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SSIE 419/519: Applied Soft Computing

Lecture 02: Introduction & Word Embeddings

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WARNING

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Overview

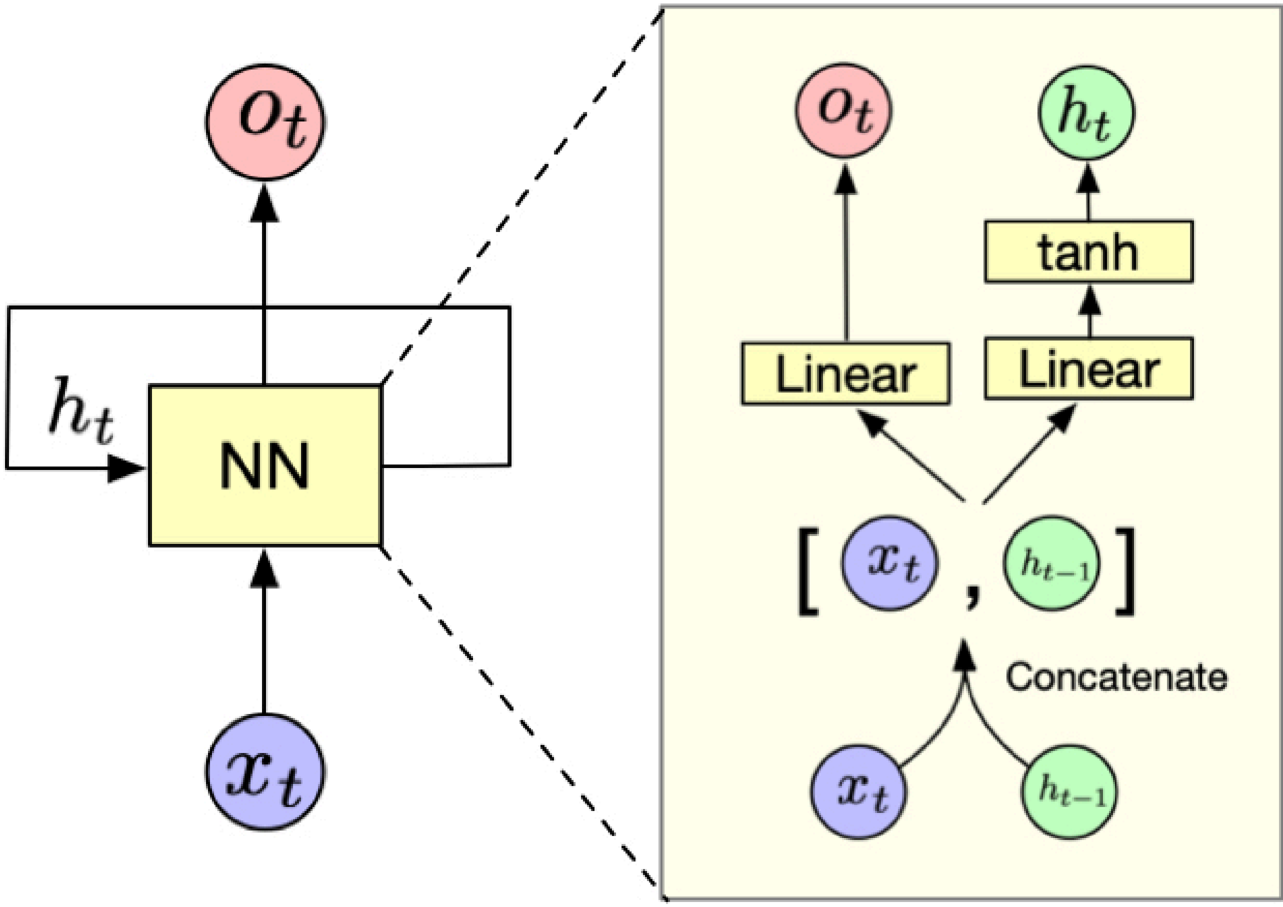
- Recurrent Neural Networks (RNN)
- Long Short-Term Memory (LSTM)
- Embeddings from Language Models (ELMo)
- Sequence-to-Sequence (Seq2Seq)
- Attention Mechanisms

The Core Idea of RNNs 💡

- **Intuition**:
  Neural Network + a working memory
- **Working memory**:
  Represented as a vector h_t of a fixed size
- **Update & Output**:

$$h_t = f(h_{t-1}, x_t)$$
$$o_t = g(h_t)$$

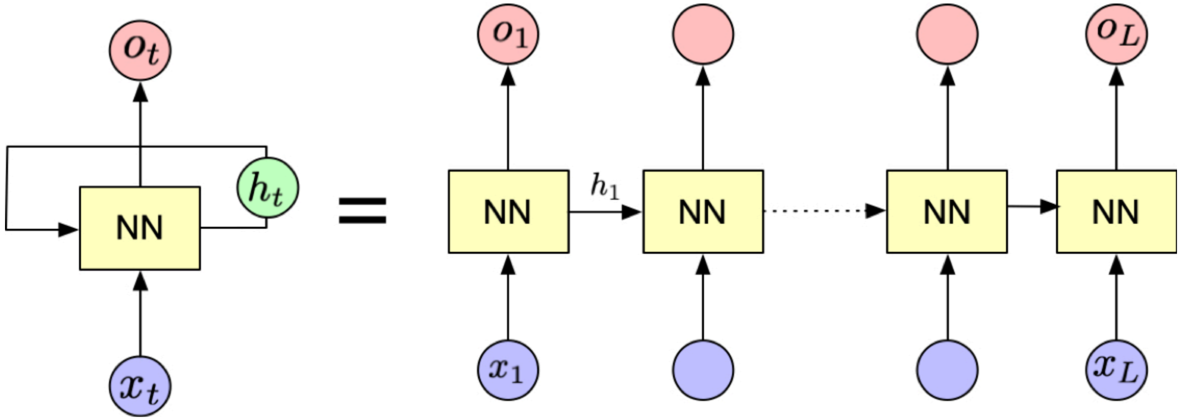
  - h_{t-1}: previous hidden state
  - x_t: current input
  - f: memory update function
  - o_t: output
  - g: output function



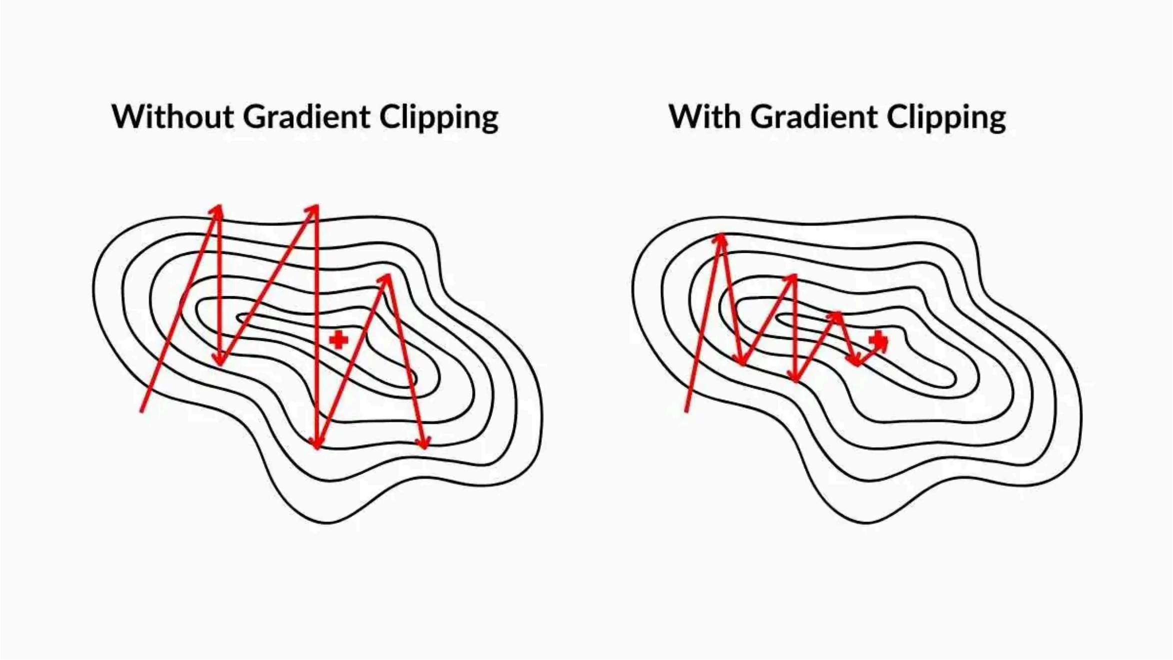
RNN Hands on

RNN Forward Pass & Unrolling ➡️

- **Unrolled view**:
  RNN can be seen as a deep network with many copies of the same layer

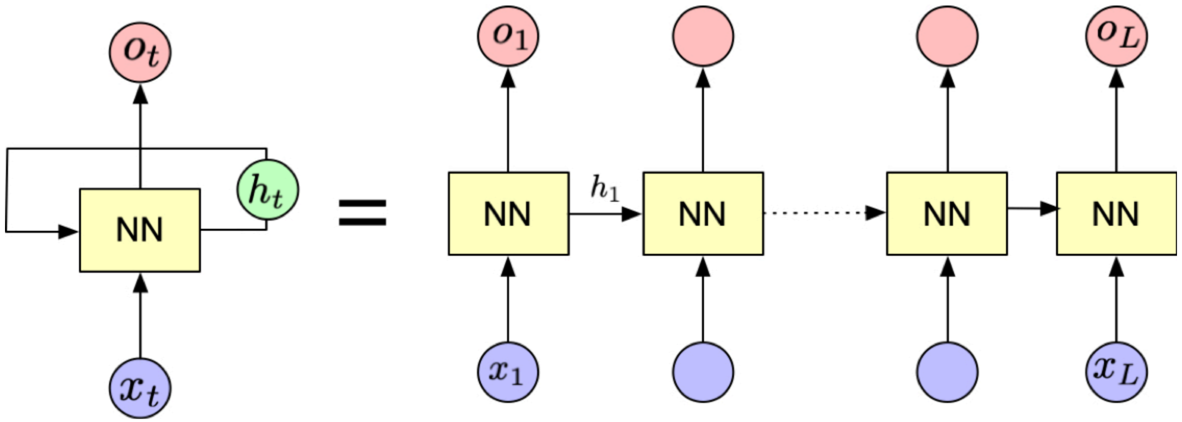


- **Backpropagation Through Time (BPTT)**:
  The gradient is backpropagated backward through time



How to train RNN

- **Unrolled view**:
  RNN can be seen as a deep network with many copies of the same layer



- **Backpropagation Through Time (BPTT)**:
  The gradient is backpropagated backward through time

- We train an RNN with parameter W to minimize objective $\mathcal{L}$.
- $\mathcal{L}$ is a function of the last output o_T from RNN at time T (e.g., MSE).
- Update the weight based on the gradient:

$$W := W - \underbrace{\eta}_{\substack{\text{learning}\\\text{rate}}} \underbrace{\frac{\partial \mathcal{L}}{\partial W}}_{\text{gradient}}$$

Because W is reused at each time step, we need to accumulate gradients.

$$\frac{\partial L}{\partial W} = \sum_{t=1}^{T} \frac{\partial \mathcal{L}}{\partial h_t} \frac{\partial h_t}{\partial W}$$

How to train RNN (cont.)

Using the chain rule, we can calculate how changes in a hidden state h_t affect the final loss $\mathcal{L}$:

$$\frac{\partial \mathcal{L}}{\partial h_t} = \frac{\partial \mathcal{L}}{\partial o_T} \frac{\partial o_T}{\partial h_T} \frac{\partial h_T}{\partial h_{T-1}} \cdots \frac{\partial h_{t+1}}{\partial h_t}$$

where:

- $\frac{\partial \mathcal{L}}{\partial o_t}$ shows how the loss changes with the output
- $\frac{\partial o_T}{\partial h_T}$ captures how the hidden state influences the output

🤔 **Question**

Compute the gradient:

$$\frac{\partial \mathcal{L}}{\partial h_1}$$

for the following setting:

- $T = 2$
- $\mathcal{L} = (y_T - o_T)^2$
- $o_t = w_1 h_t$
- $h_t = \tanh(w_2 x_t + w_3 h_{t-1})$

Hint: $\partial \tanh(x)/\partial x = 1 - \tanh(x)^2$

💡 Answer

First, using the chain rule:

$$\frac{\partial \mathcal{L}}{\partial h_1} = \frac{\partial \mathcal{L}}{\partial o_2}\frac{\partial o_2}{\partial h_2}\frac{\partial h_2}{\partial h_1}$$

Let's solve each term:

- $\dfrac{\partial \mathcal{L}}{\partial o_2} = -2(y_2 - o_2)$
- $\dfrac{\partial o_2}{\partial h_2} = w_1$
- $\dfrac{\partial h_2}{\partial h_1} = w_3(1 - \tanh^2(w_2 x_2 + w_3 h_1))$

Putting it all together:

$$\frac{\partial \mathcal{L}}{\partial h_1} = -2(y_2 - o_2)w_1 w_3 \times (1 - \underline{\tanh}^2(w_2 x_2 + w_3 h_1))$$

Vanishing Gradient Problem 📉

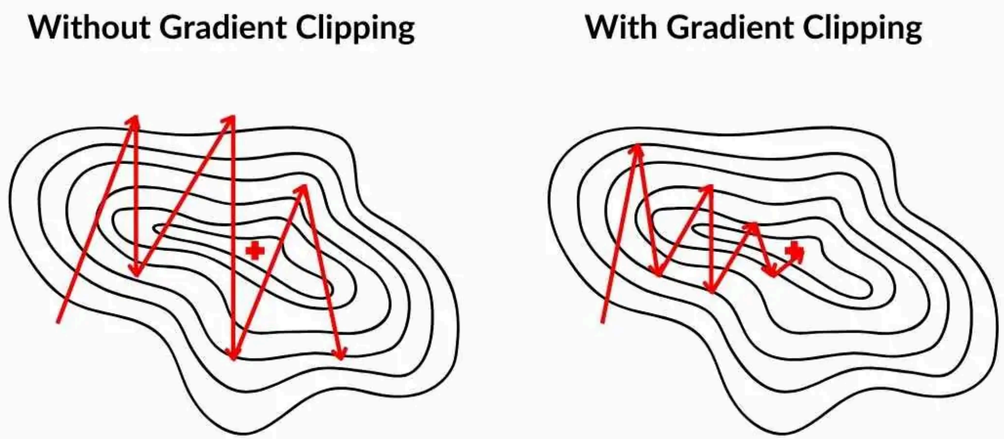
- Gradients shrink (or explode) through many time steps
- *Example* :
  - If $\tanh(x) = 0.5$ and $T = 10$, then the gradient is reduced by a factor of $(0.25)^{10} \approx 0.0000001$

> ### 💭 Intuition
>
> An RNN forgets some bits of information through time, and the final state becomes effectively independent of early inputs, leading to nearly zero gradients for them.

Gradient Clipping

- Normalize the gradient to have a fixed norm.
- Example (clipping by norm):
  If the gradient norm exceeds a threshold α, scale parameters by dividing by their norm:

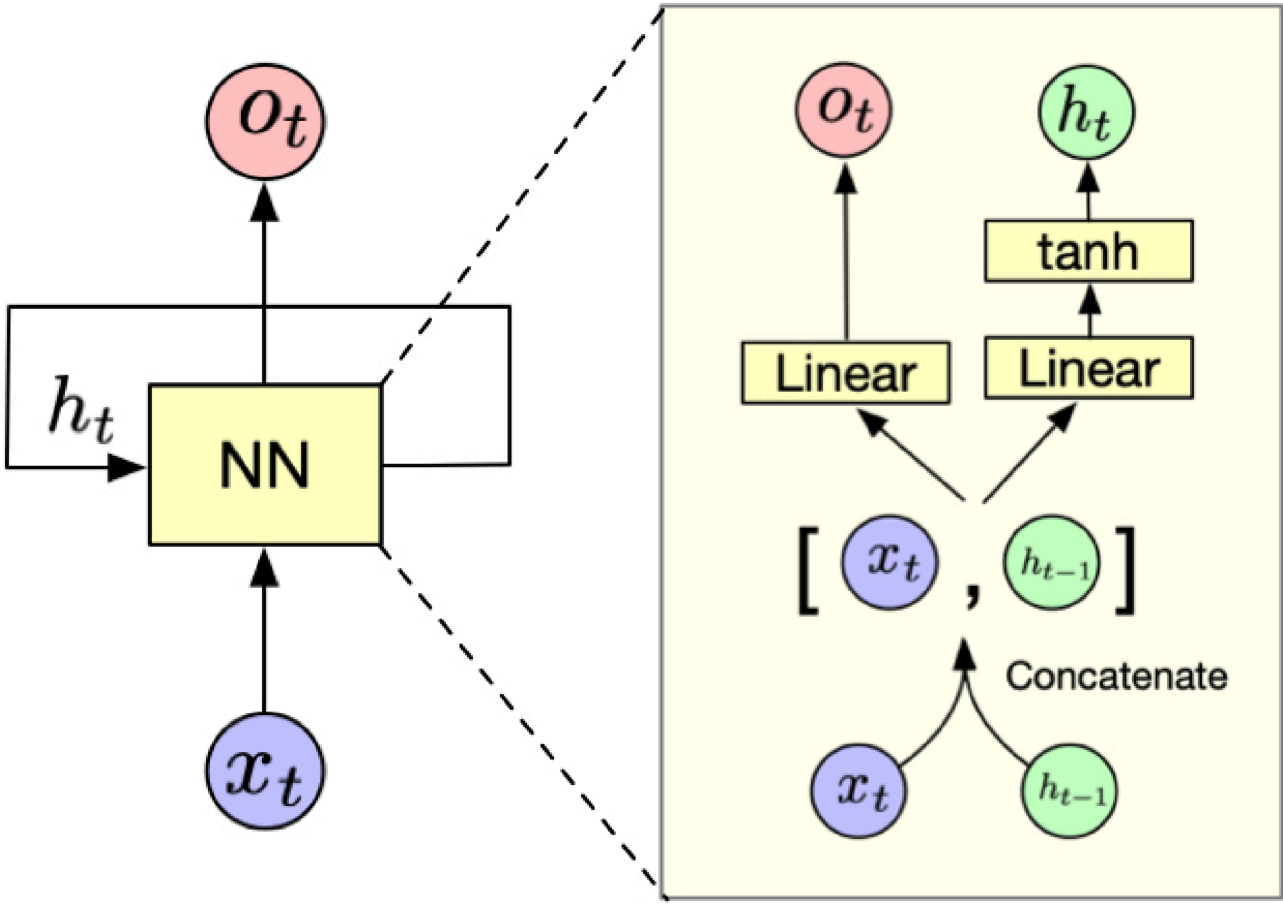
$$w_i \leftarrow \alpha \frac{w_i}{\sqrt{\sum_j w_j^2}}$$



Demo: Training an RNN with PyTorch

LSTM (1)

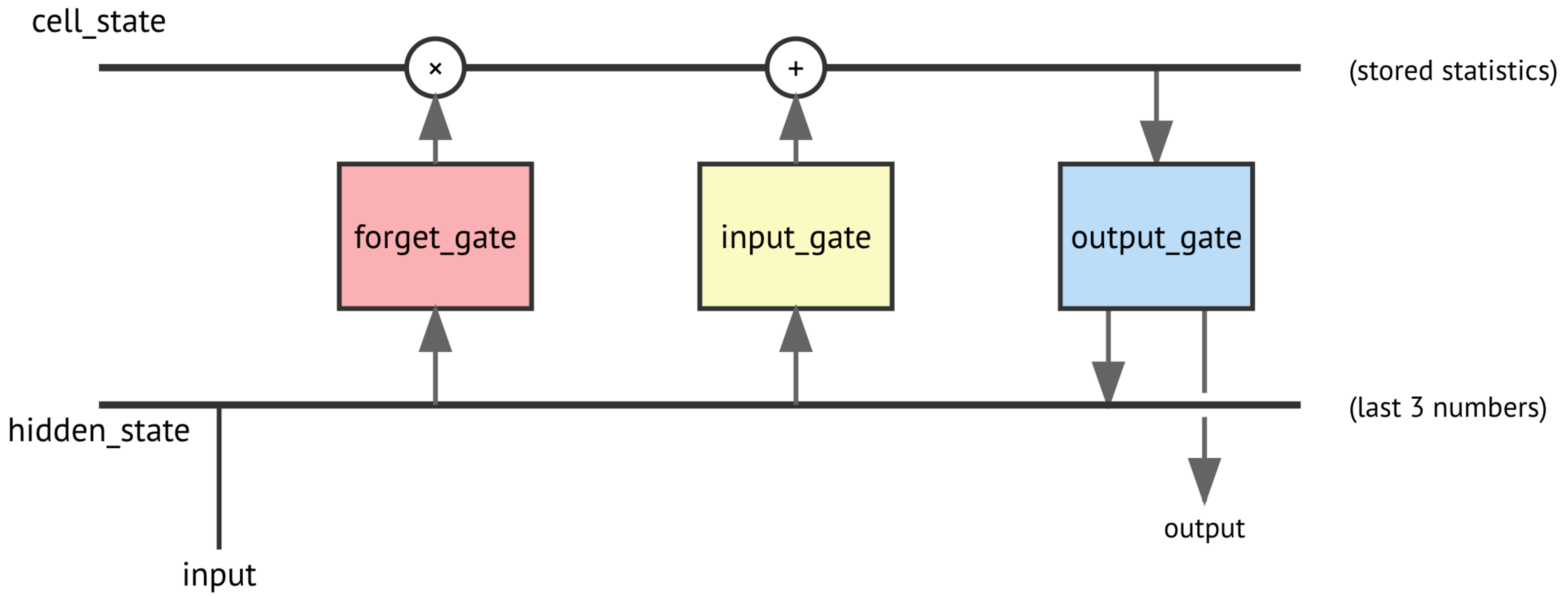
- In a simple RNN, we let a neural network to figure out how to structure and update the memory (hidden state) 🧠
  - Not easy for a neural network to learn how to do this from scratch
- We can introduce a structure to learn how to update the memory (hidden state) 🔄
- What are the key operations in human memory systems? 🤔



LSTM (2)

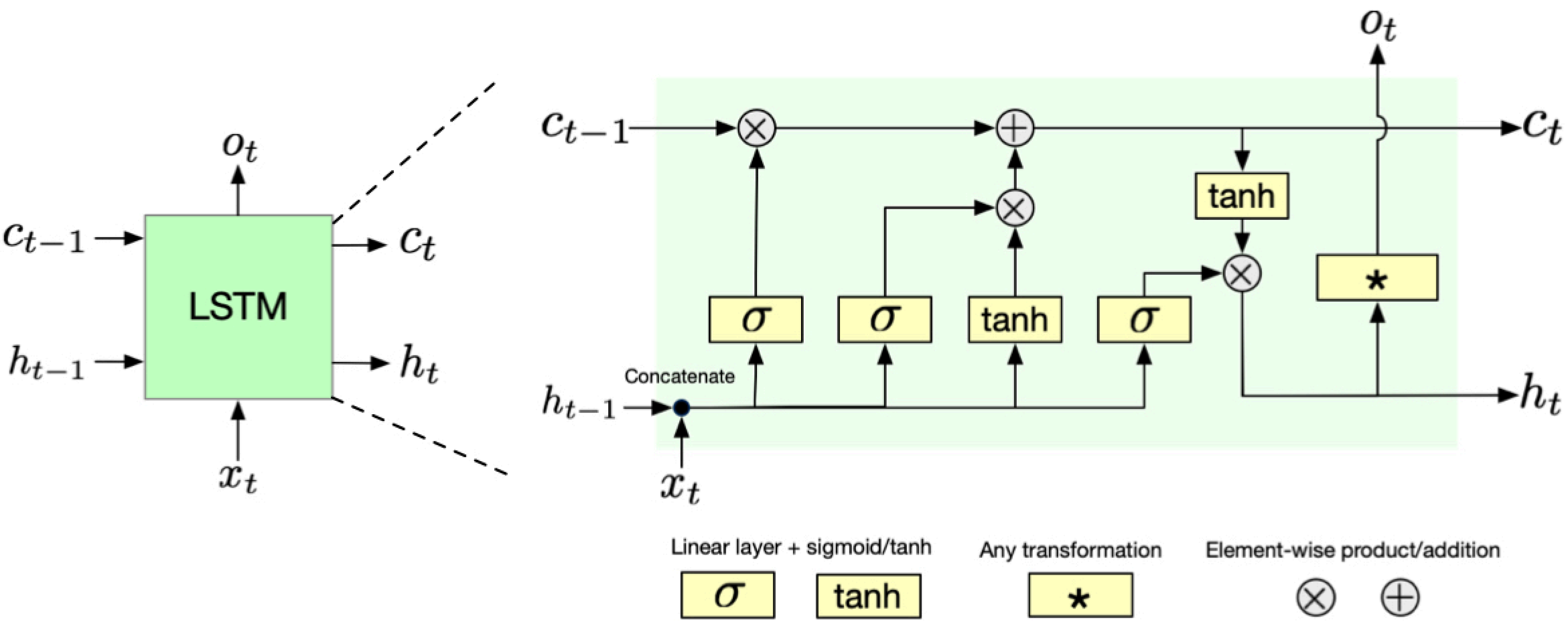
- Memory operations 🧠:
  - **Forget** 🗑️: discard old info
  - **Add** ➕: store new info
  - **Retrieve** 🔍: access stored info
- Memory types 💭:
  - **Long-term** 📚: knowledge & experiences
  - **Short-term** 💡: current processing

LSTM (3)



cell_state
×
+
(stored statistics)
forget_gate
input_gate
output_gate
hidden_state
(last 3 numbers)
input
output

LSTM (4)


o_t
c_{t-1}
c_t
LSTM
h_{t-1}
h_t
x_t
o_t
c_{t-1}
c_t
tanh
*
σ
σ
tanh
σ
Concatenate
h_{t-1}
h_t
x_t
Linear layer + sigmoid/tanh
σ
tanh
Any transformation
*
Element-wise product/addition

LSTM (5)

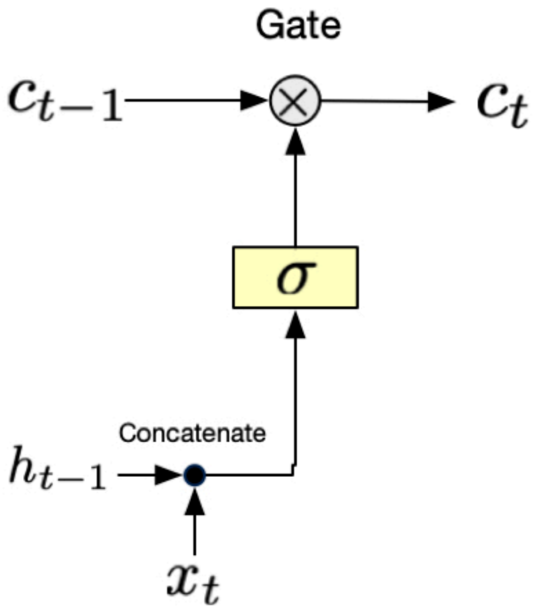
Forget Gate

Decides what to forget from cell state

$$f_t = \sigma(W_f \cdot [h_{t-1}, x_t] + b_f)$$

- Simoid σ squashes values between 0 and 1
- W_f and b_f are learnable parameters
- h_{t-1} and x_t are the inputs

> 💭 **Intuition**
>
> Think of it as a filter 🧠 that looks at previous (h_{t-1}) and new (x_t) info, deciding what to keep (1) or forget (0).



Example

$$c_{t-1} = [0.1, 0.3, -0.9]$$

$$\sigma(x_t, h_t) = [1.0, 0.2, 0.0]$$

$$c_t = [0.1, 0.06, 0.0]$$

LSTM (6)

Input Gate

Decide what new information to store in cell state.

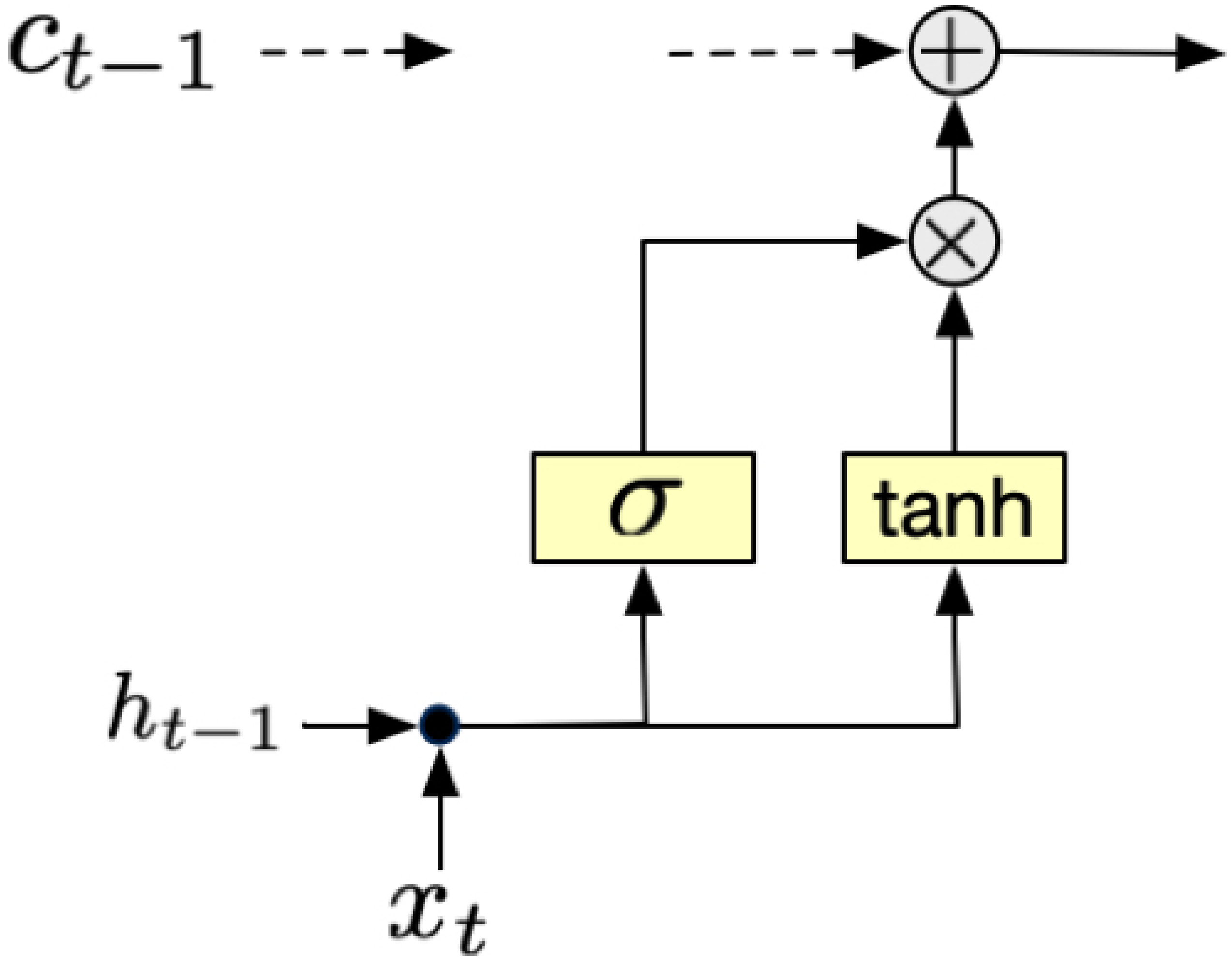
$$C_t = \underbrace{i_t}_{\text{Filter}} \quad \underbrace{\odot}_{\substack{\text{Element-wise} \\ \text{multiplication}}} \quad \underbrace{\tilde{C}_t}_{\text{Candidate update}}$$

Where the candidate update:

$$\tilde{C}_t = \tanh(W_c[h_{t-1}, x_t] + b_c)$$

And filter:

$$i_t = \sigma(W_i \cdot [h_{t-1}, x_t] + b_i)$$



LSTM (7)

Output Gate

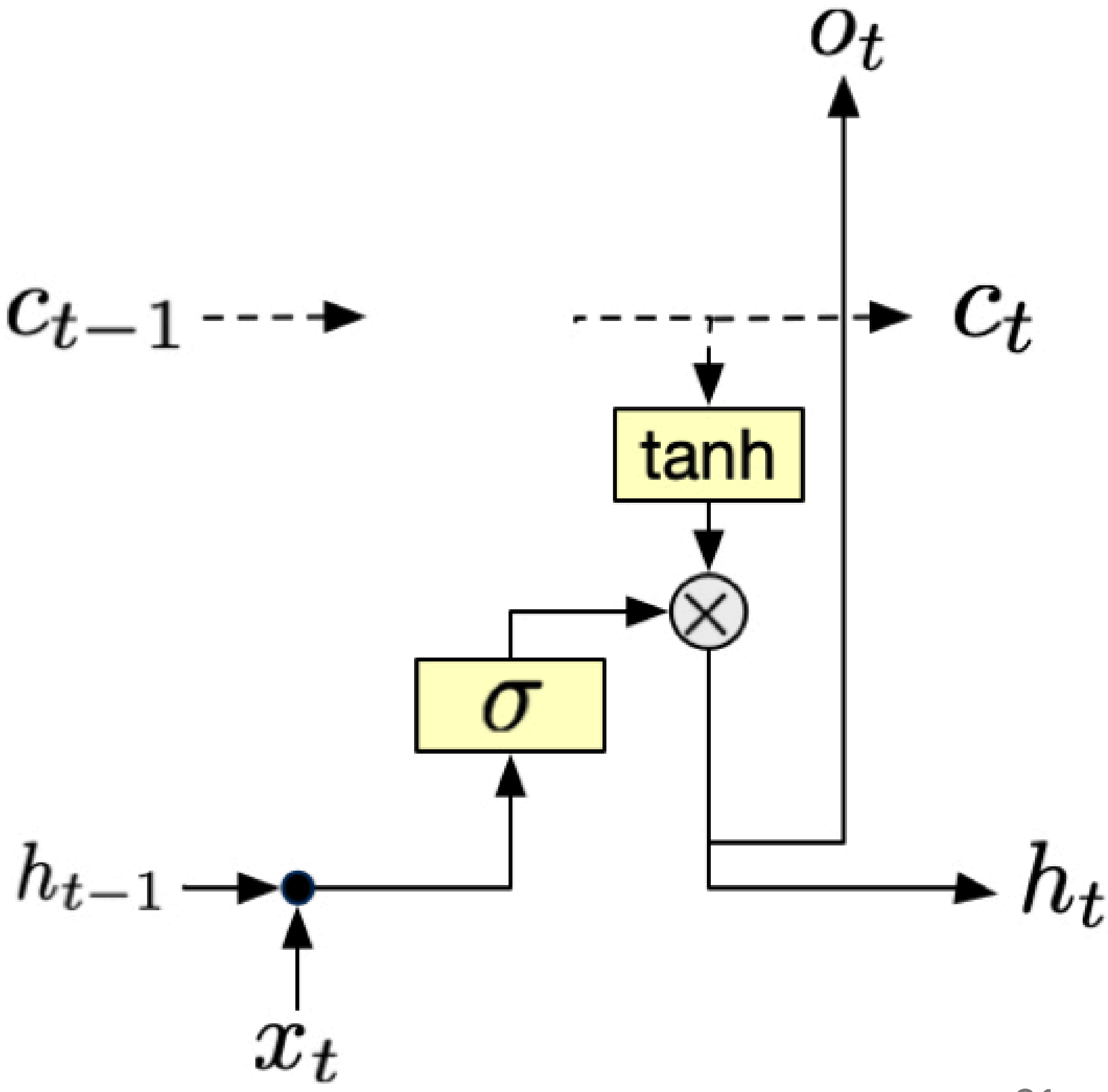
Decides what to output from the cell state.

$$o_t = \sigma(W_o \cdot [h_{t-1}, x_t] + b_o)$$

- Sigmoid σ squashes values between 0 and 1
- W_o and b_o are learnable parameters
- h_{t-1} and x_t are the inputs

and the hidden state is updated as:

$$h_t = o_t \odot \tanh(C_t)$$



LSTM (8)

Putting it all together:

Cell State Update

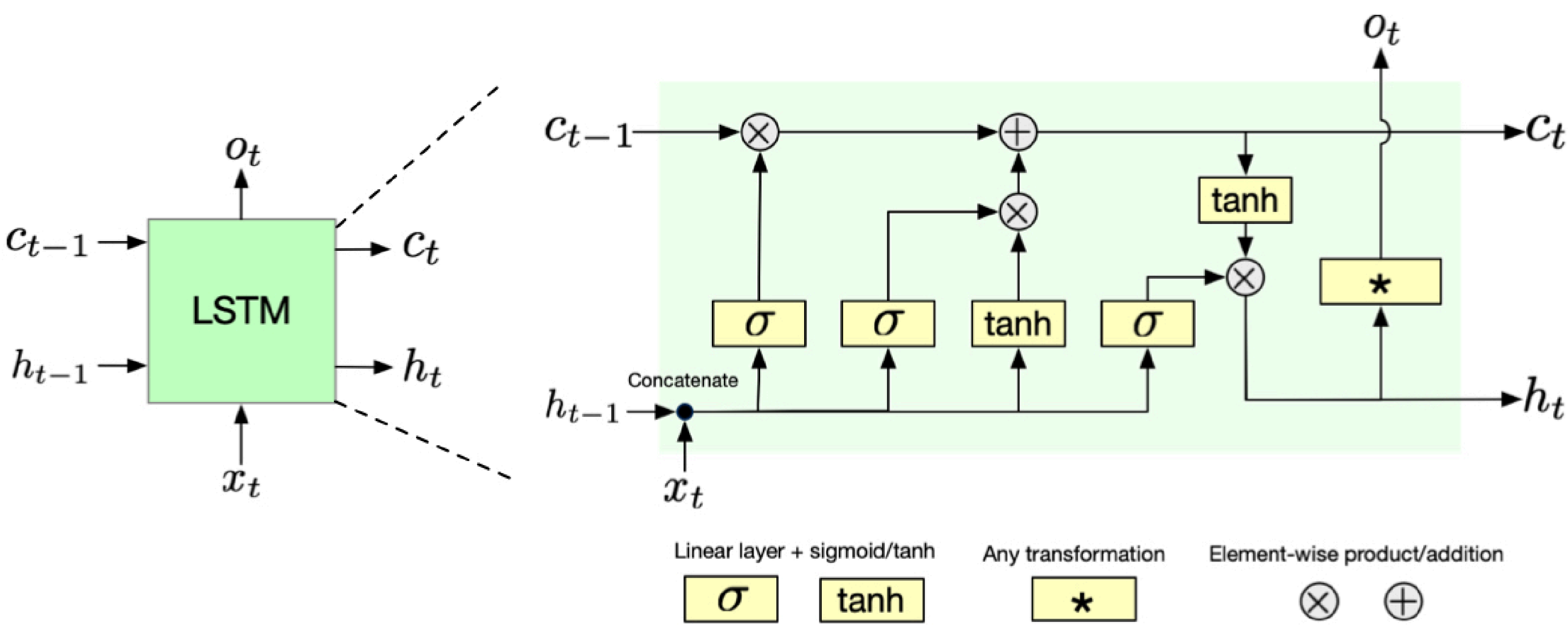
$$C_t = f_t \odot C_{t-1} + i_t \odot \tilde{C}_t$$

Hidden State Update

$$h_t = o_t \odot \tanh(C_t)$$

Gates

$$f_t = \sigma(W_f[h_{t-1}, x_t] + b_f)$$
$$i_t = \sigma(W_i[h_{t-1}, x_t] + b_i)$$
$$o_t = \sigma(W_o[h_{t-1}, x_t] + b_o)$$



Interactive Notebook: Memory Challenge

Key advantage of LSTM

🤔 **Question**

LSTM mitigates the problem of gradient vanishing problem. To see this, let us calculate:

$$\frac{\partial C_t}{\partial C_{t-1}}$$

where:

$$C_t = f_t \odot C_{t-1} + i_t \odot \tilde{C}_t$$

- f_t is the forget gate
- i_t is the input gate
- $\tilde{C}_t$ is the candidate update
- $\odot$ is the element-wise product

💡 **Answer**

The derivative of the cell state is:

$$\frac{\partial C_t}{\partial C_{t-1}} = f_t$$

where f_t is time-varying but controlled by the forget gate. If the long-term memory is useful for the task, LSTM can easily retain the memory by setting f_t to 1.

For RNN with $h_t = \tanh(Wh_{t-1} + Ux_t + b)$, the derivative of the hidden state is:

$$\frac{\partial h_t}{\partial h_{t-1}} = \mathrm{diag}(1 - h_t^2)W.$$

- When $h_t^2 \simeq 1$ (which is the case when $h_t \gg 0$ or $h_t \ll 0$), the gradient vanishes.

💡 **Answer**

> (Cont) For RNN with $h_t = \tanh(Wh_{t-1} + Ux_t + b)$:
> $$\frac{\partial h_t}{\partial h_{t-1}} = \mathrm{diag}(1 - h_t^2)W.$$

- Even if $h_t^2 \simeq 0$, the gradient can still vanish or explode. To see this, notice that W is time-invariant, and multiplied many times through backpropagation (cont). To simplify, let us assume $h_t = 0$ for all t. Then the gradient is:

$$\frac{\partial \mathcal{L}}{\partial h_t} = \frac{\partial \mathcal{L}_t}{\partial h_t} + W^T \frac{\partial \mathcal{L}_{t+1}}{\partial h_{t+1}} + (W^T)^2 \frac{\partial \mathcal{L}_{t+2}}{\partial h_{t+2}} + \cdots + (W^T)^{T-t} \frac{\partial \mathcal{L}_T}{\partial h_T}$$

- The gradient magnitude depends on the spectrum radius ρ of W (its largest eigenvalue in absolute value). When this radius exceeds 1, the gradient explodes, and vice versa.
- Only when $\rho(W) = 1$, the gradient does not vanish or explode, which is hard to achieve unless we constrain W to be so.

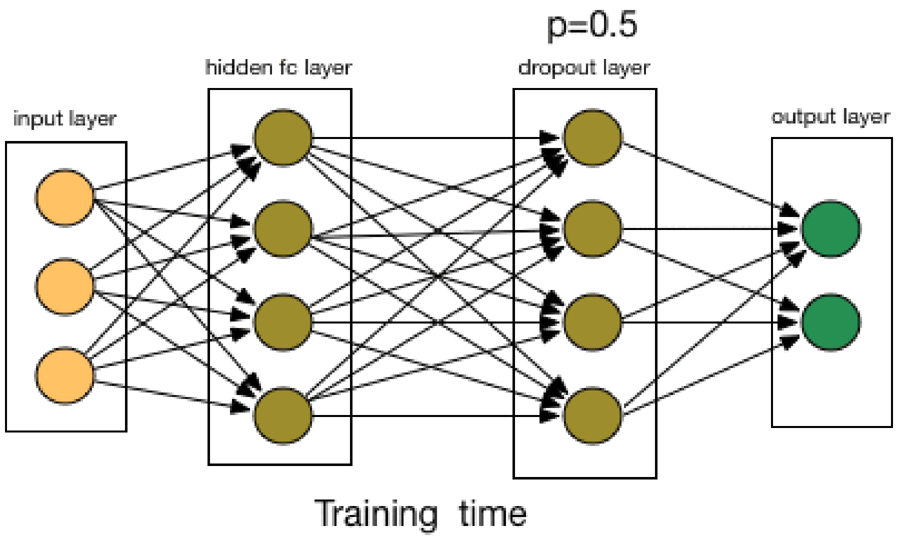
Another issue: Overfitting

- Simple RNN with D_h dimensional hidden state and D_i dimensional input:
  - Weight matrix for hidden state update: $D_h \times (D_h + D_i)$
  - Bias term: D_h
  - Total parameters: $D_h(D_h + D_i + 1)$
- For LSTM:
  - Three gates (input, forget, output) + (candidate cell state generation)
  - Each has a weight matrix of size $D_h \times (D_h + D_i)$ and bias term of size D_h
  - Total parameters: $4D_h(D_h + D_i + 1)$
  - Large number of parameters can lead to overfitting
- LSTM has more parameters, more expressiveness, and thus is more prone to overfitting.

Dropout Regularization

- Randomly "drop" (set to 0) some neurons during training
- Forces network to be redundant, more robust
- Prevents the model to be dependent on a few neurons

> ℹ️ **Note**
>
> During inference (testing), we don't drop any neurons but scale outputs by p to maintain expected value.



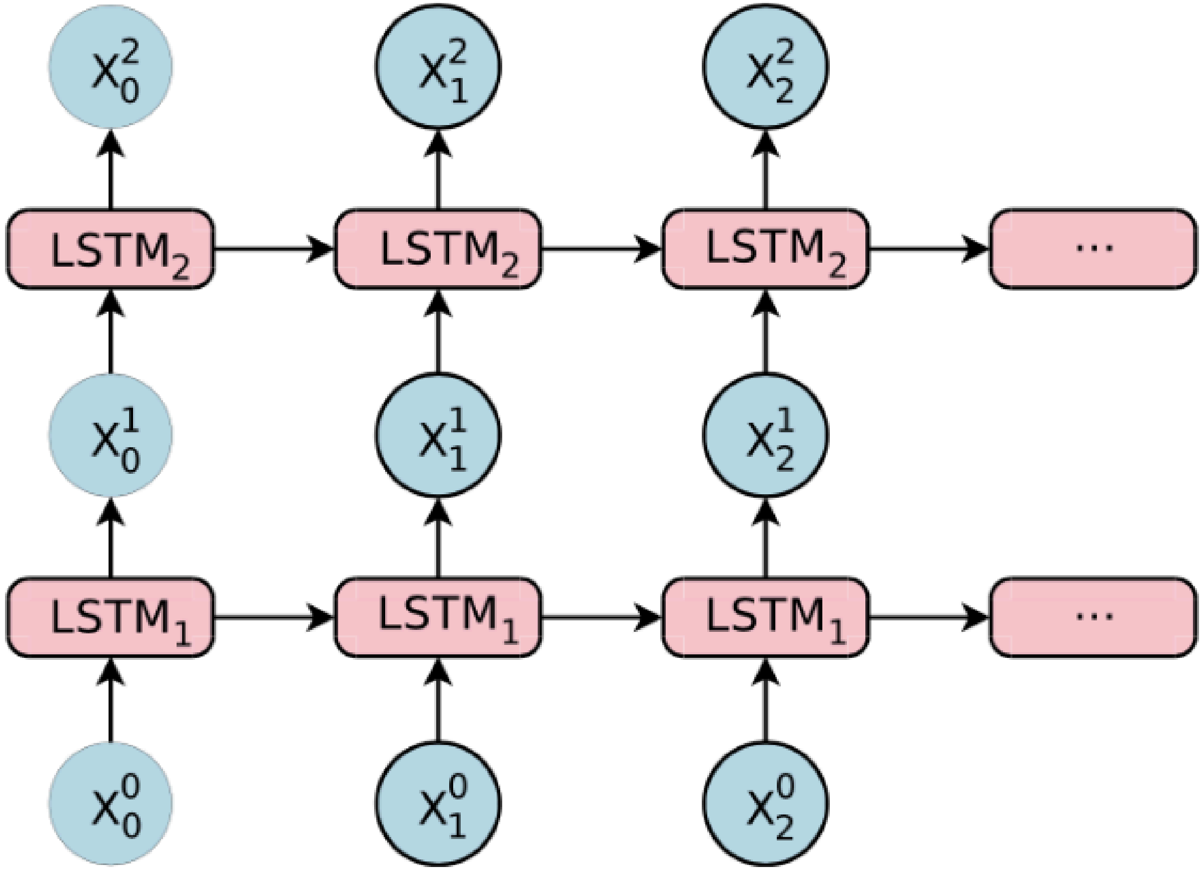
GRU (Gated Recurrent Unit)

- A simplified version of LSTM
- Less parameters and easier to train
- But less powerful than LSTM

> ℹ️ **Note**
>
> GRU has only the hidden state h_t.

Stacked LSTM

- Multiple LSTM layers stacked vertically
- Each layer's hidden state becomes input for the next layer
- **Progressive Abstraction**:
  - Each layer learns increasingly complex temporal representations
  - Lower layers capture concrete, local patterns (e.g., basic syntax, immediate trends)
  - Higher layers transform local features into abstract patterns



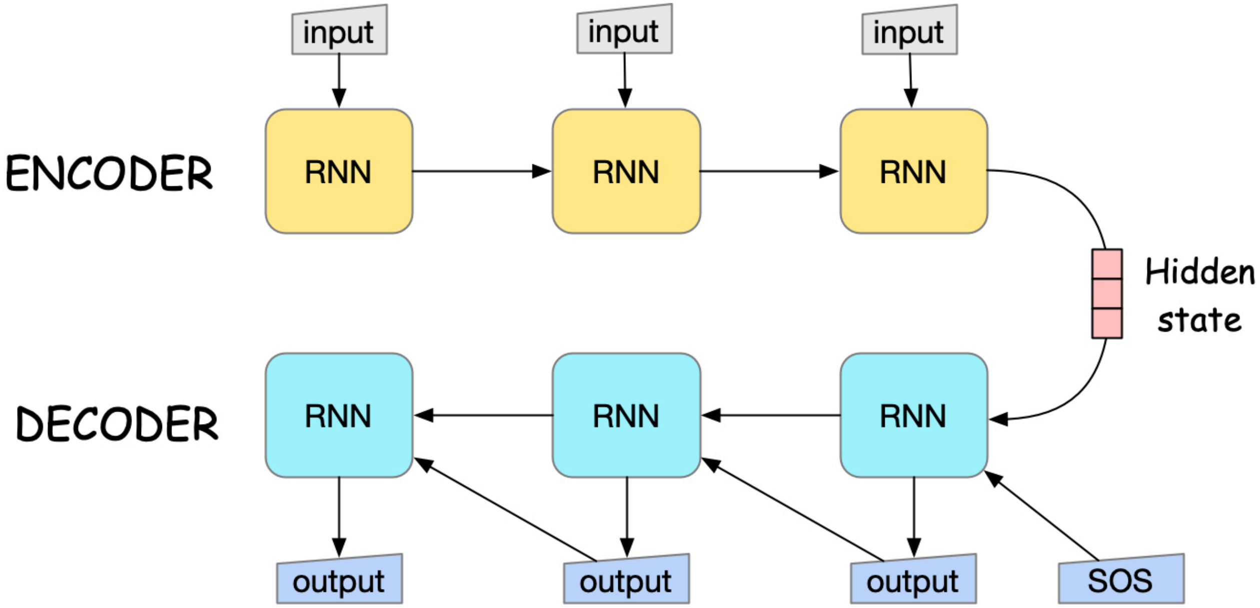
Embedding from Language Models (ELMo) 🪄

- Generate *contextualized* word embeddings:
    - Example: “Bank” in finance vs. “bank” of a river. word2vec assigns the same embedding to both. ELMo assigns different embeddings to each based on the context
- Stacked *Bidirectional* LSTMs that read words in both directions
- Character-level CNN: handle out-of-vocab words
- State-of-the-art before Transformer

Demo: LSTM

Sequence-to-Sequence (Seq2Seq) ➡️

- *For translation, summarization, Q&A…*
- **Encoder**: reads input, outputs “context vector”
- **Decoder**: uses that context to generate new sequence
- [SOS] (Start of Sequence) token is used to indicate the beginning of the sequence for the decoder



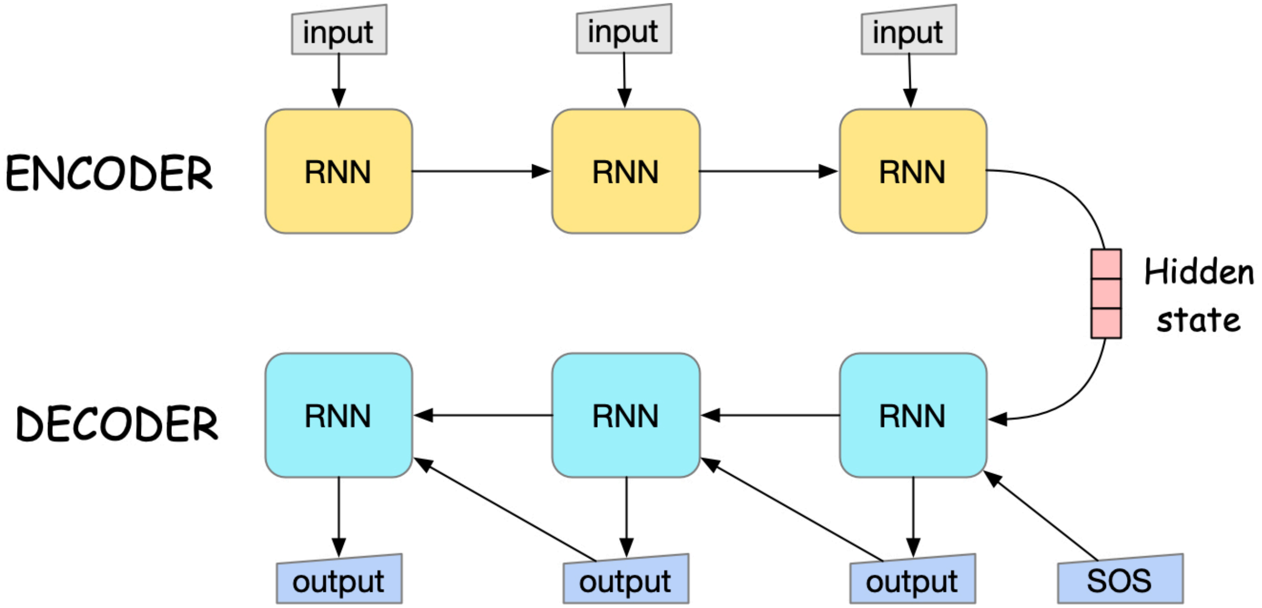
The hidden state of the encoder represents a "summary" of the input sequence.

right:100%

(Taken from Sutskever, I. (2014). Sequence to Sequence Learning with Neural Networks. arXiv preprint arXiv:1409.3215.)

Issue of Seq2Seq

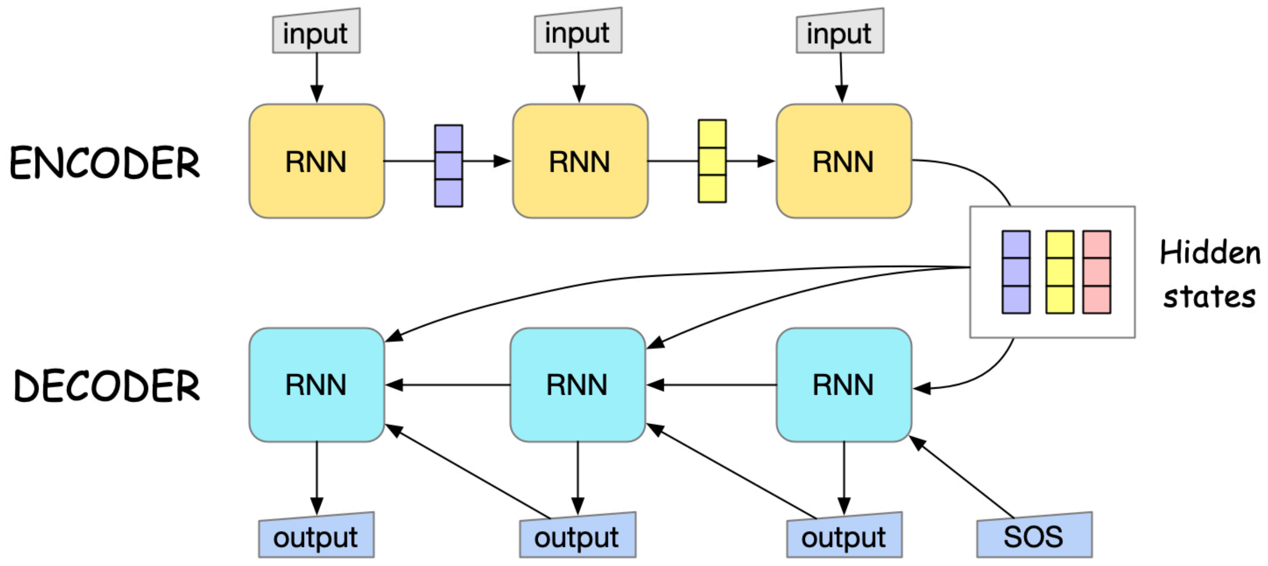
- Single "bottleneck" vector is limiting for long inputs



Attention Mechanism 👀

"Paying Focus Where It Matters"

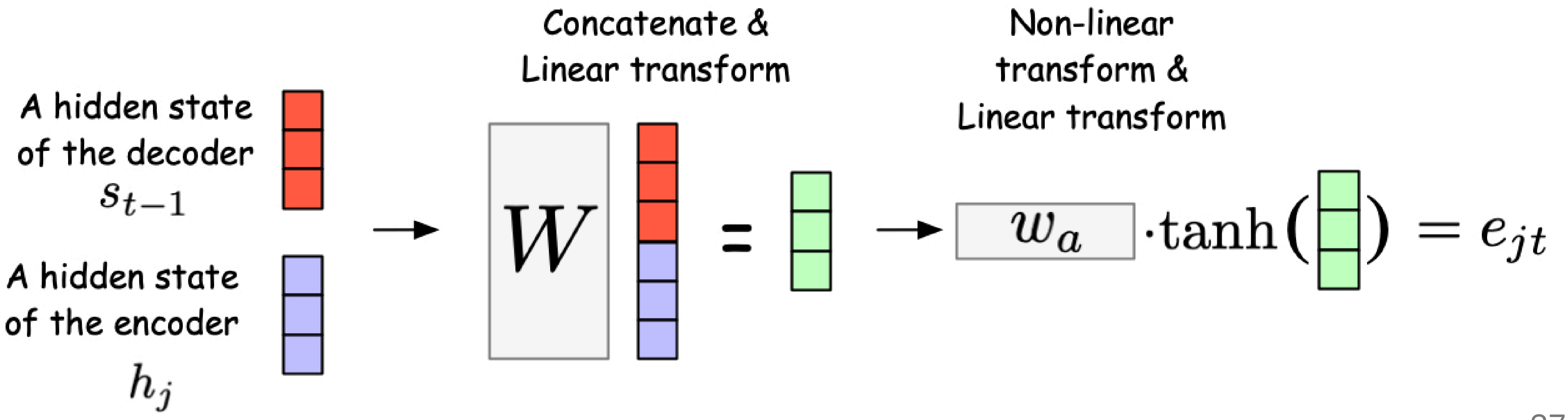
- Instead of a single context vector, **look** at all encoder states
- The decoder decides which parts to focus on each time step
- **Analogy**: A translator re-checks specific words in the source sentence as needed.



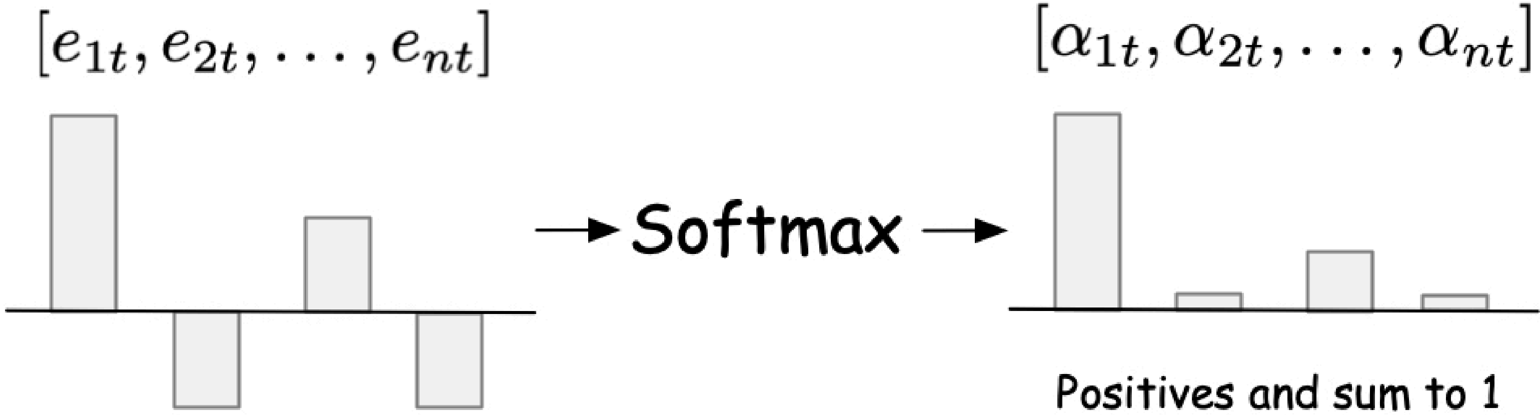
How Attention Works 🔍

1. **Compute score:** $e_{tj} = f(h_t, h_j^{\text{enc}})$

- h_t: the hidden state of the decoder at time t
- h_j^{enc}: the hidden state of the encoder at time j
- f: a function that computes the score (multilayer perceptron)

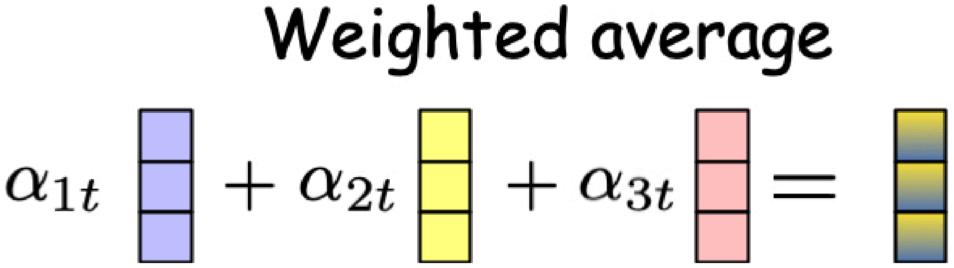


2. **Normalize** e_{tj} by softmax to get attention α_{tj} that sums to 1, i.e., $\sum_j \alpha_{tj} = 1$



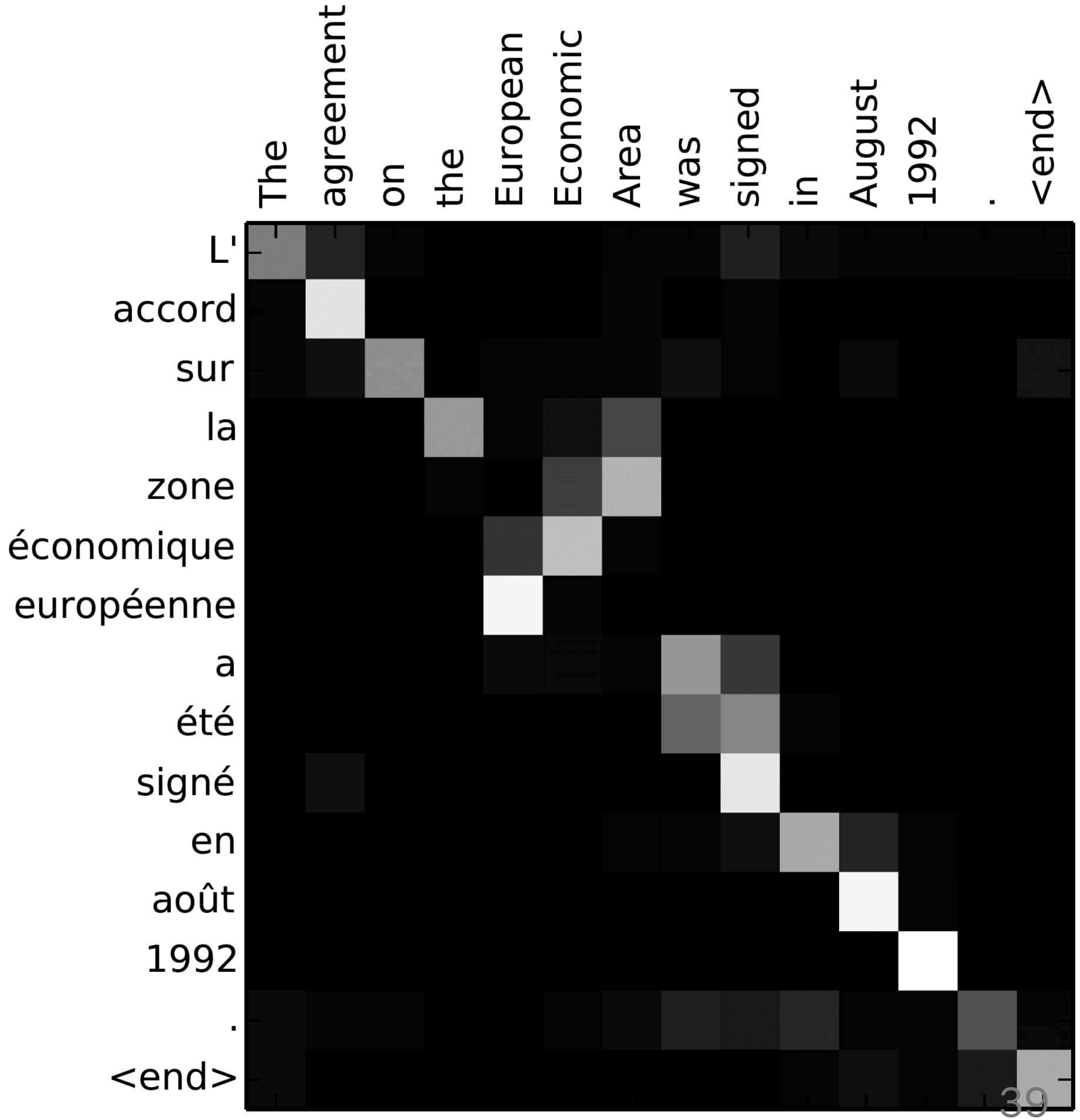
3. **Context Vector**:

$$c_t = \sum_j \alpha_{tj} h_j^{\text{enc}}$$



Example: Attention map

- Taken from the original paper: Bahdanau, D., Cho, K., & Bengio, Y. (2014). Neural Machine Translation by Jointly Learning to Align and Translate. CoRR, abs/1409.0473.
- English-French translation



Attention:

- Helps with **long-range** relationships
- Improves **interpretability** (which words are relevant?)
- Opened the door to **Transformers** (self-attention)

Conclusion & Next Steps 🎉

- **RNN**: first step for sequential data
- **LSTM**: gating for long-term memory
- **ELMo**: dynamic embeddings sensitive to context
- **Seq2Seq + Attention**: break free from bottleneck, focus on relevant parts

Beyond:

- **Transformers** (GPT, BERT)
- Large Language Models
- Advanced optimization & regularization