Neural Networks for Sequence Data

CMPUT 261: Introduction to Artificial Intelligence

GBC §10.0-10.2
P §12.1-12.2, 12.4-12.5

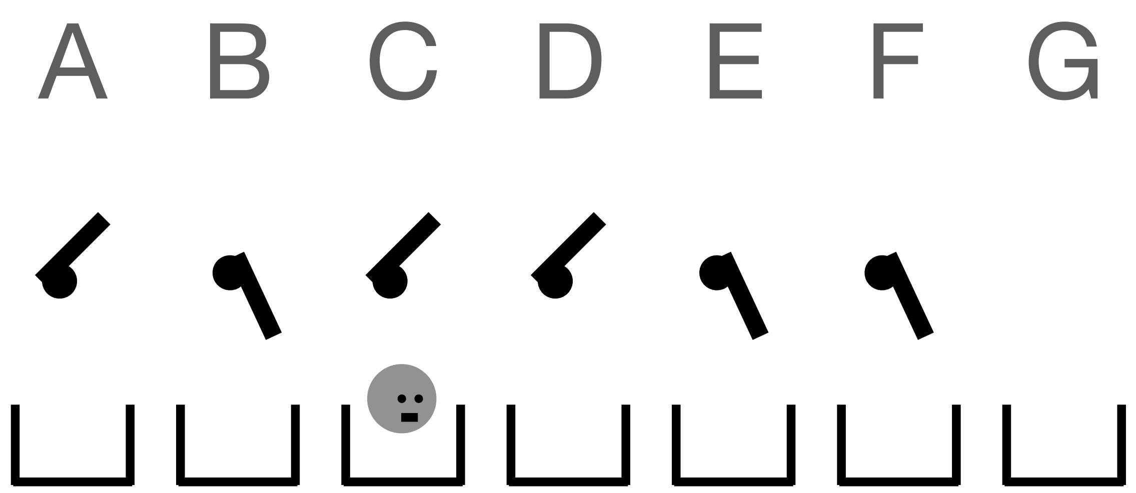
Lecture Outline

1. Midterm Review
2. Recap & Logistics
3. Unfolding Computations
4. Recurrent Neural Networks
5. Attention & Transformers

After this lecture, you should be able to:

- demonstrate unfolding a recurrent expression
- explain the problems with handling sequence input using dense or convolutional neural networks
- explain the high-level idea behind neural networks and transformers
- describe how self-attention combines inputs to generate its outputs
- describe the architecture of a transformer layer
- explain the high-level idea behind encoder-decoder architectures

Midterm Review: States

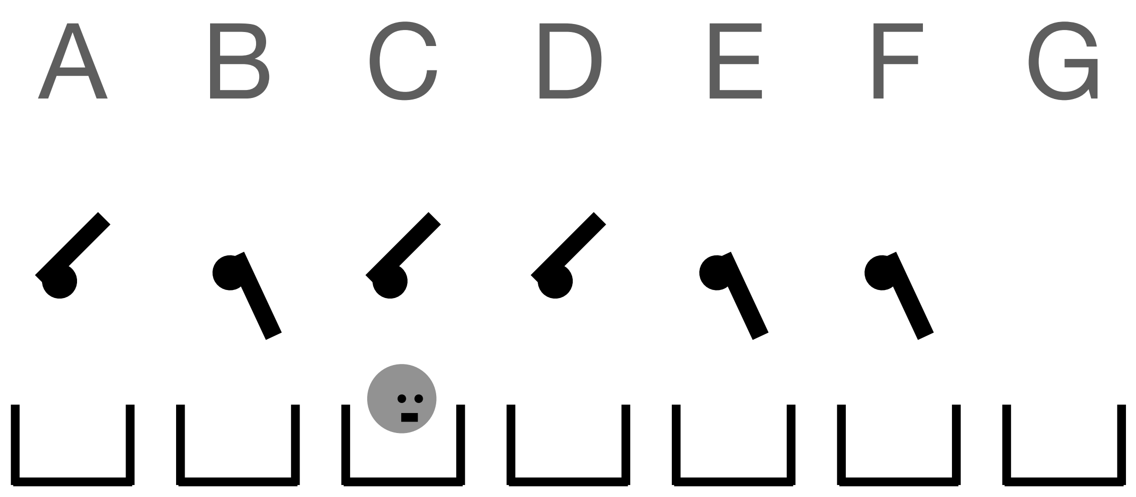


(a) [**3 points**] How would you represent the *states* for this search problem?

(b) [**2 points**] How many states does this search problem have?

- Many people tracked only the on/off states of the switches
  - You need to track the **position** of SwitchBot as well
- Many people tracked only the position of SwitchBot, plus maybe the on/off state of the switch at the current position
  - You need to track the states of **all** the switches

Midterm Review: Admissible Heuristic



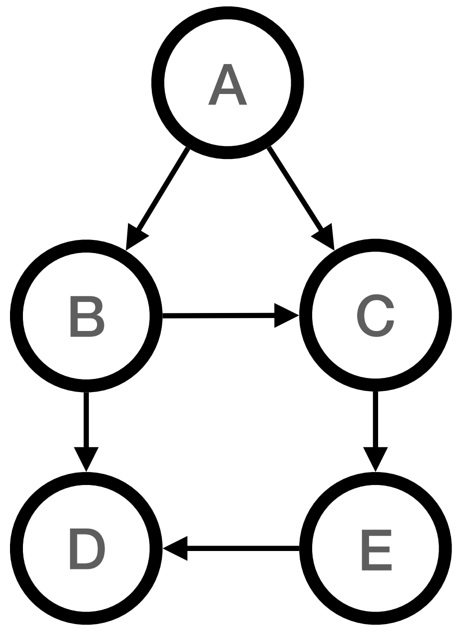
Consider the following heuristic function:

$$h(s) = \sum_{\text{positions } y} 1[\text{switch at position } y \text{ is off}]\, d(\text{pos}(s), y).$$

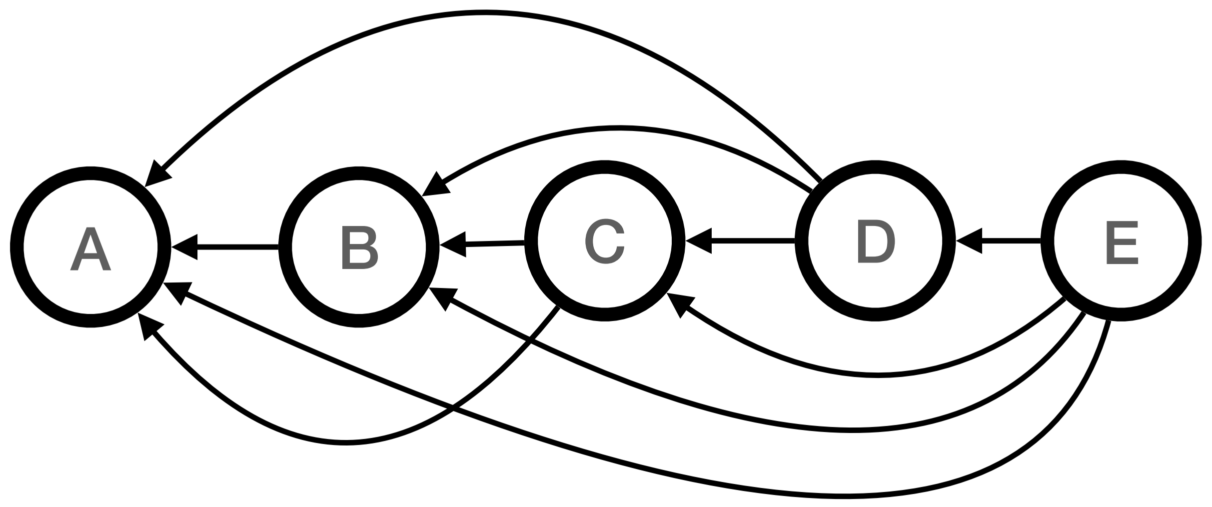
Is the heuristic function h an *admissible heuristic* for this problem? Why or why not?

- Heuristic adds up cost to get from current position to position y for every position y
- But that's more actions than you need to take for *any* solution
- **Question:** What will h return from a state where all the switches are in the **on** state and SwitchBot is in position **G**?
- **Question:** Can an admissible heuristic ever **dominate** a non-admissible heuristic?

Midterm Review: Factorings



$P(A)P(B \mid A)P(C \mid A, B)P(D \mid B, E)P(E \mid C)$



$P(A \mid B, C, D, E)P(B \mid C, D, E)P(C \mid D, E)P(D \mid E)P(E)$

- Many people spotted that these two belief networks represent **different factorings** of $P(A, B, C, D, E)$
- Not every joint distribution can be factored according to the left network (e.g., any distribution where E is **not** conditionally independent of A given only C)
- But *any* distribution over $A, \ldots, E$ can be factored according to the right network (**why?**)

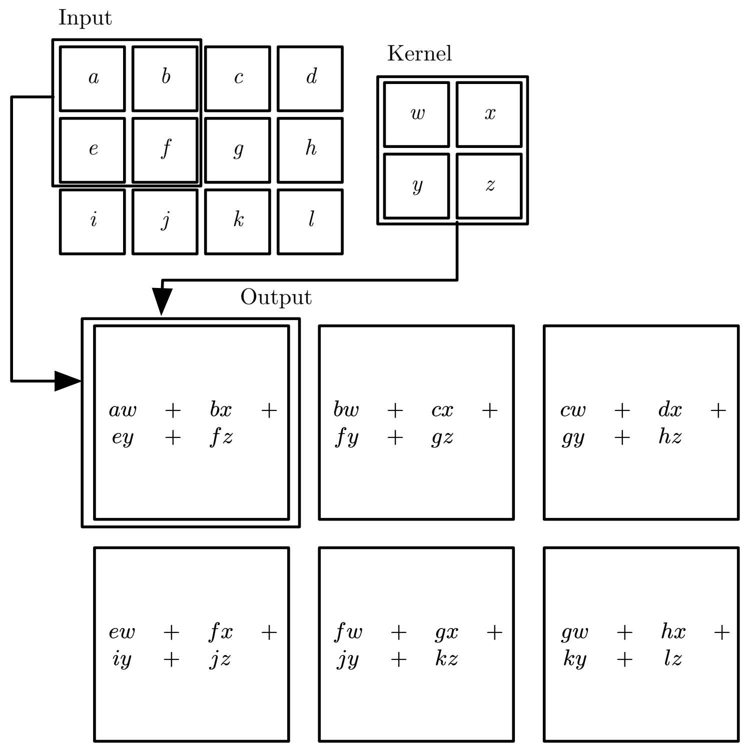
Logistics: Assignment #3

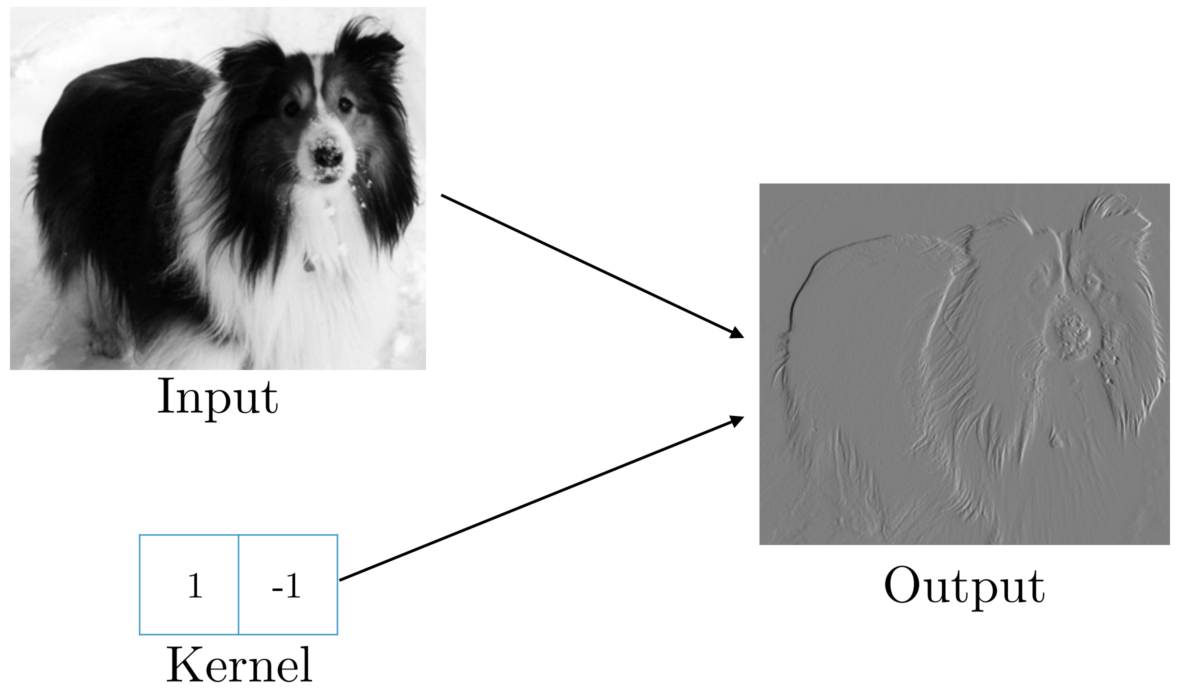
- **Assignment 3** is due **Thursday (Nov 17)** at 11:59pm
    - Late submissions until the following Monday with 20% deduction
- See eClass for corrections:
    - Minor typos in question 3
    - Install torch using

```
pip3 install --user torch torchvision
```

Recap:
Convolutional Neural Networks

- Convolutional networks: Specialized architecture for **images**
- Number of **parameters** controlled by using **convolutions** and **pooling** operations instead of **dense connections**
- Fewer parameters means more **efficient to train**





(Images: Goodfellow 2016)

Sequence Modelling

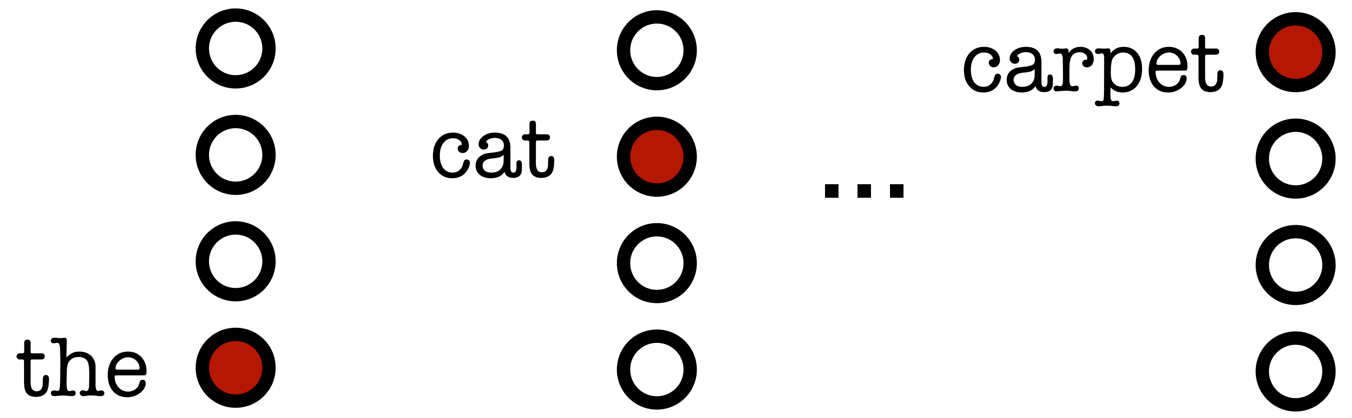
- For many tasks, especially involving language, we want to model the behaviour of **sequences**
- **Example:** Translation
  - The cat is on the carpet $\Longrightarrow$ Le chat est sur le tapis
- **Example:** Sentiment analysis
  - This pie is great $\Longrightarrow$ POSITIVE
  - This pie is okay, not great $\Longrightarrow$ NEUTRAL
  - This pie is not okay $\Longrightarrow$ NEGATIVE

Sequential Inputs

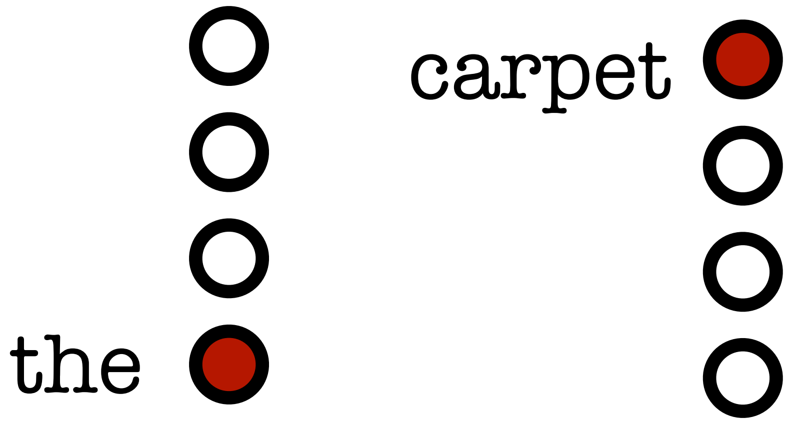
The cat is on the carpet

Question: How should we **represent** sequential input to a neural network?

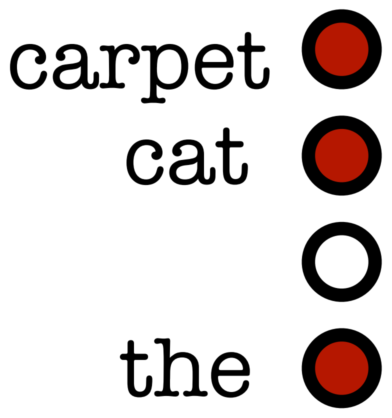
1. 1-hot vector for **each word**
   (Sequence must be a specific length?)



2. 1-hot vector for **last few words**
   (n-gram)



3. **Single vector** indicating each word that is present
   (bag of words)



One-Hot Representations

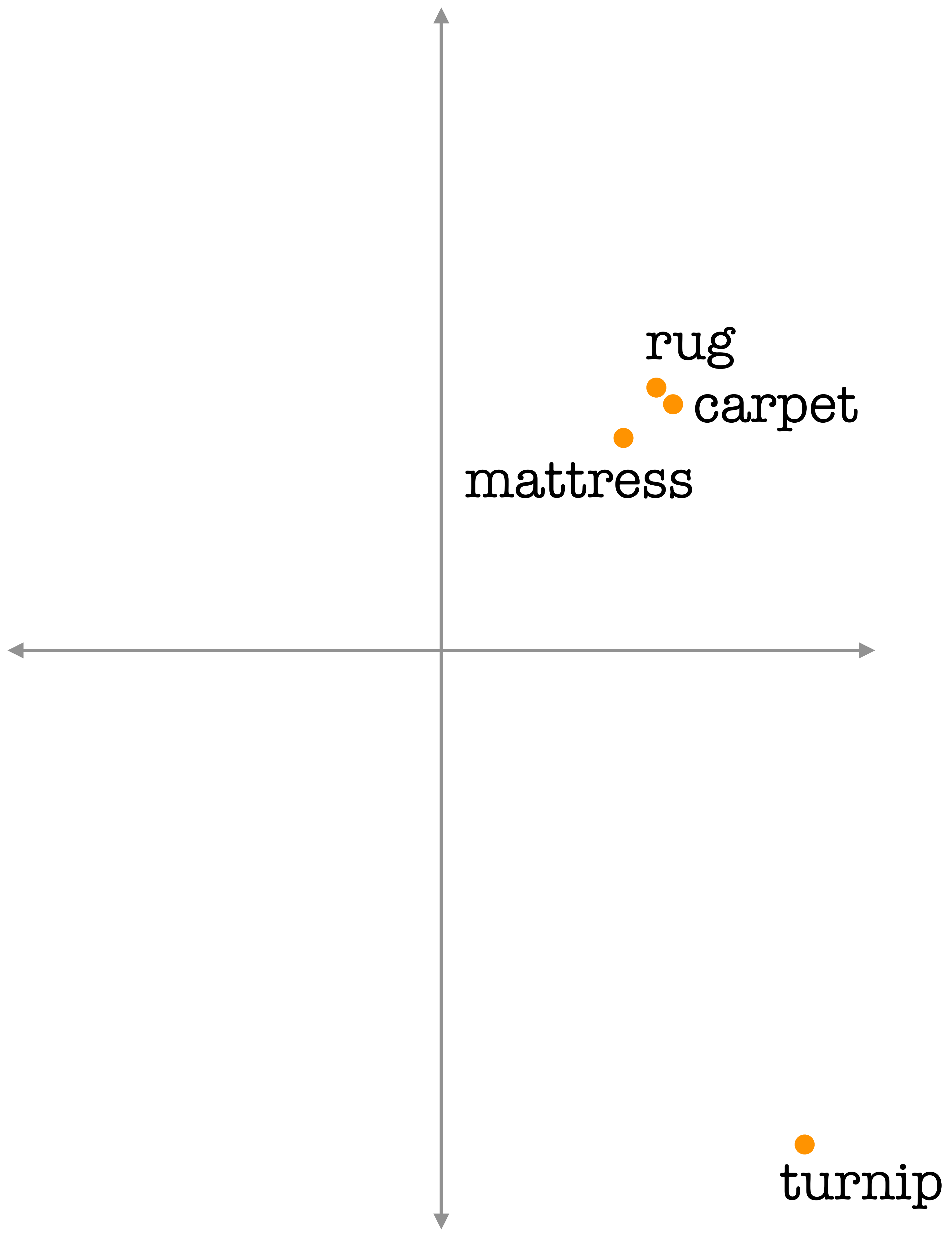
One-hot representations of words have some problems:

1. **Wasteful:** Each input vector must have a dimension equal to the size of the vocabulary (possible words)
    - If vocabulary has 30,000 words, then each vector has 29,999 zeros
2. **Poor generalization:** Ideally, similar words would be treated similarly
    - Exploiting meaningful similarity between images was an important feature of convolutional neural networks

$$\begin{array}{r c} & \\ & \\ & \\ & \\ & \\ & \\ & \\ \texttt{carpet} & \\ & \\ & \\ & \\ & \\ & \\ & \\ & \\ & \\ & \\ & \\ & \\ & \\ & \\ & \\ & \\ & \\ & \\ & \\ & \end{array}\left[\begin{array}{c} 0 \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \\ \mathbf{1} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \\ 0 \\ 0 \end{array}\right]$$

Semantic Embeddings

- The usual approach is to first learn a **semantic embedding** for one-hot vectors
- Every word gets represented as a **dense vector** with smaller dimension than the vocabulary (typical size: 1,024)
- **Goal:** Words with similar **meanings** will have small **distance** between embedded vectors; words with different meanings will have large **distance** between embedded vectors



(Pre-)Training Semantic Embeddings

Question: How many **parameters** are required to convert a one-hot encoding for vocabulary of V words into a D-dimensional embedding?

- Embeddings require the training of a lot of parameters
- Fortunately, this can be done with **unlabeled** data
- **Trick:** "Pre-train" neural network for a task that we don't care about
  - But which can be evaluated using unlabeled data
  - Predicting words from k nearby words
  - Predicting "masked" words
- Keep the weights that convert the one-hot layer into a dense embedding layer
- Throw away the weights that convert the embedding layer into output

Processing
Variable-Length Sequences

- Image inputs can be restricted to a **standard size** (20x20, 1024x768, etc.)
- Sequence inputs (e.g., text) are **variable-length**
    - And often **very long**
- **Solution:** Apply the same operations to each position in the sequence
- Two such approaches:

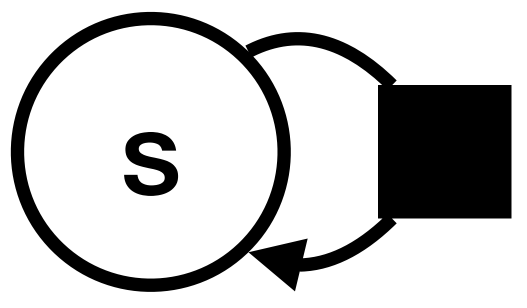
1. **Recurrent neural networks:**
   input is current token + fixed-dimension "state" from previous operation
2. **Transformers / self-attention:** Size of state varies with size of sequence

Dynamical Systems

- A **dynamical system** is a system whose state at time $t + 1$ depends on its state at time t:

$$\mathbf{s}^{(t)} = f(\mathbf{s}^{(t-1)}; \theta)$$

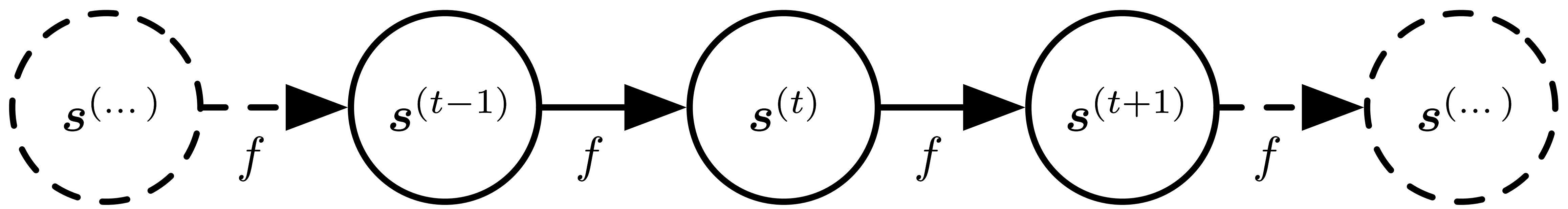
- An expression that depends on the same expression at an earlier time is **recurrent**.



Unfolding Computations

- A recurrent expression can be converted to a non-recurrent expression by **unfolding**:

$$\begin{aligned}\mathbf{s}^{(3)} &= f(\mathbf{s}^{(2)}; \theta) \\ &= f(f(\mathbf{s}^{(1)}; \theta); \theta)\end{aligned}$$



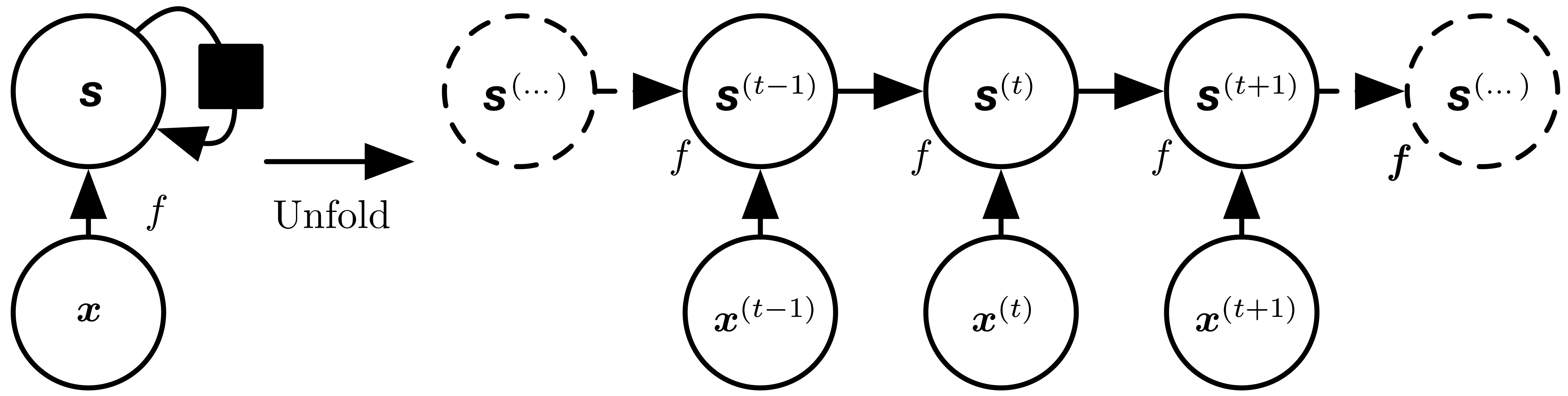
(Image: Goodfellow 2016)

External Signals

- Dynamical systems can also be driven by **external signals**:

$$\mathbf{s}^{(t)} = f(\mathbf{s}^{(t-1)}, \mathbf{x}^{(t)}; \theta)$$

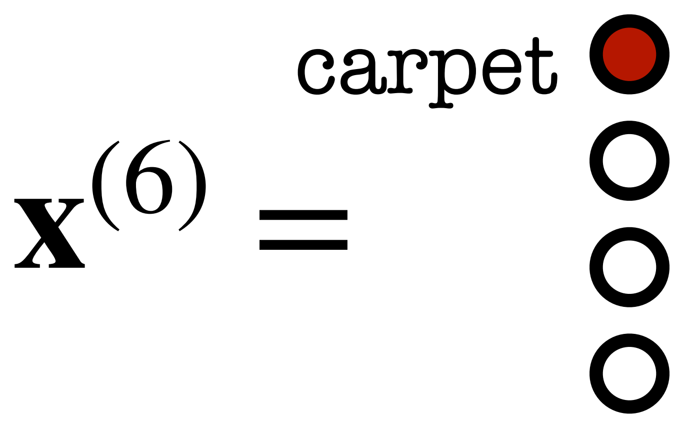
- These systems can also be represented by non-recurrent, unfolded computations:



(Image: Goodfellow 2016)

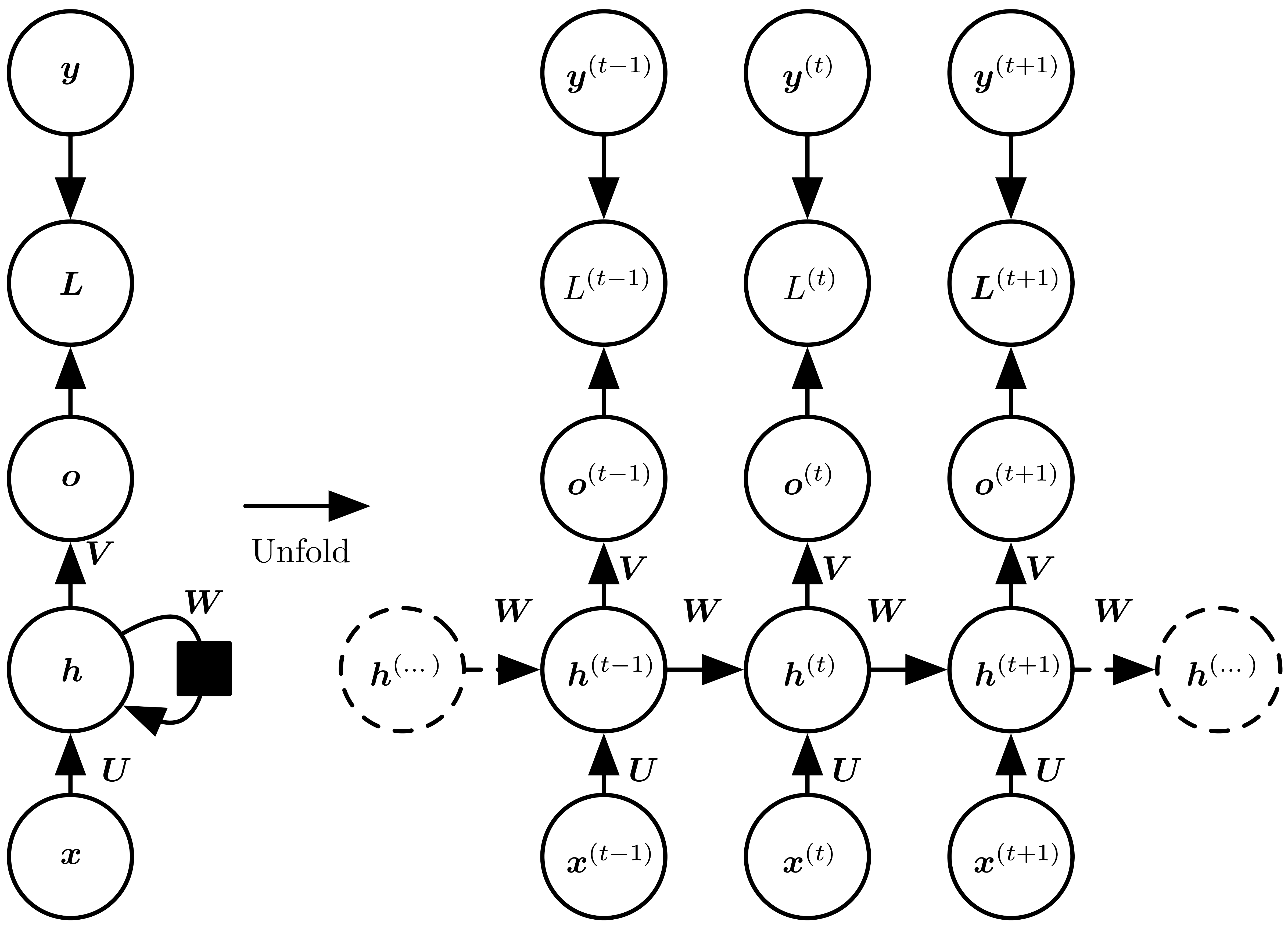
Recurrent Neural Networks

- Recurrent neural network: a specialized architecture for modelling **sequential data**
- Input presented **one element at a time**



- Parameter sharing by:
  - Treating the sequence as a system with **state**
  - Introducing hidden layers that **represent** state
  - Computing **state transitions** and **output** using **same functions** at each stage
- The **same computation** is applied to each pair of state and input
  - But the state is different after each application

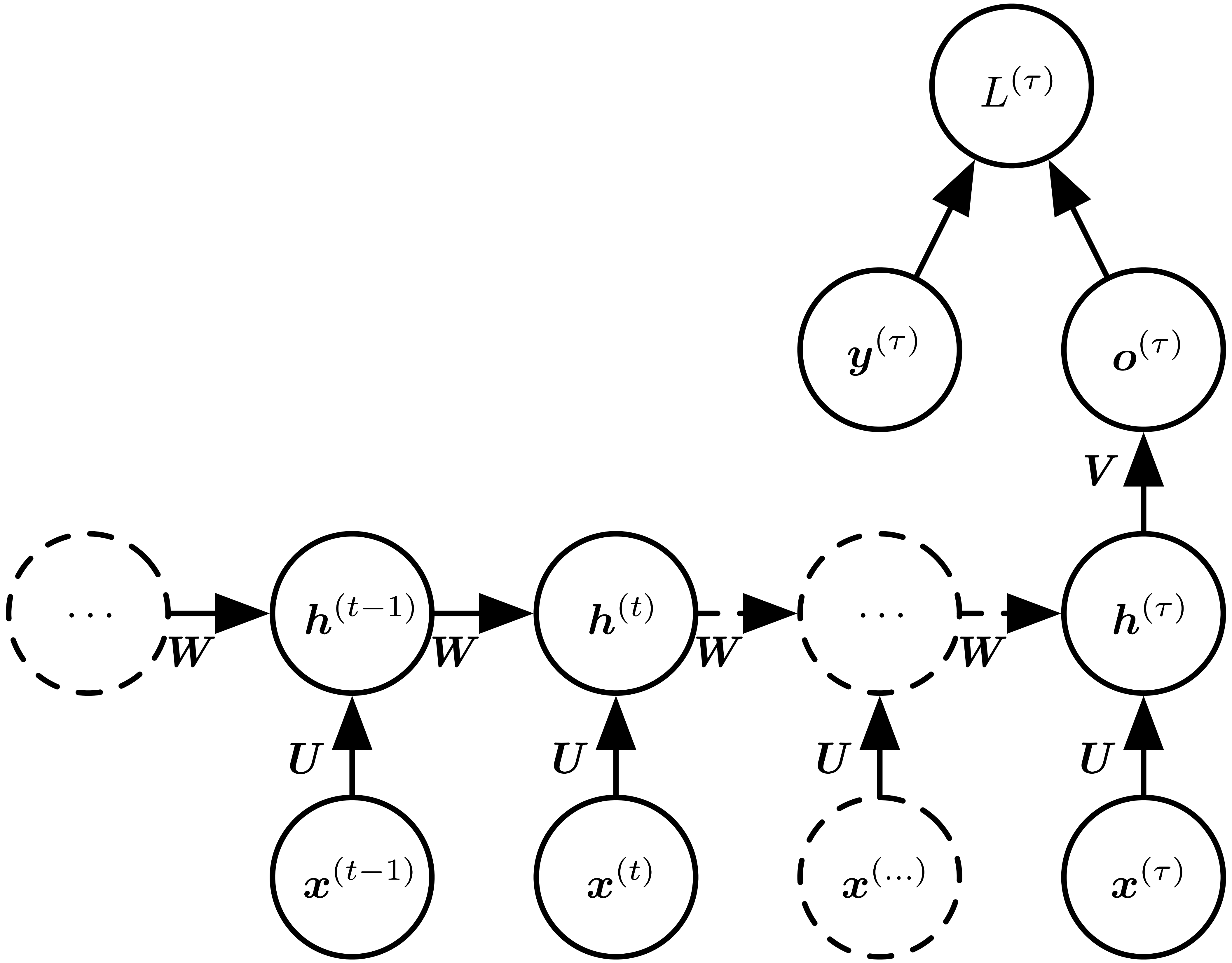
Recurrent Hidden Units: Sequence to Sequence



- **Input values x** connected to **hidden state h** by weights $\mathbf{U}$
- Hidden state **h** mapped to **output o** by weights $\mathbf{V}$
- Hidden state $\mathbf{h}^{(t-1)}$ connected to hidden state $\mathbf{h}^{(t)}$ by weights $\mathbf{W}$
- Gradients computed by **back propagation through time**: from final loss all the way back to initial input.
- All hidden states computed must be **stored** for computing gradients

(Image: Goodfellow 2016)

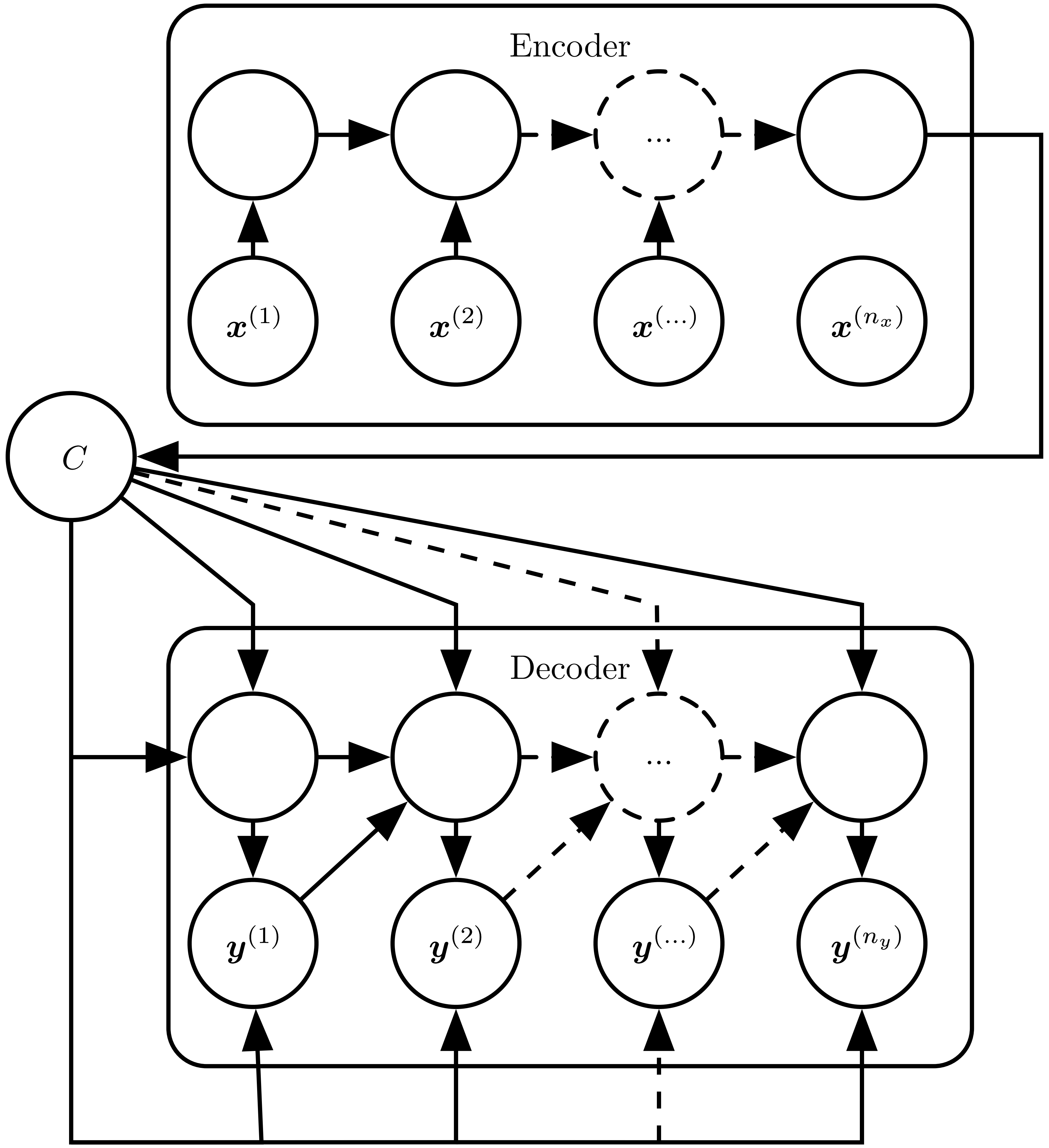
Recurrent Hidden Units: Sequence to Single Output



- Update state as inputs are provided
- Only compute a **single** output at the **end**
- $\mathbf{W}, \mathbf{U}$ still shared at every stage
- Back propagation through time still requires **evaluating every state** in gradient computation

(Image: Goodfellow 2016)

Encoder/Decoder Architecture for Sequence to Sequence



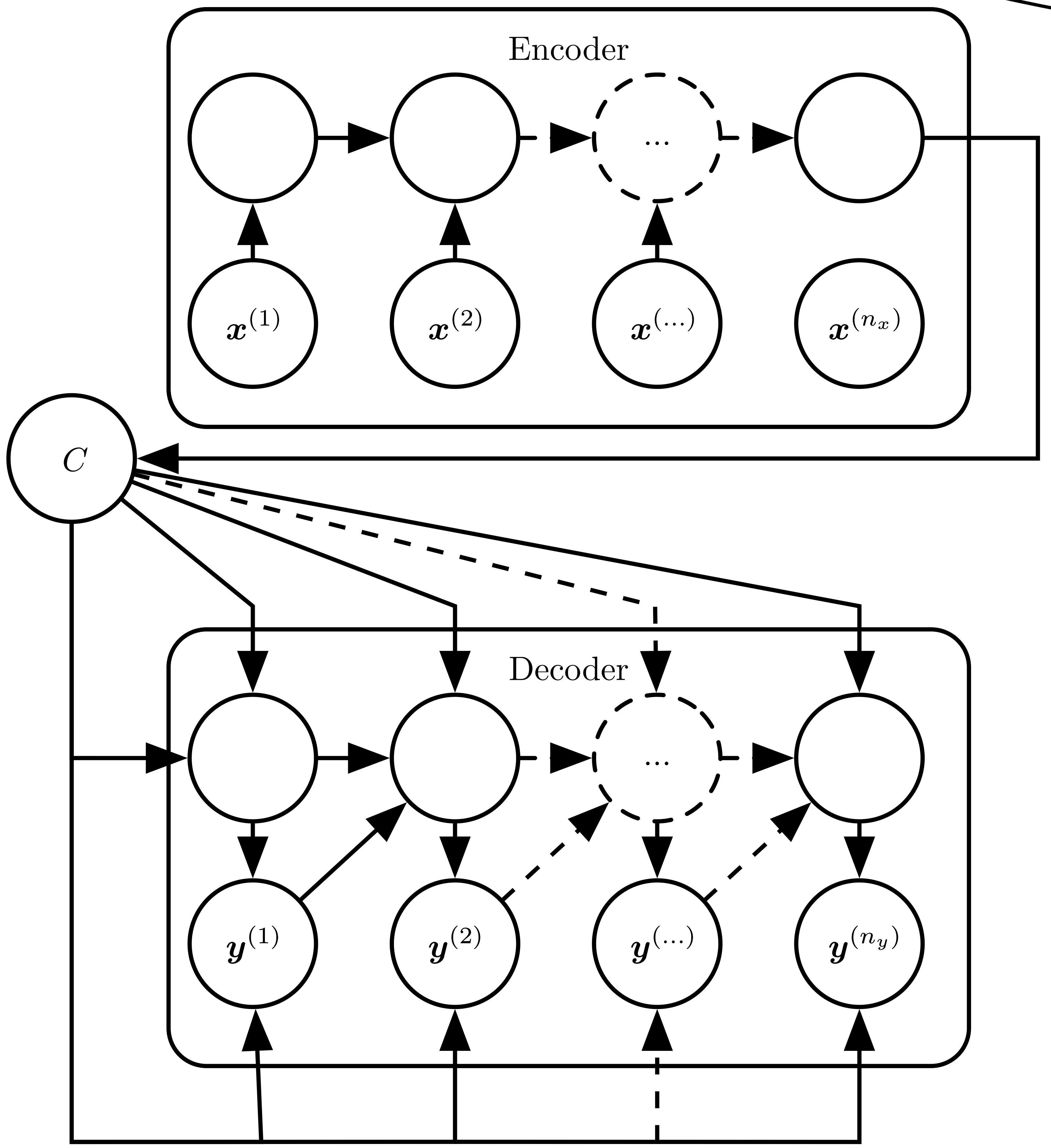
Can **combine approaches** for sequence-to-sequence:

1. Accept entire input to construct a single "**context**" output $\mathbf{C}$
2. Construct new sequence using context $\mathbf{C}$ as **only input**

(Image: Goodfellow 2016)

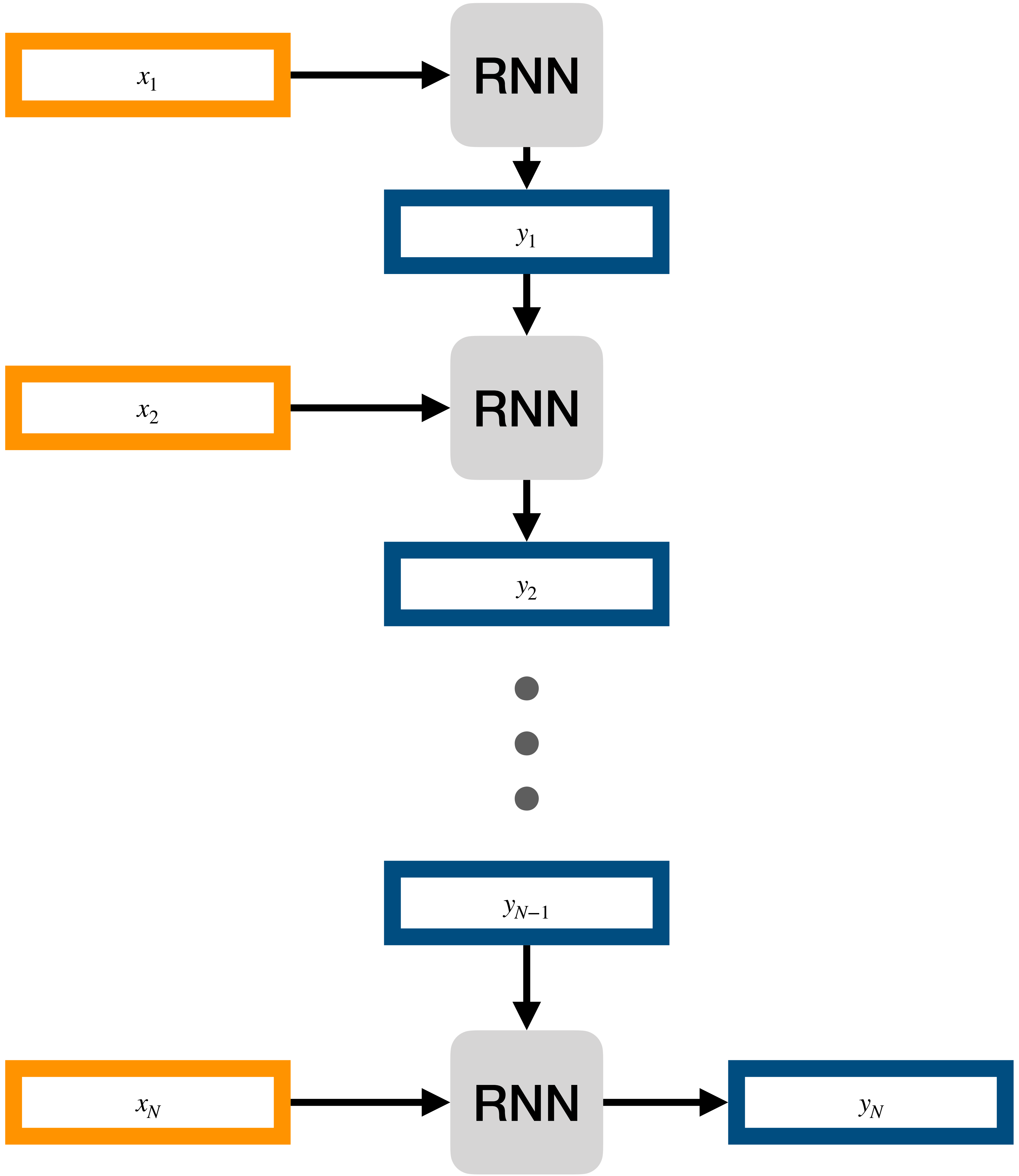
Long-Range Dependence

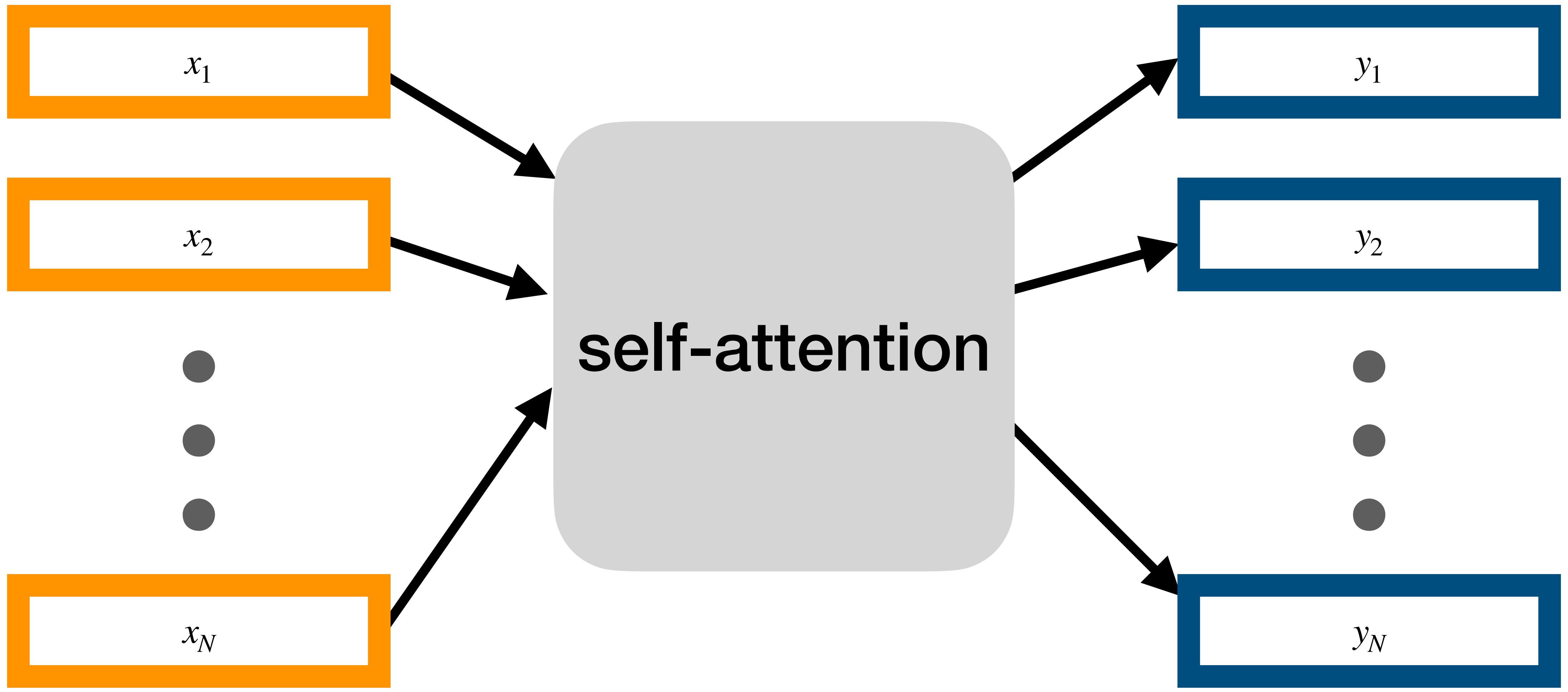
The submarine, which was the subject of a well known song by the Beatles, was yellow.



- Information sometimes needs to be **accumulated** for a long part of the sequence
- But **how long** an individual piece of information should be accumulated is **context-dependent**
- Long-range dependence can be difficult for a recurrent network
  - Often need to **accumulate** information in the state, and then **forget** it later

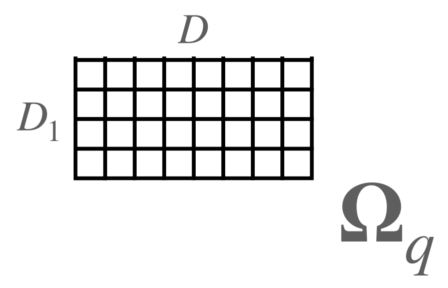
Self-Attention vs. RNN





- **RNN:** accept "previous" state and current input; output "next" state
    - Final output is last state
- **Self-attention:** Accept ALL inputs
    - Final output is ALL states

Self-Attention

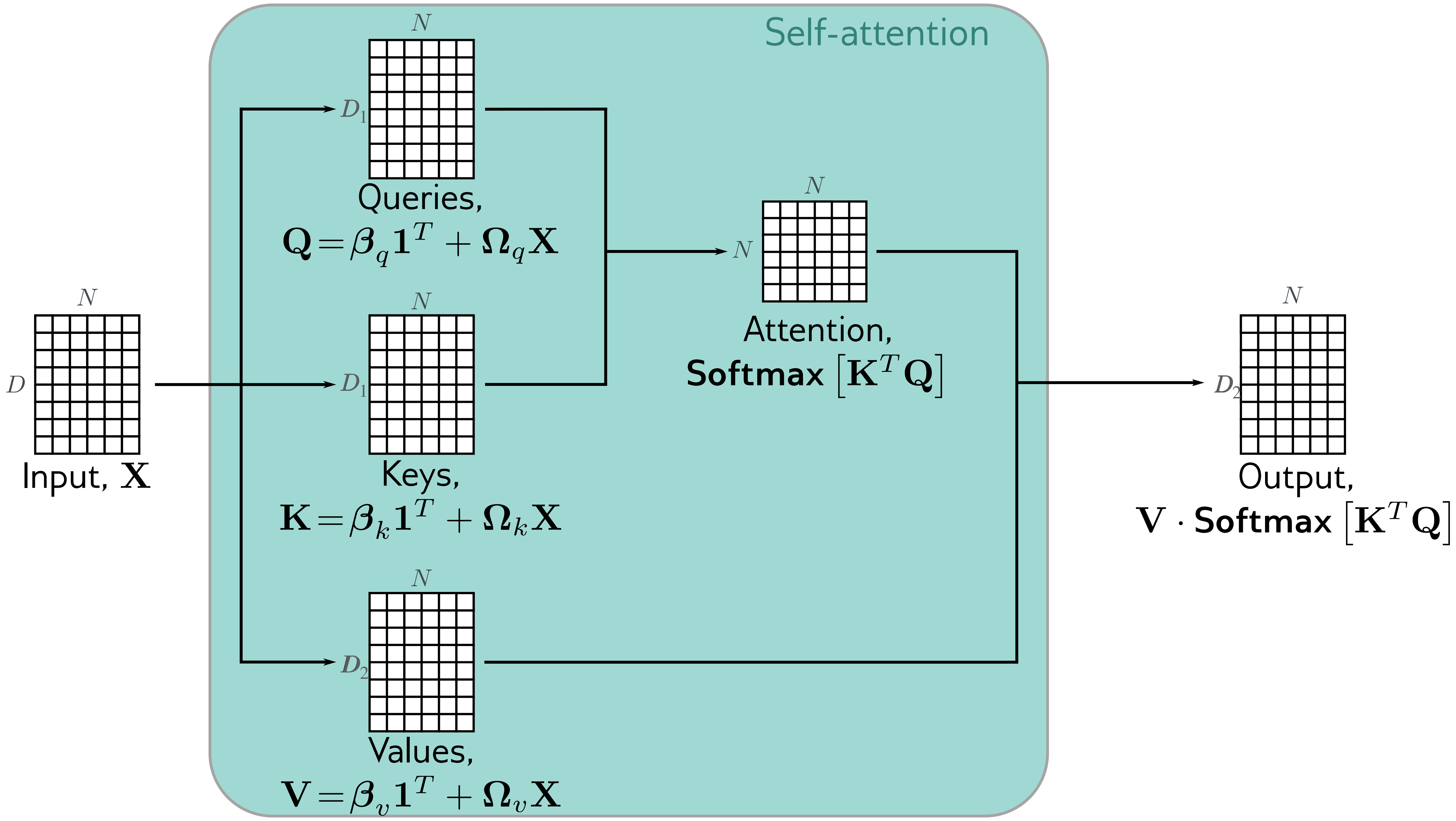


- A **self-attention unit** computes **three values** for each input i:
  - **Query** q_i, **Key** k_i, and **Value** v_i
  - These values are computed in the **same way** for each input
- Each output is a **weighted** combination of the **values** of all inputs:

$$y_j = \sum_i w_{ij} v_i$$

- Weight for output j of **value** i is the dot-product of j's **query** and i's **key**

$$w_{ij} = q_j^\top k_i$$



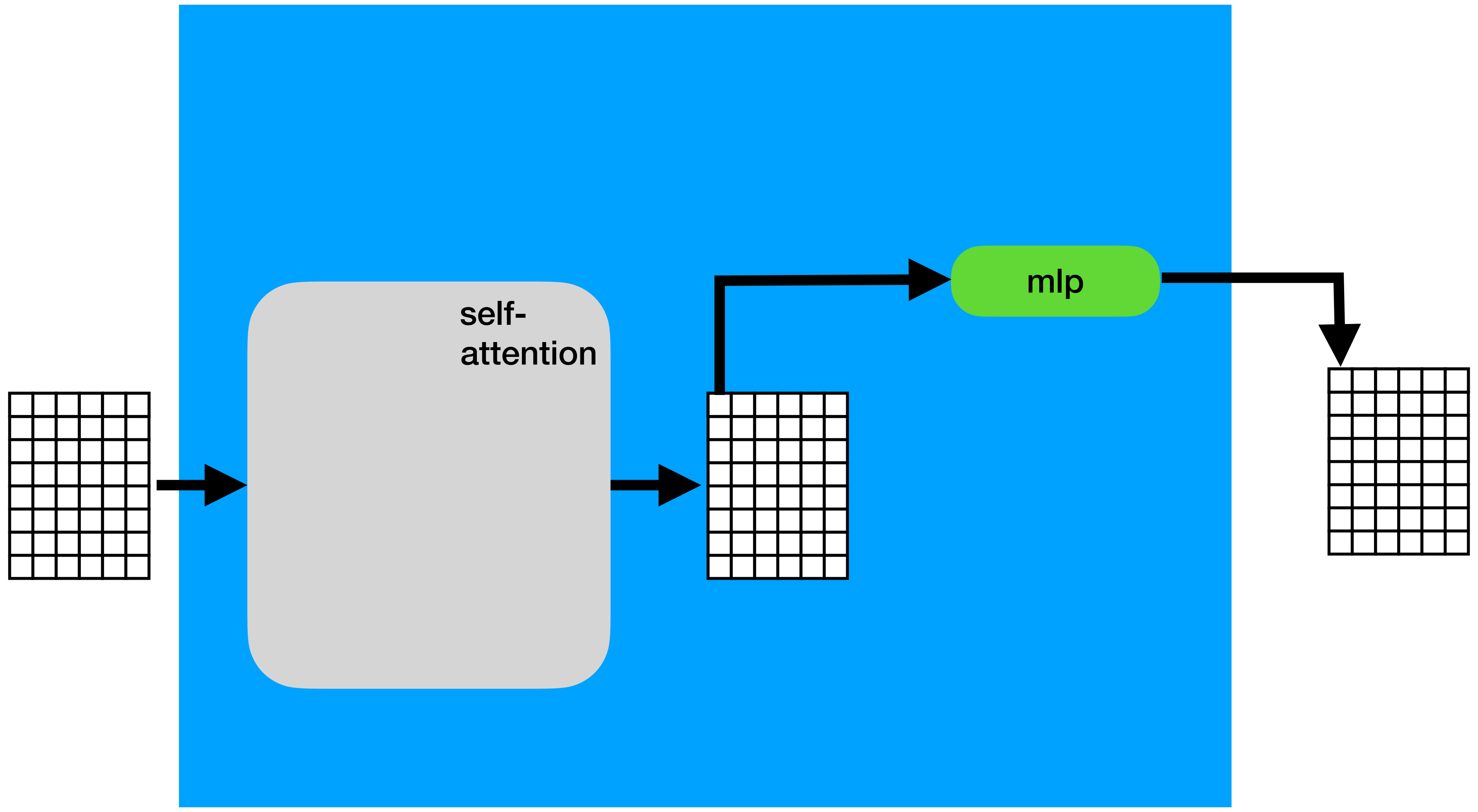
(Image: Prince 2022)

Transformer Blocks

- A **transformer layer** is a **self-attention** unit followed by a **dense feedforward network**
  - The **same** feedforward network gets applied to each output of the self-attention unit:

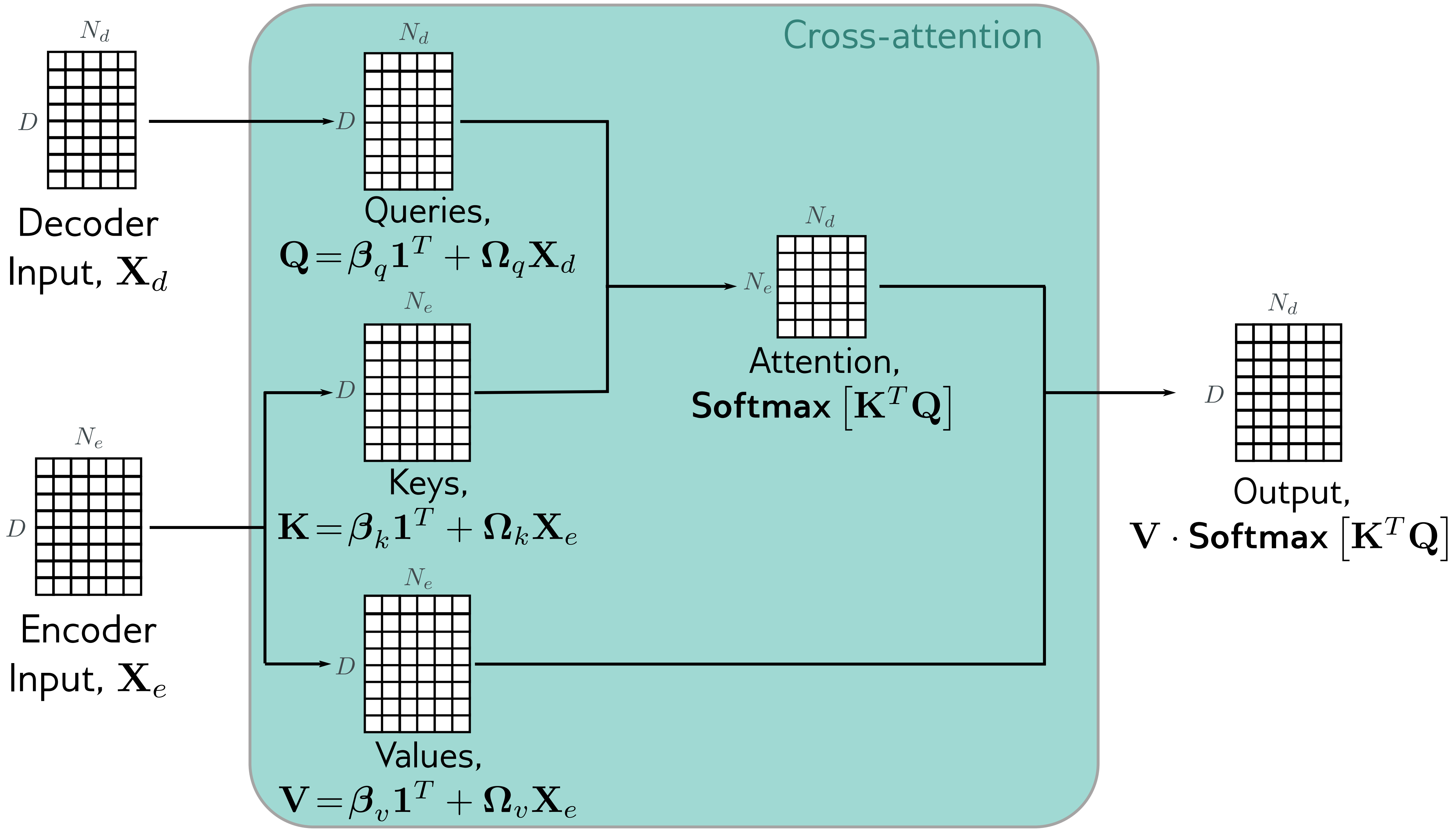
$$y_j = \mathrm{mlp}(x_j; \Omega) \quad \text{for } j = 1, \ldots, N$$

- In a typical transformer architecture, several transformer blocks will be strung together in parallel



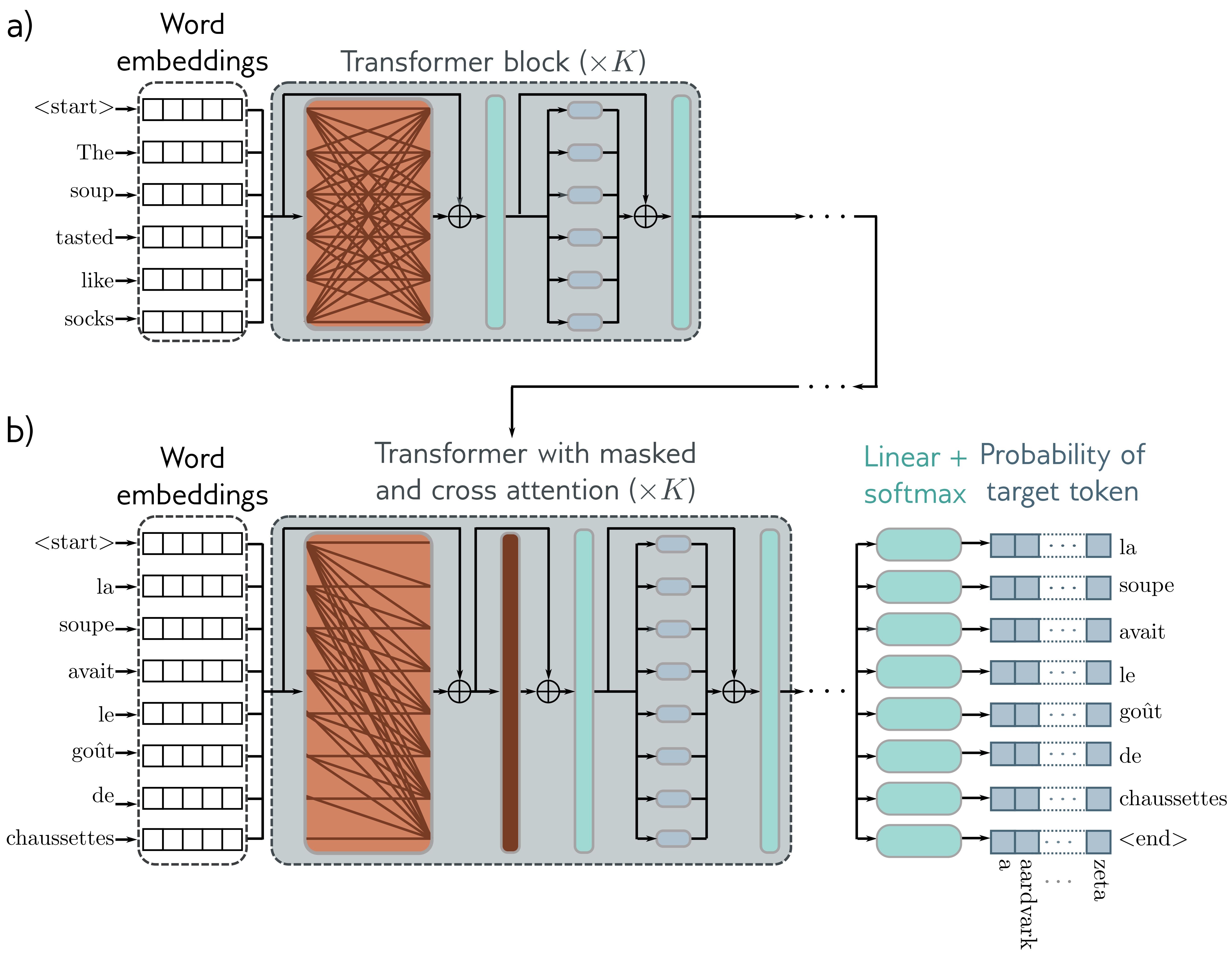
Cross-Attention

- The transformers described so far will construct a **context**: an **encoding** of the sequence
- For some tasks (e.g., translation), this encoding must then be **decoded**
- Decoder looks almost identical to encoder, except that it attends to the context as well as the previous input
- This is accomplished using **cross-attention**



(Image: Prince 2022)

Example Encoder-Decoder



(Image: Prince 2022)

Summary

- Naïvely representing **sequential inputs** for a neural network requires infeasibly many input nodes (and hence **parameters**)
- **Recurrent neural networks** are a **specialized architecture** for sequential inputs
  - **State** accumulates across input elements
  - Each stage computed from **previous stage** using **same parameters**
- **Transformers** are another specialized architecture!
  - **Self-attention** to combine inputs instead of accumulating state
  - All states output (not just last in a sequence)
  - Improved ability to attend to long-range dependence
  - Admits of better parallel evaluation