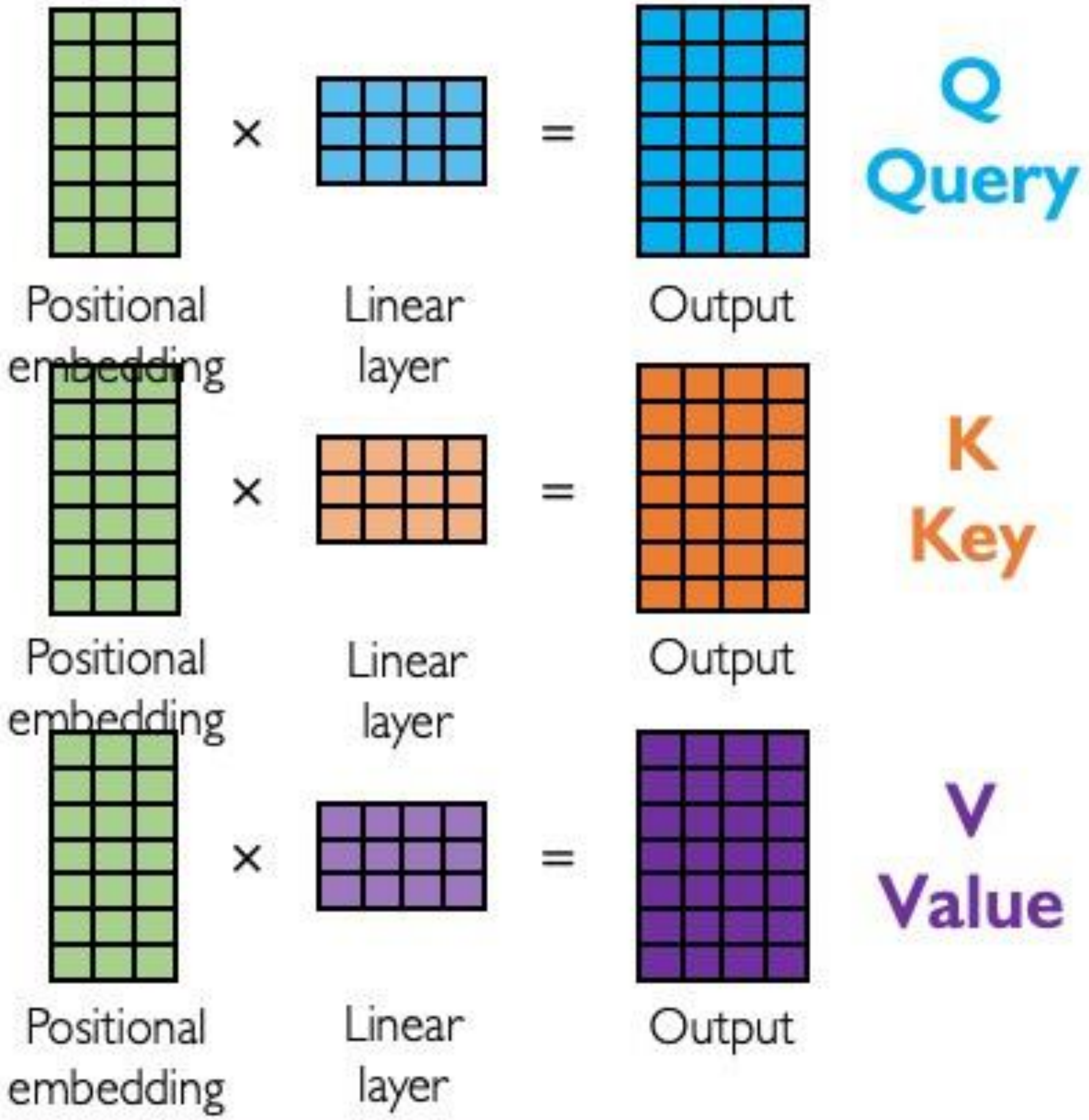

Learning Self-Attention with Neural Networks

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

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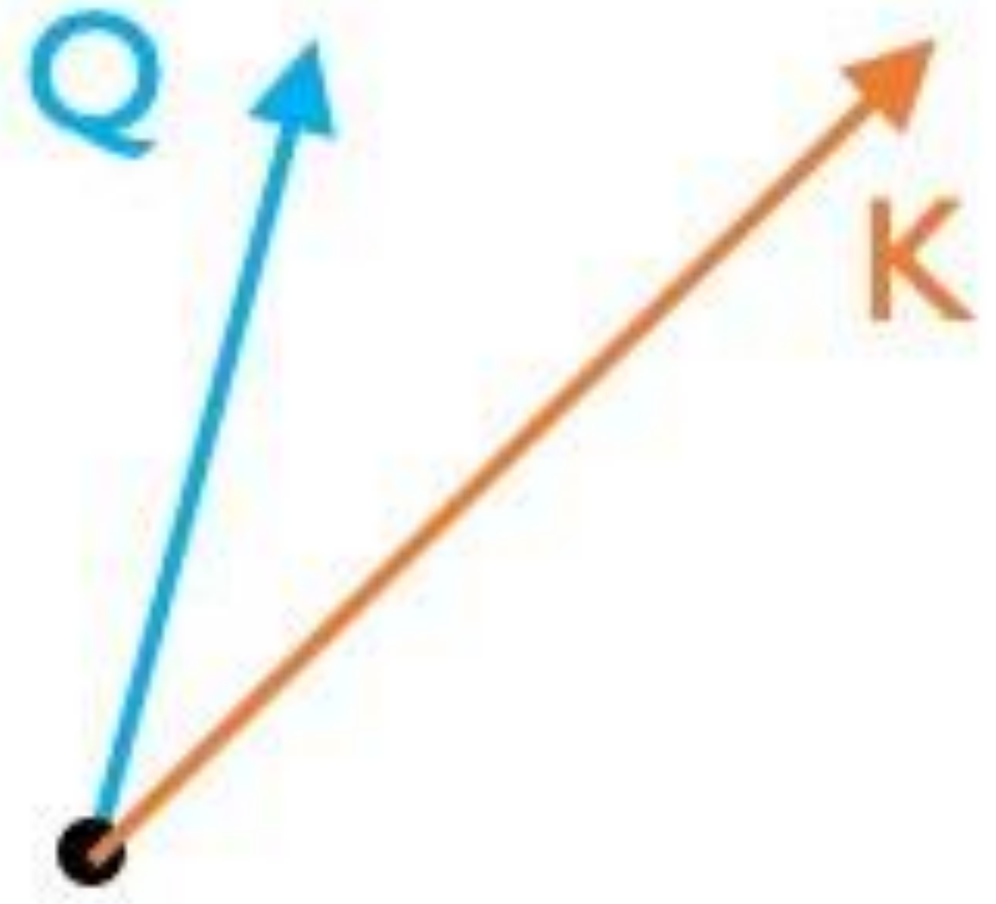
Attention score: compute pairwise similarity between each query and key

How to compute similarity between two sets of features?



Dot product → Scale

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

Similarity metric

Also known as the "cosine similarity"

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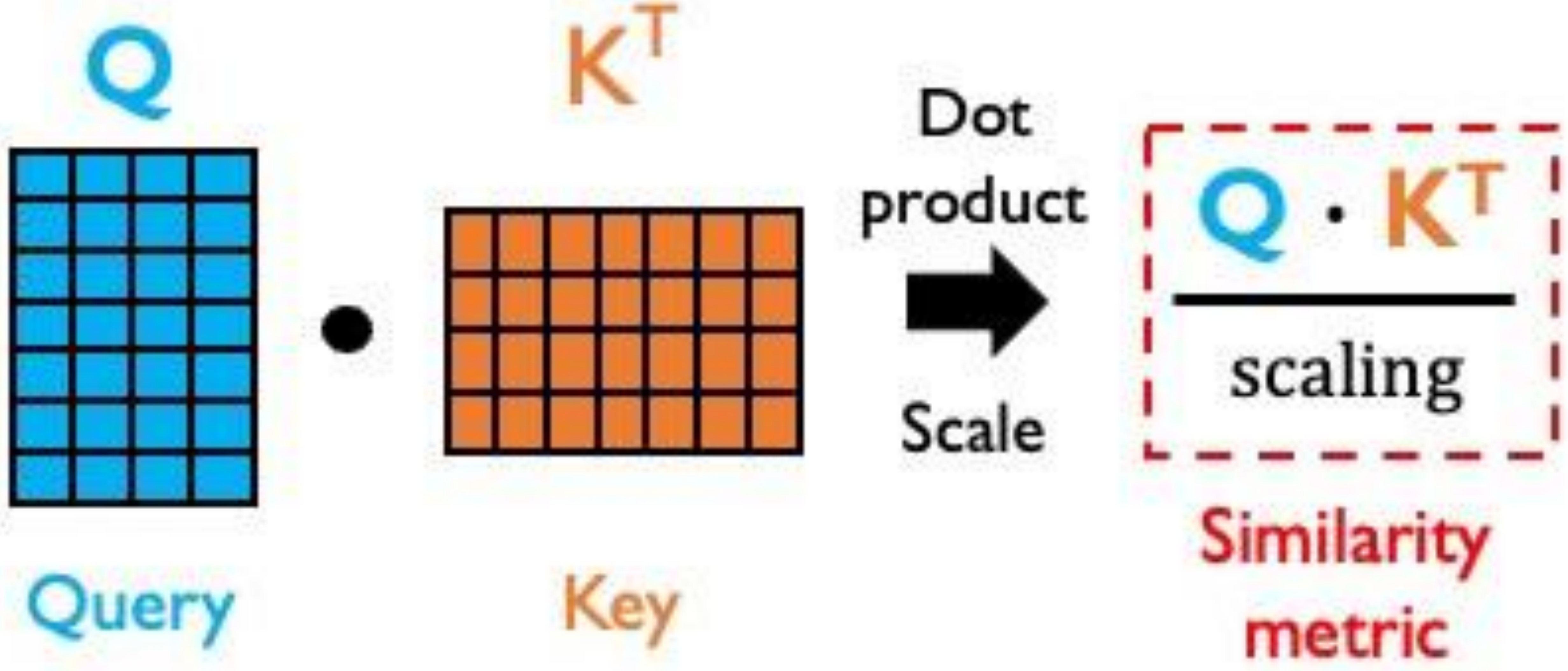

Also known as the "cosine similarity"

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
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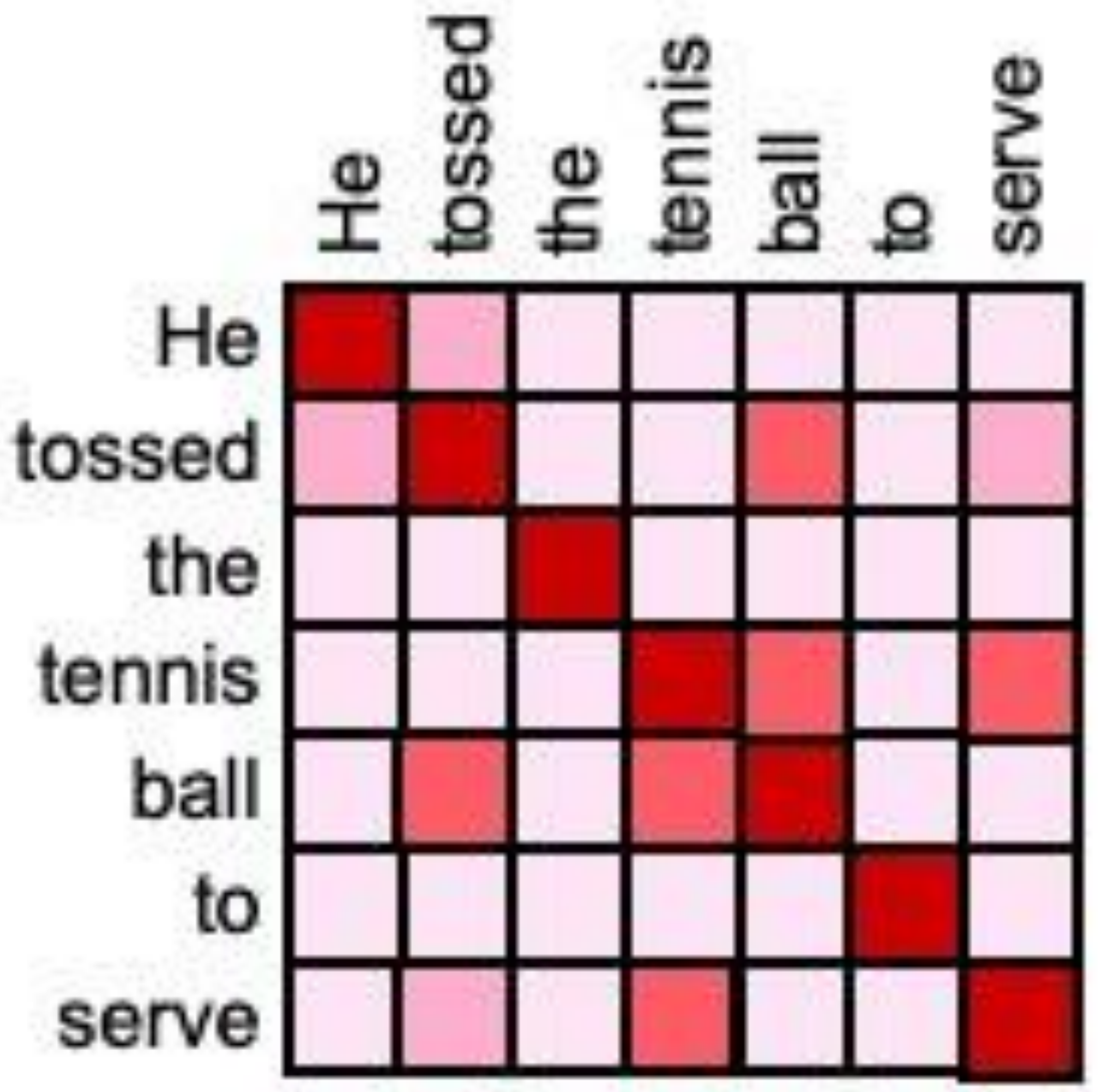
Attention weighting: where to attend to! How similar is the key to the query?



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

Attention weighting

Learning Self-Attention with Neural Networks

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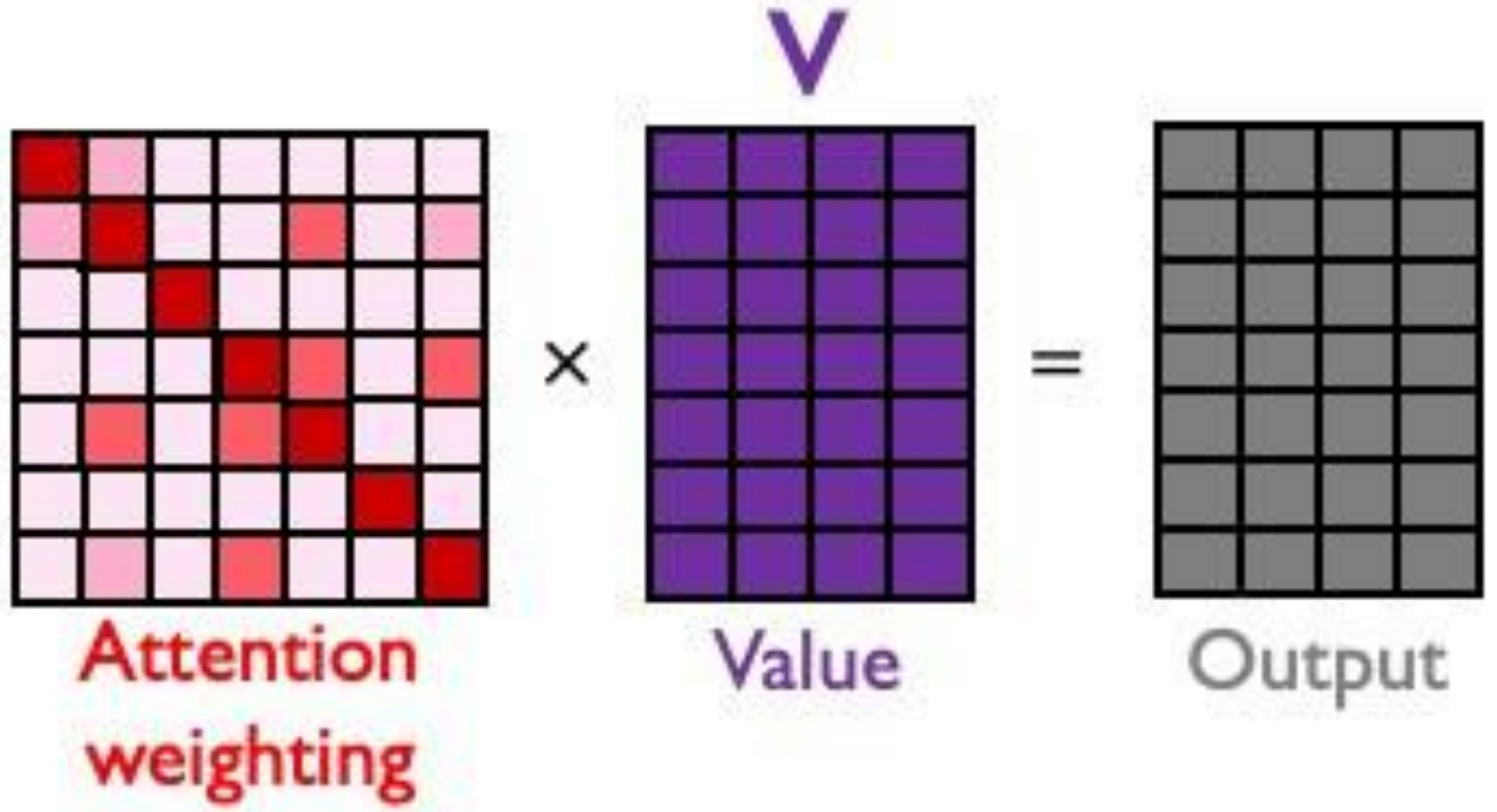
Last step: self-attend to extract features



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

Learning Self-Attention with Neural Networks

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

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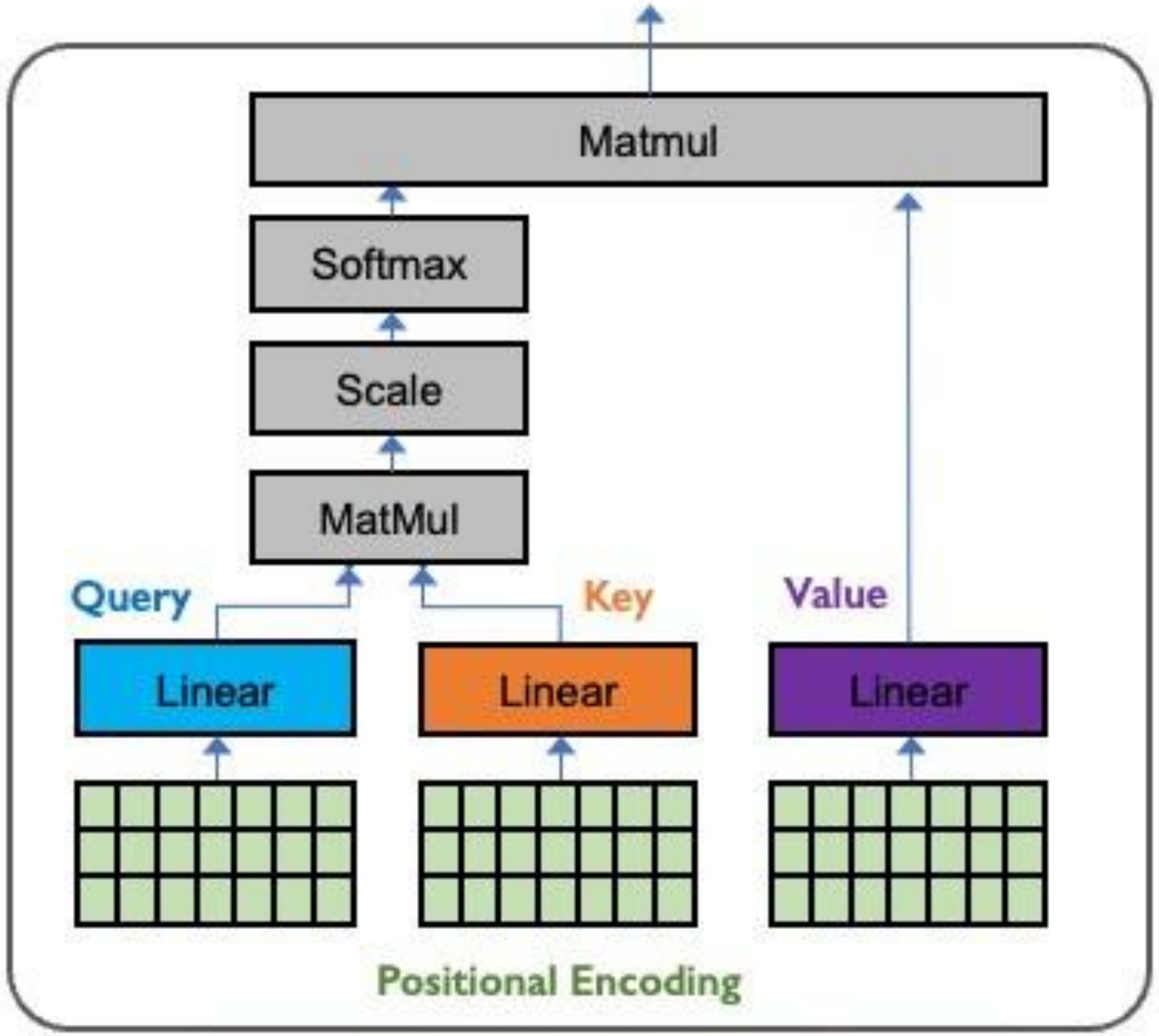
4. Extract **features with high attention**

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

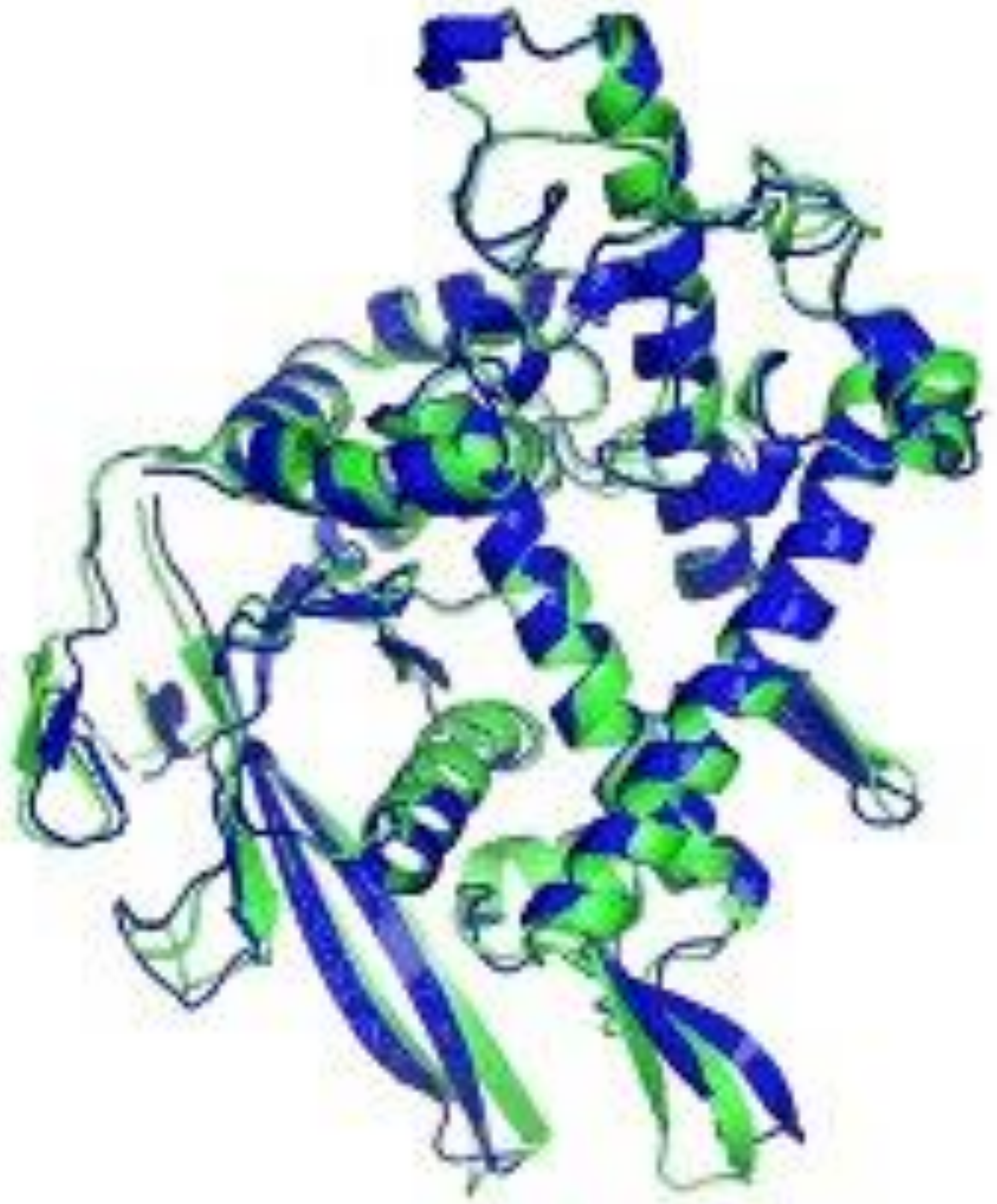
Language Processing

An armchair in the shape
of an avocado

Transformers: BERT, GPT

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**
6. Self-attention is the basis for many **large language models** – stay tuned!