# Sequence-to-Sequence (Seq2Seq) Models

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#### Motivation



#### Why Do We Need Seq2Seq and Attention?

- Many real-world problems require transforming one sequence to another:
  - Translation: "Bonjour" → "Hello"
  - Dialogue systems: Question → Response
  - Speech: Audio → Text

Standard RNNs struggle with input/output sequences of different lengths and long-term dependencies.

Seq2Seq models + attention solve this with a powerful encoder-decoder framework.

#### Learning Outcomes



By the end of this session, you should be able to:

- Explain the Seq2Seq architecture and encoder-decoder framework
- Understand the bottleneck problem in fixed-size representations
- Describe the motivation for and core idea behind attention mechanisms
- Appreciate how attention improves performance in NLP tasks
- Recognize future directions in attention-based modeling

#### Seq2Seq Architecture



**Key Idea:** Map input sequence  $\rightarrow$  intermediate vector  $\rightarrow$  output sequence.

- Encoder RNN: Processes input sequence and compresses it into a fixed-length vector (context).
- ▶ Decoder RNN: Generates output sequence from the context vector.

#### **Applications:**

- ► Machine translation
- Summarization
- Dialogue systems
- Speech recognition

#### Sequence to sequence models

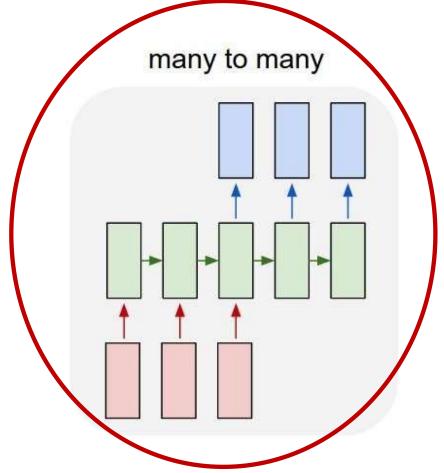






- Sequence goes in, sequence comes out
- No notion of "time synchrony" between input and output
  - May even not even maintain order of symbols
    - E.g. "I ate an apple" [] "Ich habe einen apfel gegessen"
  - Or even seem related to the input
    - E.g. "My screen is blank" [] "Please check if your computer is plugged in."



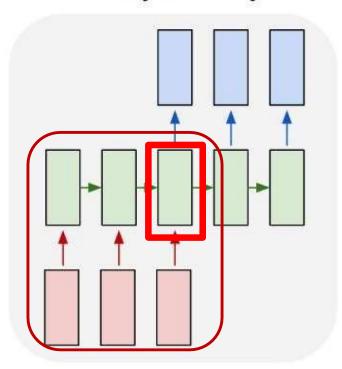


• *Delayed* sequence to sequence



#### many to many

First process the input and generate a hidden representation for it

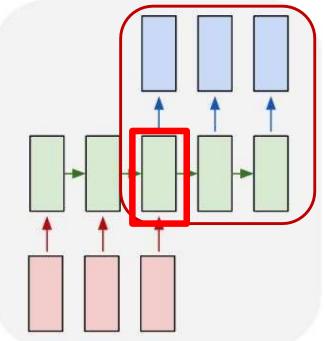


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many to many

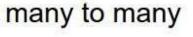
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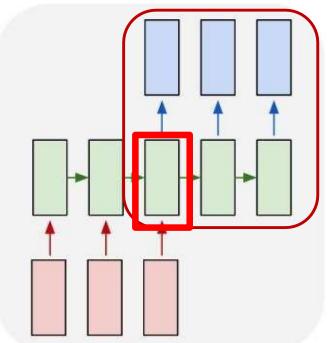
Then use it to generate an output

• *Delayed* sequence to sequence





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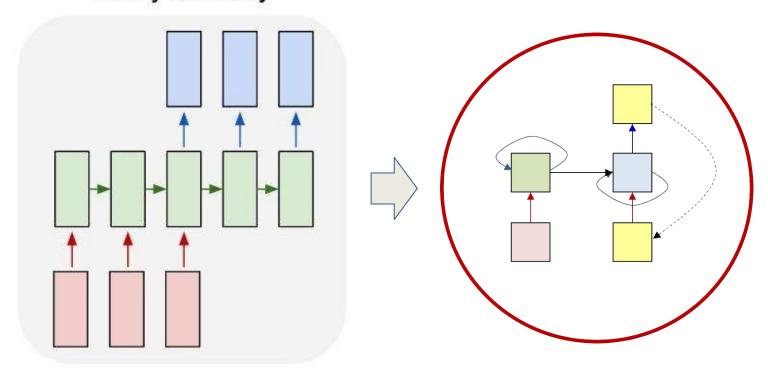


Then use it to generate an output

• *Problem:* Each word that is output depends only on current hidden state, and not on previous outputs

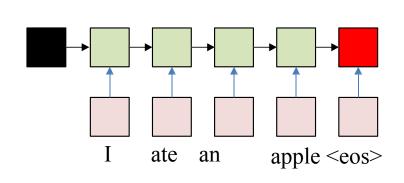


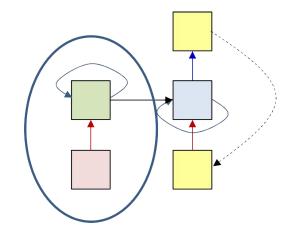
#### many to many



- *Delayed* sequence to sequence
  - Delayed self-referencing sequence-to-sequence

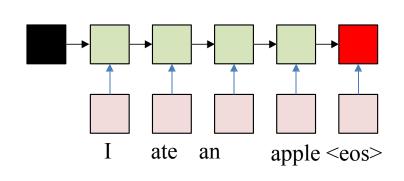


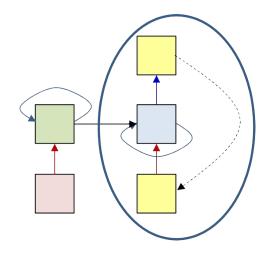




- The input sequence feeds into a recurrent structure
- The input sequence is terminated by an explicit <eos> symbol
  - The hidden activation at the <eos> "stores" all information about the sentence

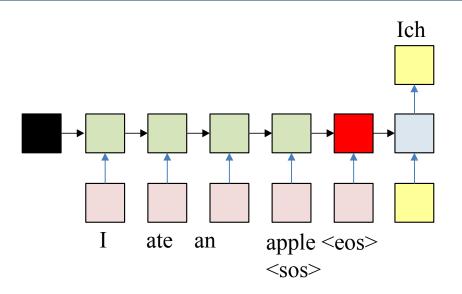






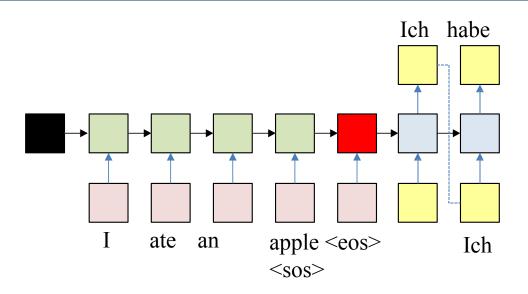
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- The input sequence is terminated by an explicit <eos> symbol
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- Subsequently a second RNN uses the hidden activation as initial state, and
   <sos> as initial symbol, to produce a sequence of outputs
  - The output at each time becomes the input at the next time
  - Output production continues until an <eos> is produced





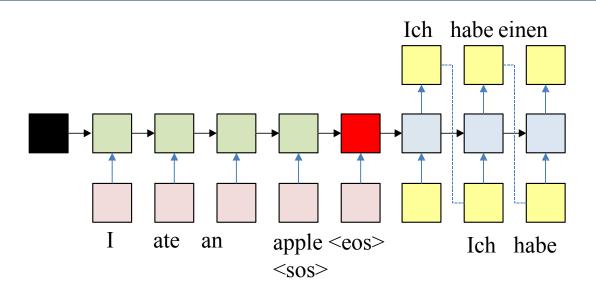
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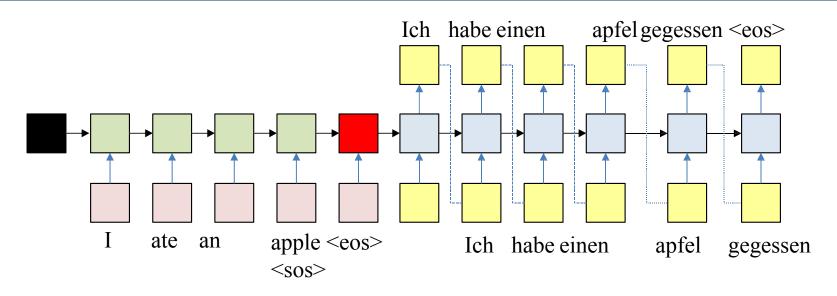
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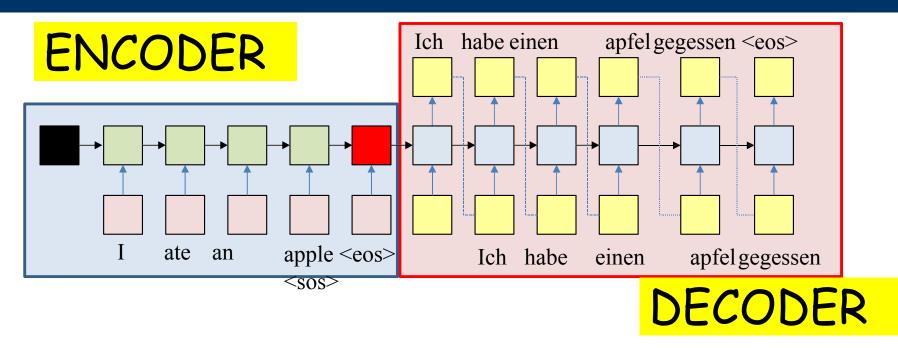
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- The recurrent structure that extracts the hidden representation from the input sequence is the *encoder*
- The recurrent structure that utilizes this representation to produce the output sequence is the *decoder*

#### The Bottleneck Problem



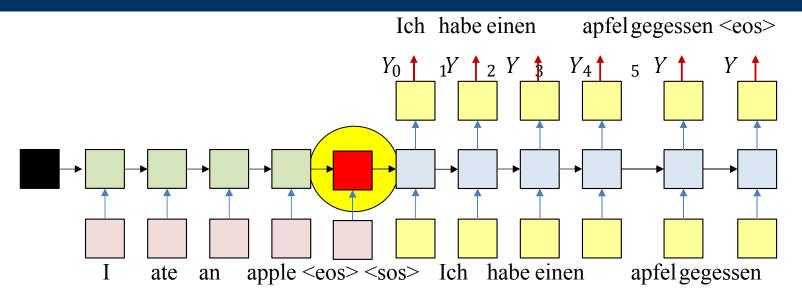
#### Fixed-length context vector = information bottleneck

- Encoder must compress entire input sequence into a single vector
- ▶ Longer or more complex inputs → information loss
- Decoder relies solely on that vector to produce outputs

Leads to poor performance on long sentences or tasks requiring high context awareness

#### A problem with this framework

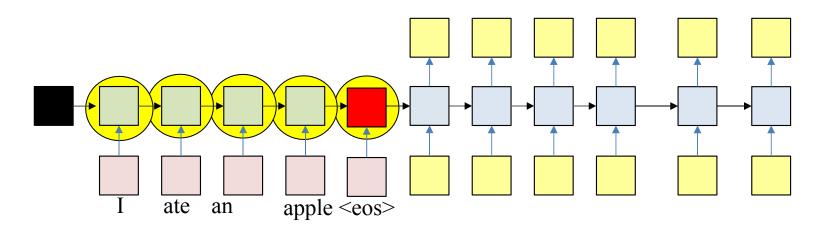




- All the information about the input sequence is embedded into a single vector
  - The "hidden" node layer at the end of the input sequence
  - This one node is "overloaded" with information
    - Particularly if the input is long

## A problem with this framework

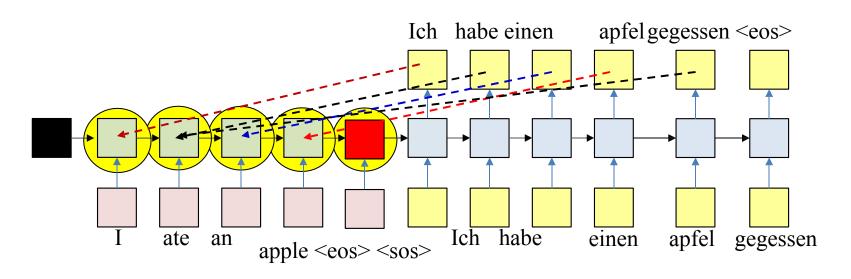




- In reality: All hidden values carry information
  - Some of which may be diluted by the time we get to the final state of the encoder

#### A problem with this framework





- In reality: All hidden values carry information

   Some of which may be diluted by the time we get to the final state of the encoder
- Every output is related to the input directly
  - Not sufficient to have the encoder hidden state to *only* the initial state of the decoder
  - Misses the direct relation of the outputs to the inputs

#### Realization: We Need More Context!



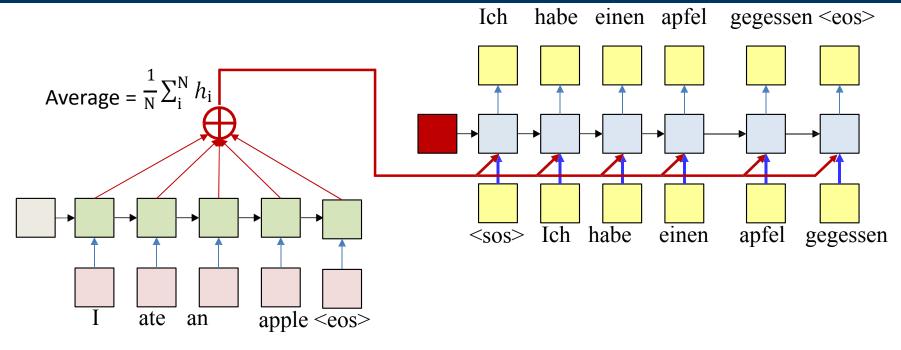
Decoder should have access to all encoder states, not just the final one.

This inspired the development of the attention mechanism.

Instead of passing only the final state, allow the decoder to "look back" at all input positions.



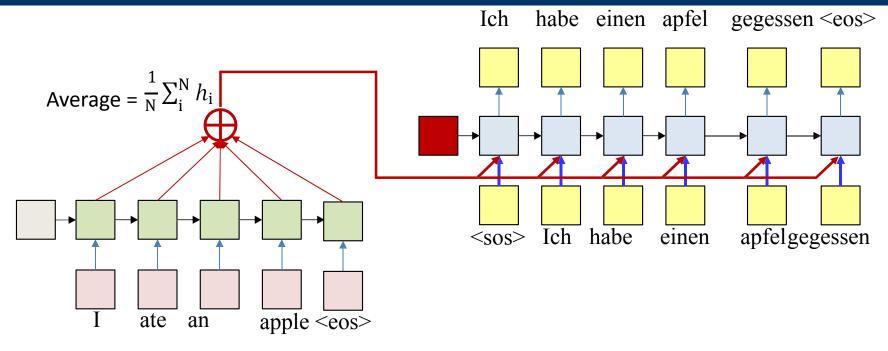




- Simple solution: Compute the average of all encoder hidden states
- Input this average to every stage of the decoder
- The initial decoder hidden state is now separate from the encoder
  - And may be a learnable parameter

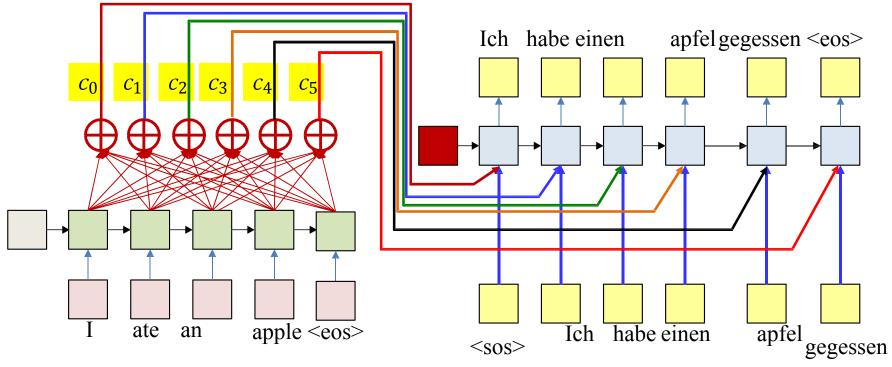






- Problem: The average applies the same weight to every input
- It supplies the same average to every output word
- In practice, different outputs may be related to different inputs
  - E.g. "Ich" is most related to "I", and "habe" and "gegessen" are both most related to "ate"

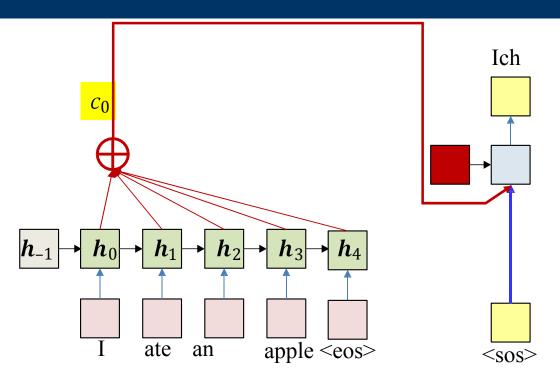




- Solution: Use a different weighted average for each output word
  - The weighted average provided for the kth output word is:

$$c = \frac{1}{N} \sum_{i}^{N} w(t)h$$

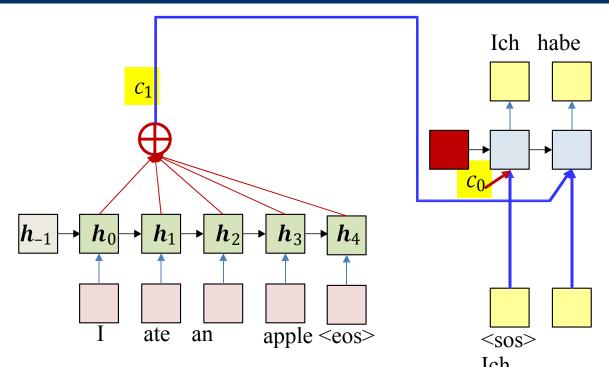




- Solution: Use a different weighted average for each output word
  - The weighted average provided for the kth output word is:

$$c_0 = \frac{1}{N} \sum_{i}^{N} w_i(0) h_i$$

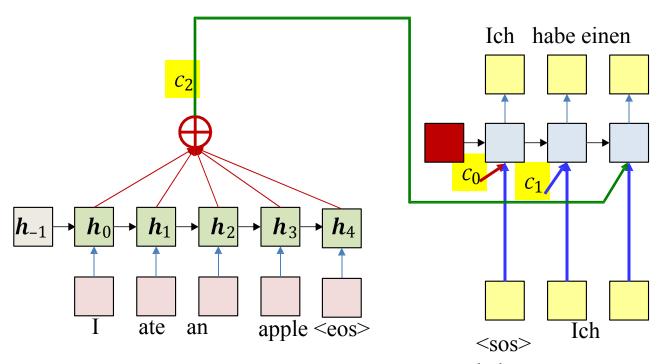




- Solution: Use a different weighted average for each output word
  - The weighted average provided for the kth output word is:

$$c_1 = \frac{1}{N} \sum_{i}^{N} w_i(1) h_i$$

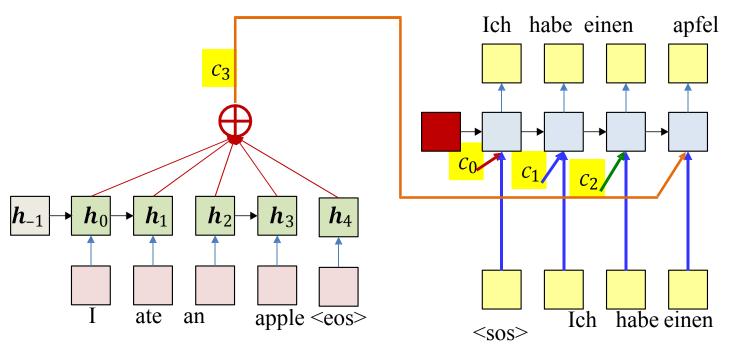




- Solution: Use a different weighted werage for each output word
  - The weighted average provided for the kth output word is:

$$c_2 = \frac{1}{N} \sum_{i}^{N} w_i(2) h_i$$

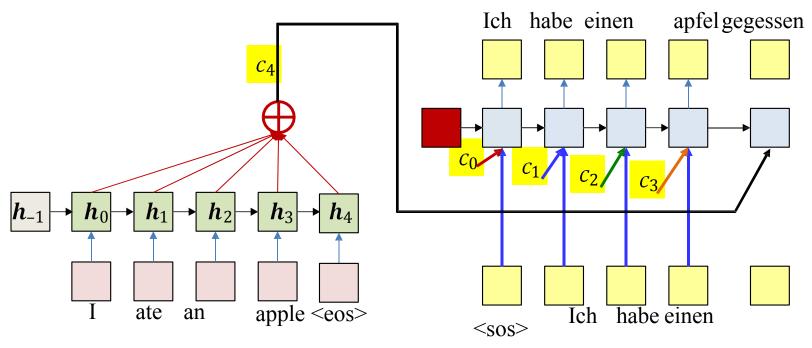




- Solution: Use a different weighted average for each output word
  - The weighted average provided for the kth output word is:

$$c_3 = \frac{1}{N} \sum_{i}^{N} w_i(3) h_i$$

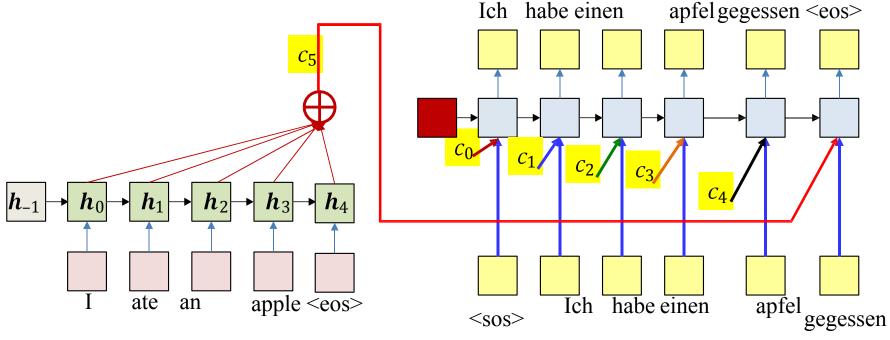




- Solution: Use a different weighted well-rage for each output word
  - The weighted average provided for the kth output word is:

$$c_4 = \frac{1}{N} \sum_{i}^{N} w_i(4) h_i$$

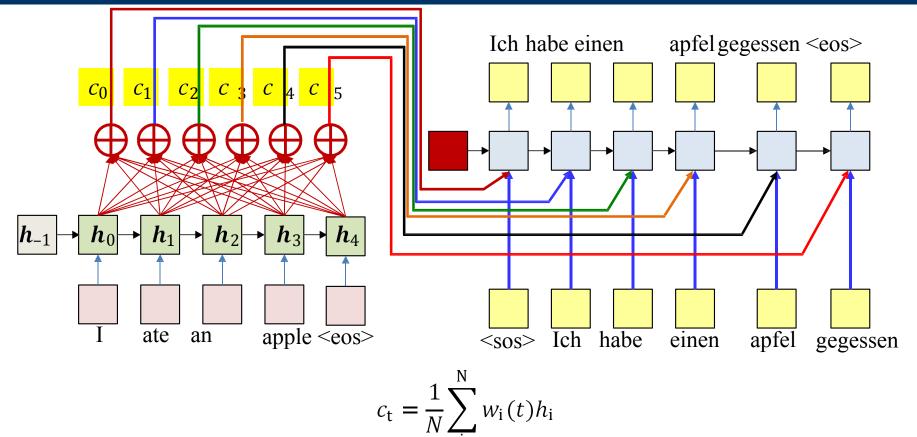




- Solution: Use a different weighted average for each output word
  - The weighted average provided for the kth output word is:

$$c_5 = \frac{1}{N} \sum_{i}^{N} w_i(5) h_i$$





- This solution will work if the weights  $w_{ki}$  can somehow be made to "focus" on the right input word
  - E.g., when predicting the word "apfel",  $w_3(4)$ , the weight for "apple" must be high while the rest must be low
- How do we generate such weights??

#### Introduction to Attention Mechanism



Core Idea: Let the decoder focus on different parts of the input sequence at each step of decoding.

- At each decoding step, compute a weighted sum over all encoder hidden states.
- Weights reflect relevance of each input word to the current output word.

"Soft search" over inputs → more context-awareness.

#### Mathematical Formulation of Attention



1. Alignment Score:

$$e_{t,s} = \text{score}(h_t^{\text{dec}}, h_s^{\text{enc}})$$

2. Attention Weights (Softmax):

$$\alpha_{t,s} = \frac{\exp(e_{t,s})}{\sum_{s'} \exp(e_{t,s'})}$$

3. Context Vector:

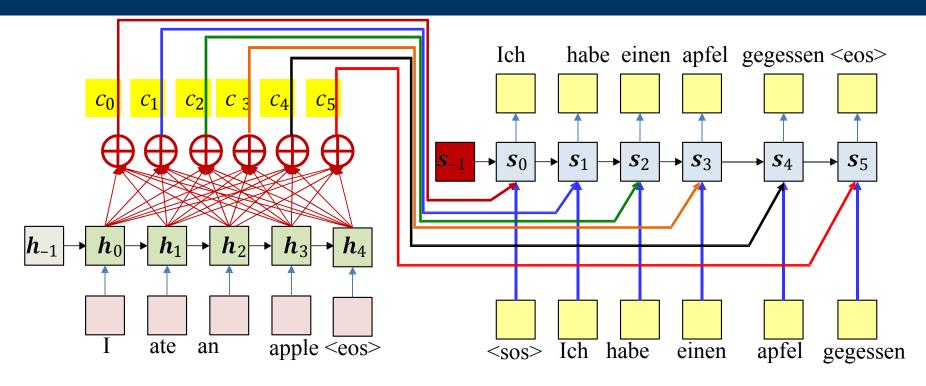
$$c_t = \sum_{s} \alpha_{t,s} h_s^{\mathsf{enc}}$$

4. Decoder Input:

$$y_t = \mathsf{Decoder}(y_{t-1}, h_{t-1}^{\mathsf{dec}}, c_t)$$

#### **Attention Models**





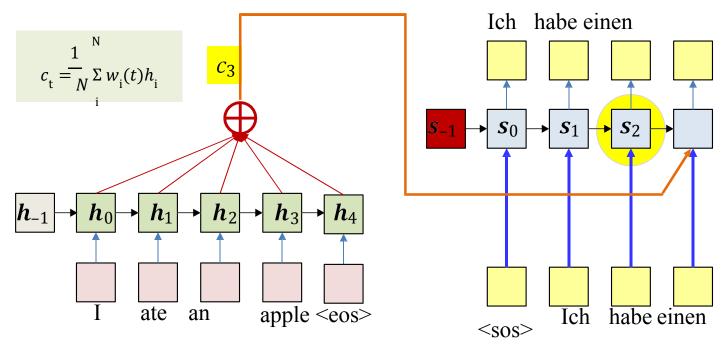
$$c_{t} = \frac{1}{N} \sum_{i}^{N} w_{i}(t) h_{i}$$

- Attention weights: The weights are dynamically computed as functions of decoder state
  - Expectation: if the model is well-trained, this will automatically "highlight" the correct input
- But how are these computed?

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# Attention weights at time



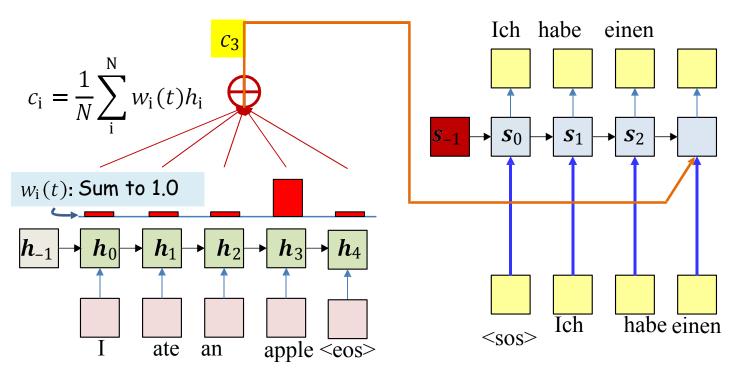


- The "attention" weights  $w_{\rm i}(t)$  at time t must be computed from available information at time t
- The primary information is  $S_{t-1}$  (the state at time time t-1)
  - Also, the input word at time t, but generally not used for simplicity

$$w_{i}(t) = a(\boldsymbol{h}_{i}, \boldsymbol{s}_{t-1})$$

### Requirement on attention weights

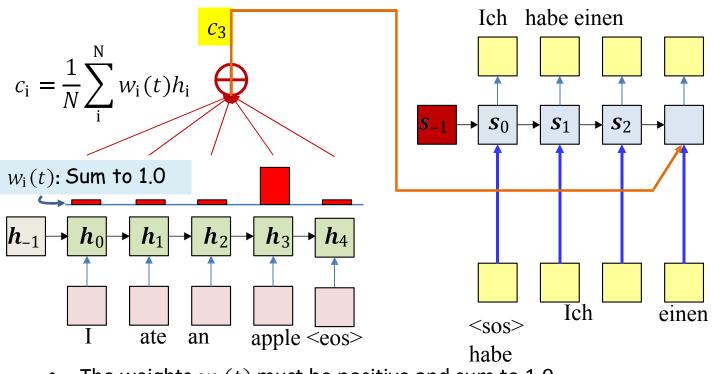




- The weights  $w_i(t)$  must be positive and sum to 1.0
  - I.e. be a distribution
  - Ideally, they must be high for the most relevant inputs for the ith output and low elsewhere

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- The weights  $w_i(t)$  must be positive and sum to 1.0
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- Solution: A two step weight computation
  - First compute raw weights (which could be +ve or -ve)
  - Then softmax them to convert them to a distribution

$$e_{i}(t) = g(\boldsymbol{h}_{i}, \boldsymbol{s}_{t-1})$$

$$w_{i}(t) = \frac{\exp(e_{i}(t))}{\sum_{j} \exp(e_{j}(t))}$$

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#### Quiz



The attention framework computes a different "context" vector at each output step (T/F)

- True
- False

The context vector is chosen as the hidden (encoder) representation of the input word that is assigned the highest attention weight (T/F)

- True
- False

The attention weight to any input word is a function of the hidden encoder representation of the word and the most recent decoder state (T/F)

- True
- False

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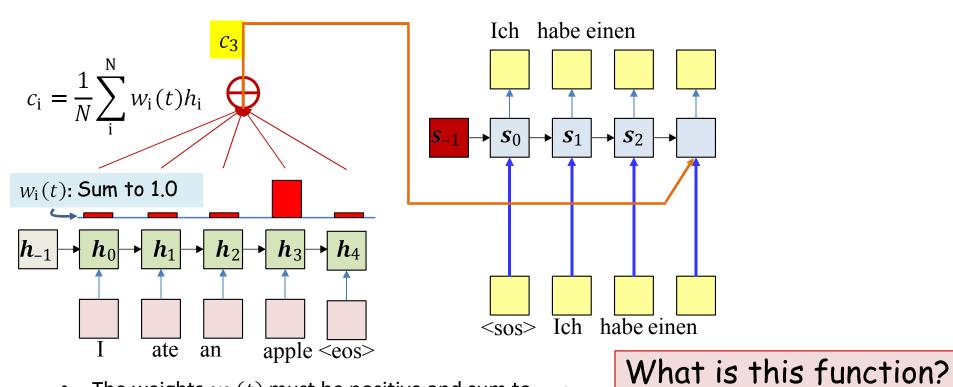
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#### Requirement on attention weights





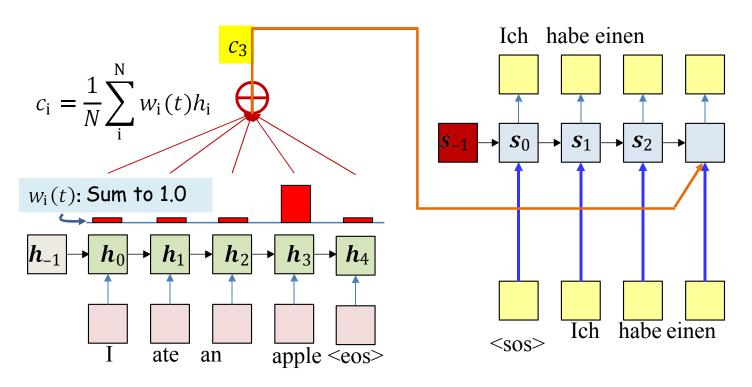
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#### Attention weights





• Typical options for g() (variables in red must learned)

$$g(\mathbf{h}_{i}, \mathbf{s}_{t-1}) = \mathbf{h}_{i}^{T} \mathbf{s}_{t-1}$$

$$g(\mathbf{h}_{i}, \mathbf{s}_{t-1}) = \mathbf{h}_{i}^{T} \mathbf{W}_{g} \mathbf{s}_{t-1}$$

$$g(\mathbf{h}_{i}, \mathbf{s}_{t-1}) = \mathbf{v}_{g}^{T} tanh \left(\mathbf{W}_{g} \begin{bmatrix} \mathbf{h}_{i} \\ \mathbf{s}_{t-1} \end{bmatrix}\right)$$

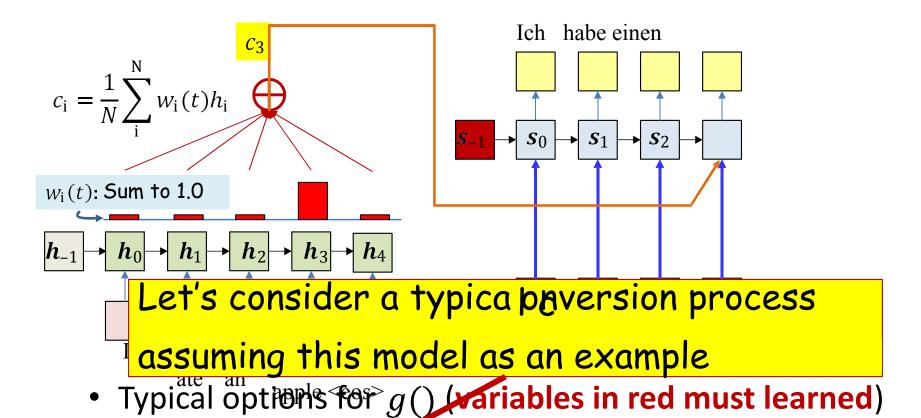
$$g(\mathbf{h}_{i}, \mathbf{s}_{t-1}) = MLP([\mathbf{h}_{i}, \mathbf{s}_{t-1}])$$

$$e_{i}(t) = g(\mathbf{h}_{i}, \mathbf{s}_{t-1})$$

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#### Attention weights





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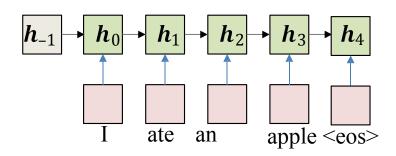
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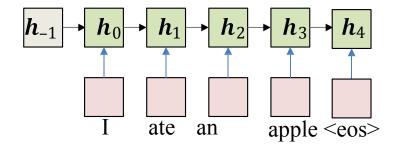
• Pass the input through the encoder to produce hidden representations  $m{h}_i$ 





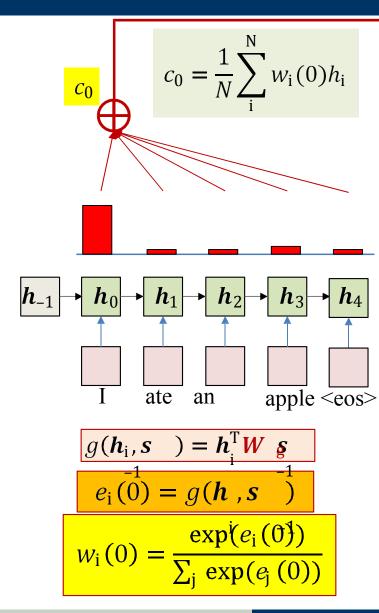
This may be

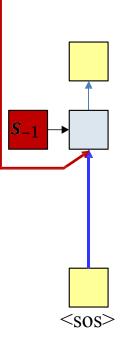
- a learned parameter, or
- Or just set to some fixed value,
   e.g. a vector of 1s or 0s, or
- Or the average of all the encoder embeddings:  $mean(h_0, ..., h_4)$
- Or  $W_{\rm init}$   $m_0ean(h, ..., h)$  where  $W_{\rm init}$  is a learned parameter



• Pass the input through the encoder to produce hidden representations  $m{h}_i$ 



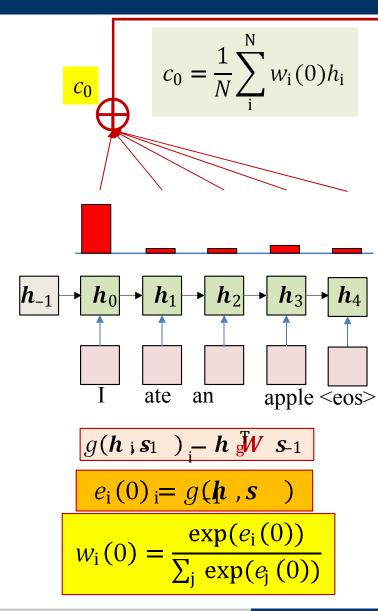


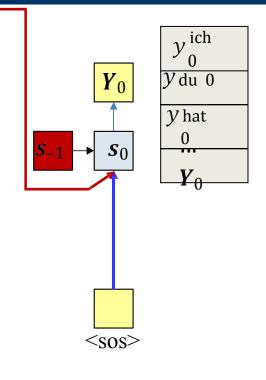


- Compute the attention weights  $w_i(0)$  for the first output using  $s_{-1}$ 
  - Will be a distribution over the input words
- Compute "context"  $c_0$ 
  - Weighted sum of input word hidden states
- Input  $c_0$  and <sos> to the decoder at time 0 <sos> because we are starting a new sequence

  - In practice we will enter the embedding of <sos>





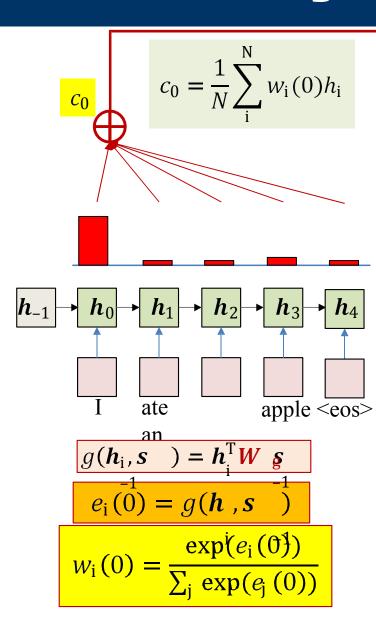


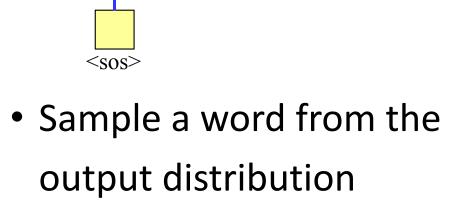
- The decoder computes
  - A probability distribution over the output vocabulary
    - Output of softmax output layer

Ich  $\sqrt{y_d}$ 

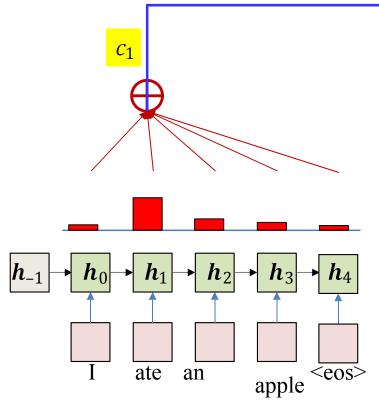
 $\boldsymbol{Y}_0$ 



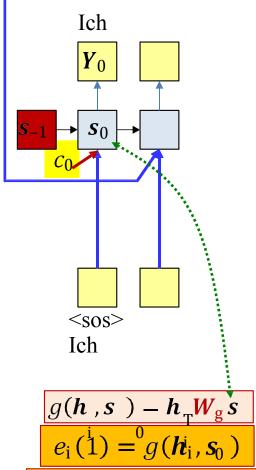






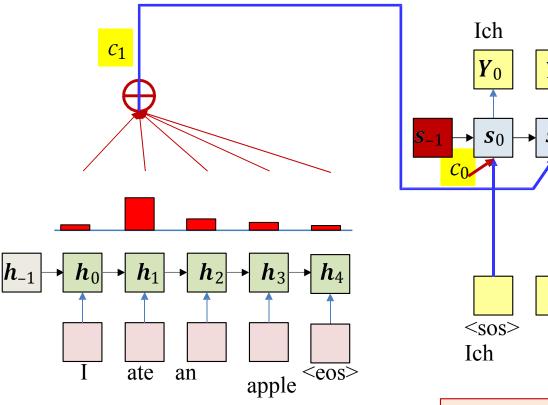


- Compute the attention weights  $w_i$  (1) over all inputs for the *second* output using  $s_0$ 
  - Compute raw weights, followed by softmax
- Compute "context"  $c_1$ 
  - Weighted sum of input hidden representations
- $\bullet \quad \text{Input $c_1$ and first output word to the } \\ \text{decoder}$ 
  - In practice we enter the *embedding* of the word



(1) = 
$$\frac{\exp(e_i(1))}{\sum_j \exp(e_j(1))}$$
  $c_1 = \frac{1}{N} \sum_i^N w_i(1)$ 





- The decoder computes
  - $s_1$
  - A probability distribution over the output vocabulary

$$g(\mathbf{h}, \mathbf{s}) - \mathbf{h}_{\mathrm{T}} W_{\mathrm{g}} \mathbf{s}$$
$$e_{\mathrm{i}}(\mathbf{1}) = {}^{0} g(\mathbf{h}_{\mathrm{i}}, \mathbf{s}_{0})$$

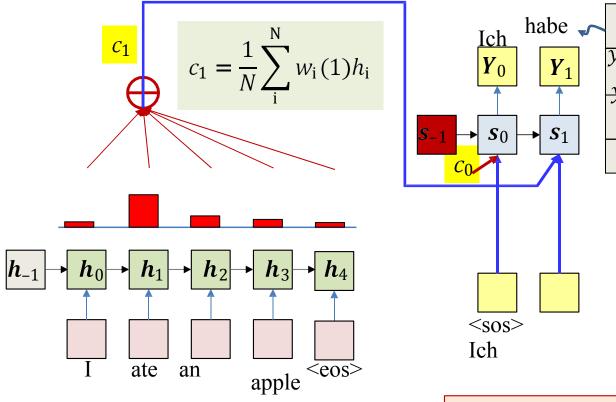
hat

 $\boldsymbol{Y}_1$ 

$$w_{i}(1) = \frac{\exp(e_{i}(1))}{\sum_{j} \exp(e_{j}(1))}$$

$$c_1 = \frac{1}{N} \sum_{i}^{N} w_i(1) h_i$$





 Sample the second word from the output distribution

$$g(\mathbf{h}, \mathbf{s}) - \mathbf{h}_{T} W_{g} \mathbf{s}$$

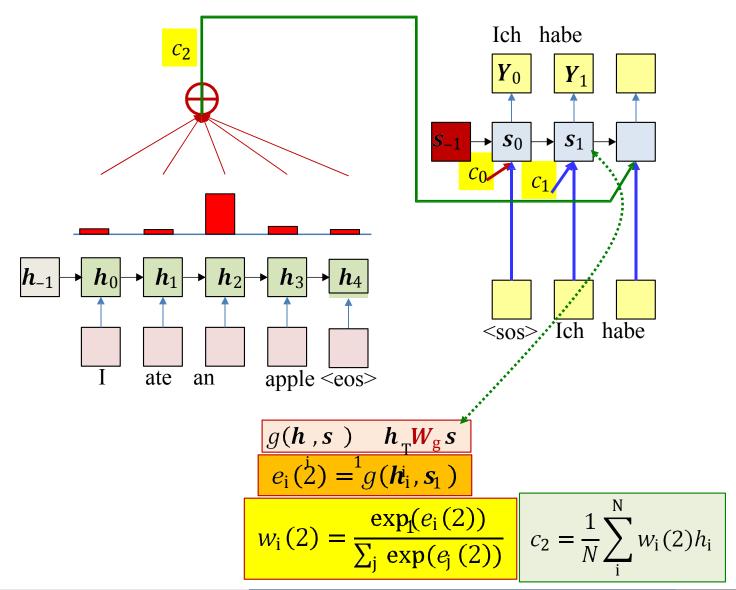
$$e_{i}(\mathbf{1}) = {}^{0}g(\mathbf{h}_{i}, \mathbf{s}_{0})$$

$$w_{i}(1) = \frac{\exp(e_{i}(1))}{\sum_{j} \exp(e_{j}(1))}$$

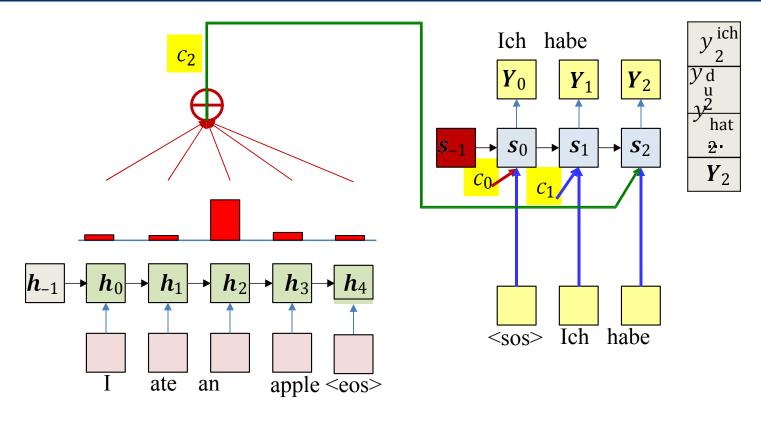
$$c_{1} = \frac{1}{N} \sum_{i}^{N} w_{i}(1)h_{i}$$

 $Y_1$ 









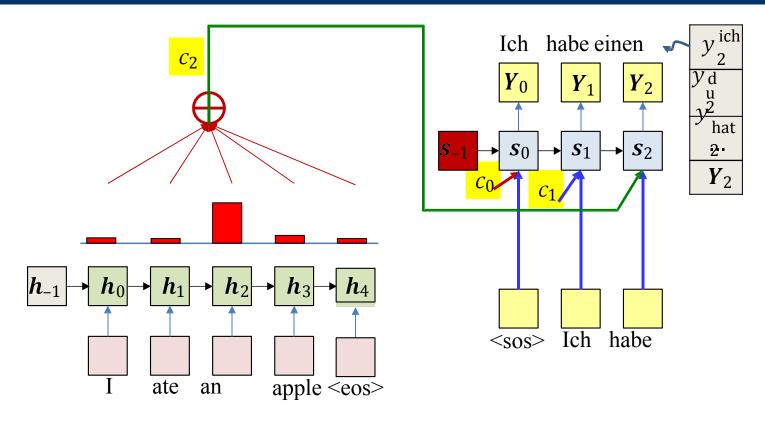
$$g(\mathbf{h}, \mathbf{s}) - \mathbf{h}_{\mathrm{T}} W_{\mathrm{g}} \mathbf{s}$$

$$e_{\mathrm{i}}(\dot{2}) = g(\mathbf{h}_{\mathrm{i}}, \mathbf{s}_{\mathrm{1}})$$

$$w_{i}(2) = \frac{\exp(e_{i}(2))}{\sum_{j} \exp(e_{j}(2))}$$

$$c_2 = \frac{1}{N} \sum_{i}^{N} w_i(2) h_i$$





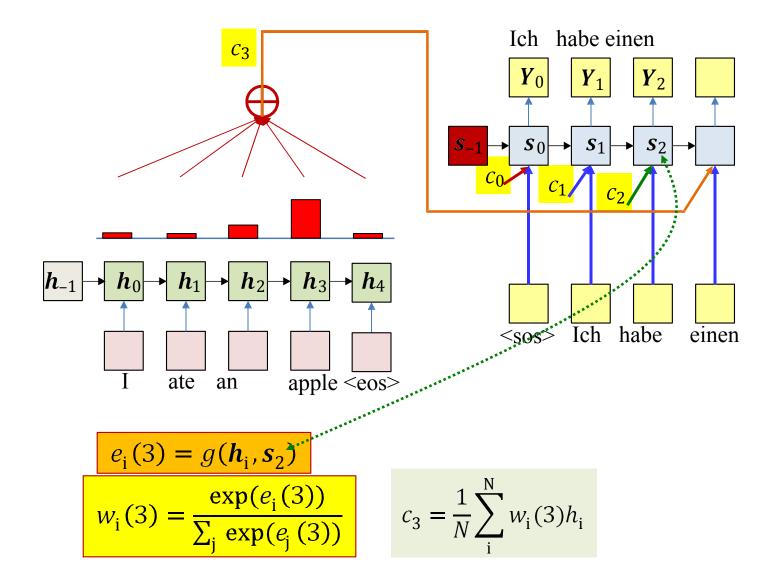
$$g(\mathbf{h}, \mathbf{s}) - \mathbf{h}_{\mathrm{T}} W_{\mathrm{g}} \mathbf{s}$$

$$e_{\mathrm{i}}(\dot{2}) = g(\mathbf{h}_{\mathrm{i}}, \mathbf{s}_{\mathrm{1}})$$

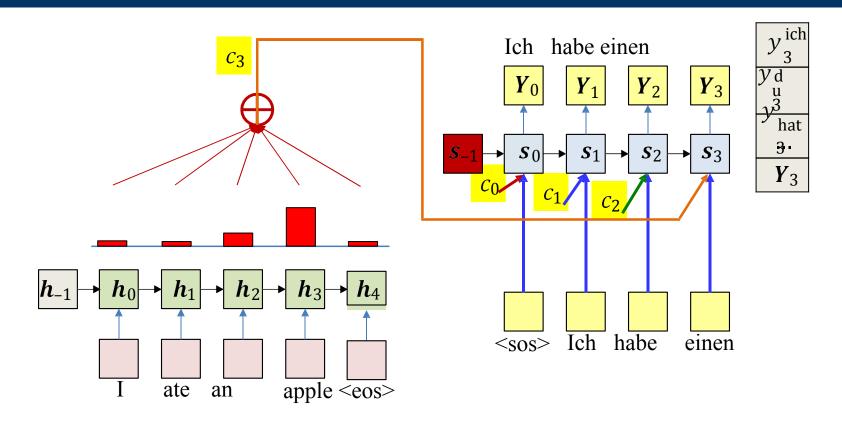
$$w_{i}(2) = \frac{\exp(e_{i}(2))}{\sum_{j} \exp(e_{j}(2))}$$
  $c_{2}$ 

$$c_2 = \frac{1}{N} \sum_{i}^{N} w_i(2) h_i$$







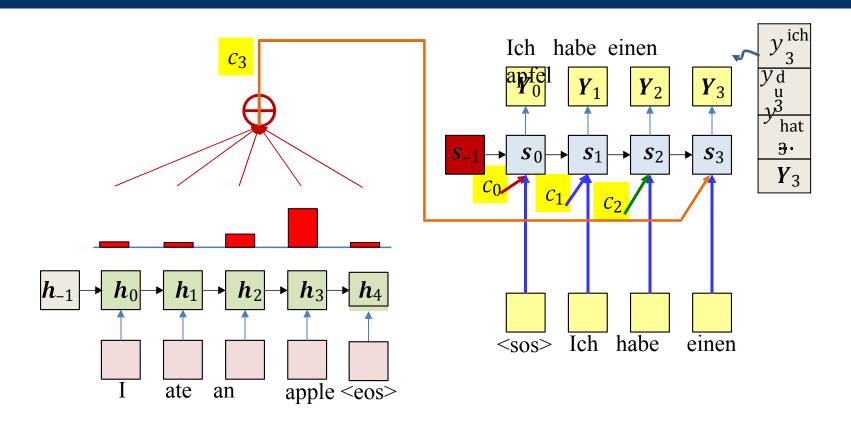


$$e_{\mathbf{i}}(3) = g(\mathbf{h}_{\mathbf{i}}, \mathbf{s}_{2})$$

$$w_{i}(3) = \frac{\exp(e_{i}(3))}{\sum_{j} \exp(e_{j}(3))} \qquad c_{3} = \frac{1}{N} \sum_{i}^{N} w(3)h_{i}$$

$$c_{3} = \frac{1}{N} \sum_{i}^{N} w(3) h_{i}$$





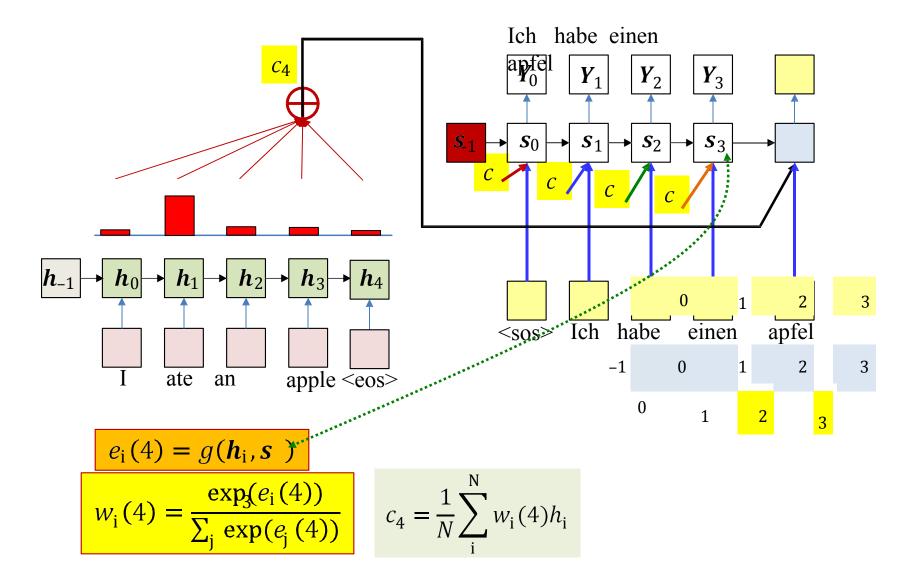
$$e_{\mathbf{i}}(3) = g(\boldsymbol{h}_{\mathbf{i}}, \boldsymbol{s}_{2})$$

$$w_{i}(3) = \frac{\exp(e_{i}(3))}{\sum_{j} \exp(e_{j}(3))}$$

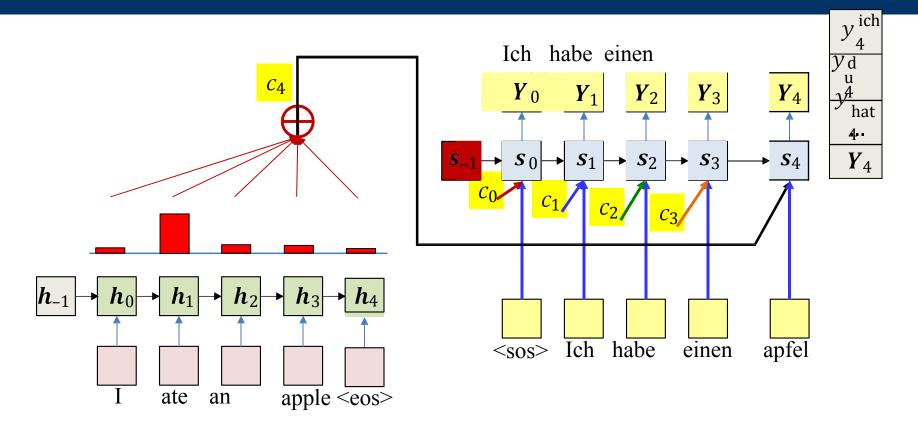
$$c_3 = \frac{1}{N} \sum_{i}^{N} w_i(3) h_i$$

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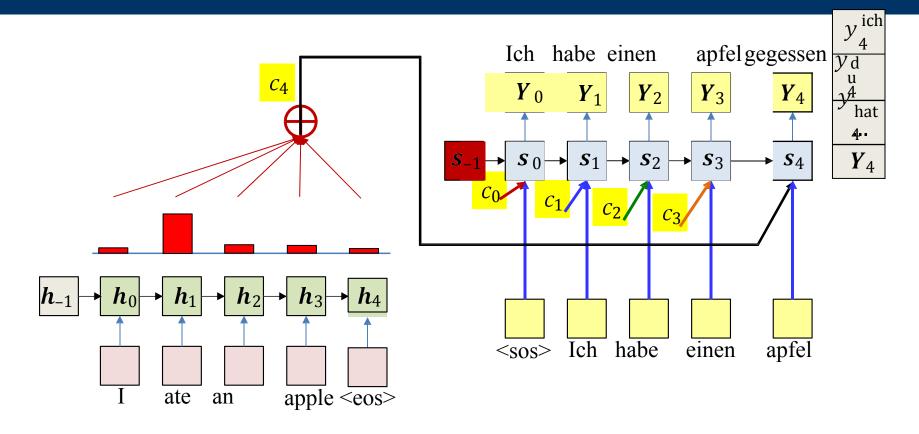


$$e_{\mathrm{i}}(4) = g(\boldsymbol{h}_{\mathrm{i}}, \boldsymbol{s}_{\mathrm{3}})$$

$$w_{i}(4) = \frac{\exp(e_{i}(4))}{\sum_{j} \exp(e_{j}(4))}$$

$$c_4 = \frac{1}{N} \sum_{i}^{N} w_i(4) h_i$$



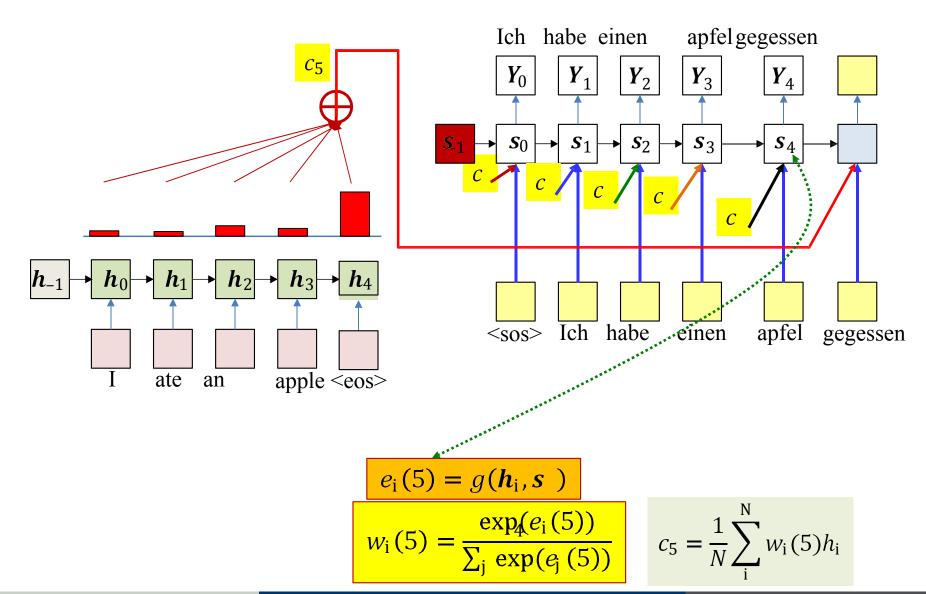


$$e_{\mathrm{i}}(4) = g(\boldsymbol{h}_{\mathrm{i}}, \boldsymbol{s}_{\mathrm{3}})$$

$$w_{i}(4) = \frac{\exp(e_{i}(4))}{\sum_{j} \exp(e_{j}(4))}$$

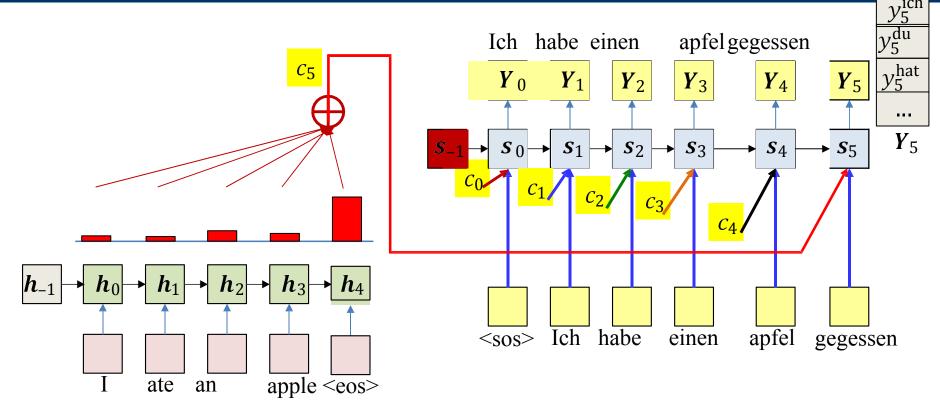
$$c_4 = \frac{1}{N} \sum_{i}^{N} w_i(4) h_i$$





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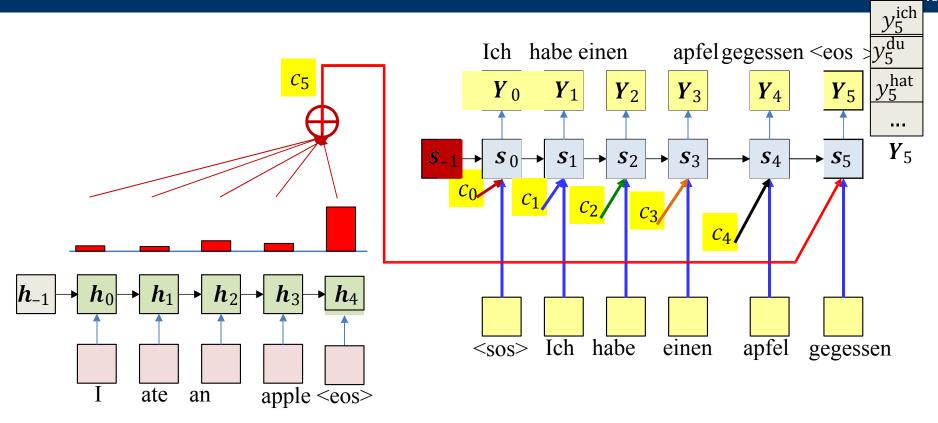


$$e_{i}(5) = g(\mathbf{h}_{i}, \mathbf{s})$$

$$w_{i}(5) = \frac{\exp(e_{i}(5))}{\sum_{j} \exp(e_{j}(5))}$$

$$c_5 = \frac{1}{N} \sum_{i}^{N} w_i(5) h_i$$





Continue this process until <eos> is drawn

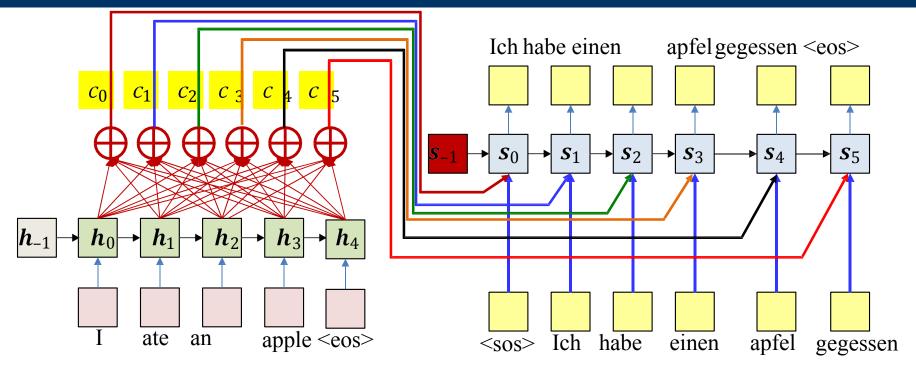
$$e_{i}(5) = g(\boldsymbol{h}_{i}, \boldsymbol{s})$$

$$w_{i}(5) = \frac{\exp(e_{i}(5))}{\sum_{j} \exp(e_{j}(5))}$$

$$c_5 = \frac{1}{N} \sum_{i}^{N} w_i(5) h_i$$

### Attention-based decoding





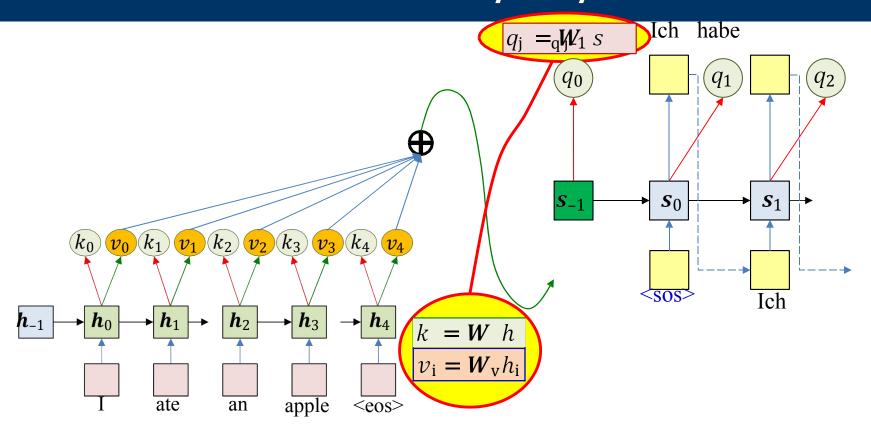
$$e_{i}(t) = g(\mathbf{h}_{i}, \mathbf{s})$$

$$w_{i}(t) = \frac{\exp(e_{i}(t))}{\sum_{j} \exp(e_{j}(t))}$$

$$c_{t} = \frac{1}{N} \sum_{i}^{N} w_{i}(t) h_{i}$$

# Modification: Query key value

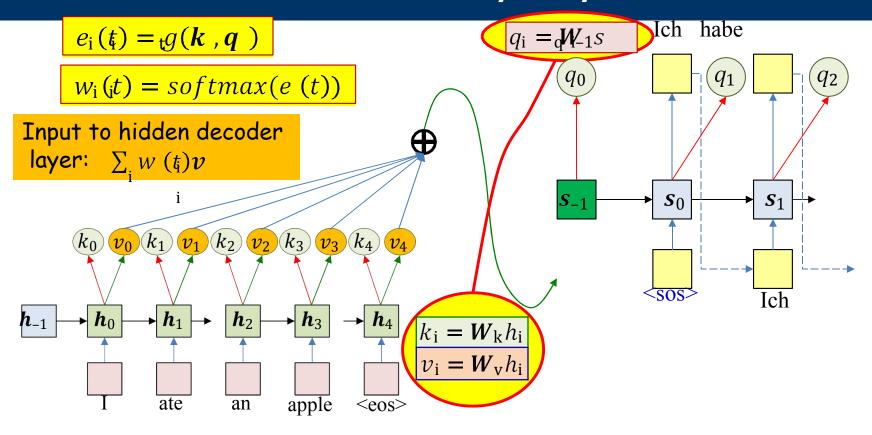




- Encoder outputs an explicit "key" and "value" at each input time
  - Key is used to evaluate the importance of the input at that time, for a given output
- Decoder outputs an explicit "query" at each output time
  - Query is used to evaluate which inputs to pay attention to
- The weight is a function of key and query
- The actual context is a weighted sum of value

## Modification: Query key value

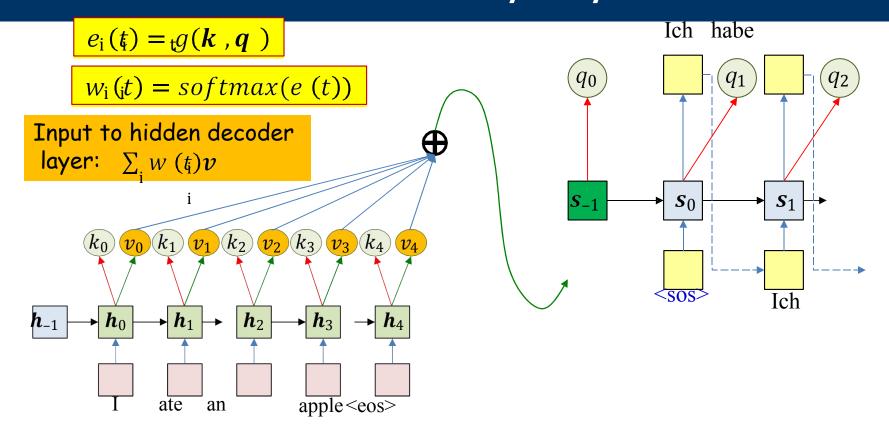




- Encoder outputs an explicit "key" and "value" at each input time
  - Key is used to evaluate the importance of the input at that time, for a given output
- Decoder outputs an explicit "query" at each output time
  - Query is used to evaluate which inputs to pay attention to
- The weight is a function of key and query
- The actual context is a weighted sum of value

### Modification: Query key value





Special case: 
$$k_i = v_i = h_i$$
  $q_t = s_{t-1}$ 

#### Pseudocode



```
# Assuming encoded input
# (K,V) = [k_{enc}[0]...k_{enc}[T]], [v_{enc}[0]...v_{enc}[T]]
# is available
t_{.} = -1
h_{out}[-1] = 0 # Initial Decoder hidden state
q[0] = 0 # Initial query
# Note: begins with a "start of sentence" symbol
# <sos> and <eos> may be identical
Y<sub>out</sub>[0] = <sos>
do
    t = t+1
    C = compute context with attention(q[t], K, V)
    y[t], h_{out}[t], q[t+1] = RNN_decode_step(h_{out}[t-1], y_{out}[t-1], C)
    y<sub>out</sub>[t] = generate(y[t]) # Random, or greedy
until y<sub>out</sub>[t] == <eos>
```

# Pseudocode: Computing context with

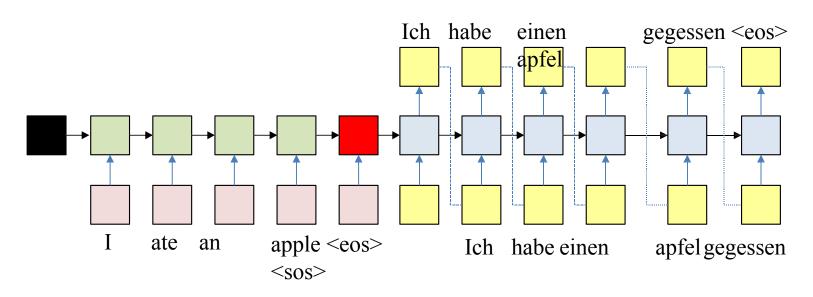


#### attention

```
# Takes in previous state, encoder states, outputs attention-weighted context
function compute context with attention(q, K, V) #
    First compute attention
   e = []
    for t = 1:T # Length of input
        e[t] = raw attention(q, K[t])
    end
   maxe = max(e) # subtract max(e) from everything to prevent underflow
    a[1..T] = exp(e[1..T] - maxe) # Component-wise exponentiation
    suma = sum(a) # Add all elements of a
    a[1..T] = a[1..T]/suma
   C = 0
    for t = 1..T
        C += a[t] * V[t]
    end
    return C
```



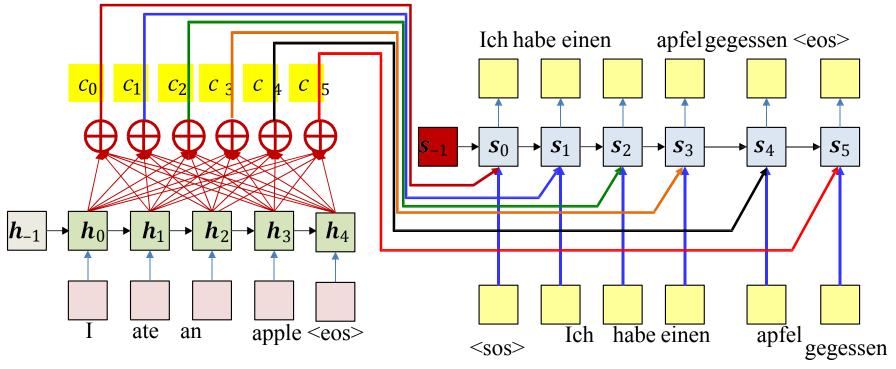
#### Recap: Seq2Seq models



- The input sequence feeds into a recurrent structure
- The input sequence is terminated by an explicit <eos> symbol
  - The hidden activation at the <eos> "stores" all information about the sentence
- Subsequently a second RNN uses the hidden activation as initial state to produce a sequence of outputs

#### Recap: Attention Models

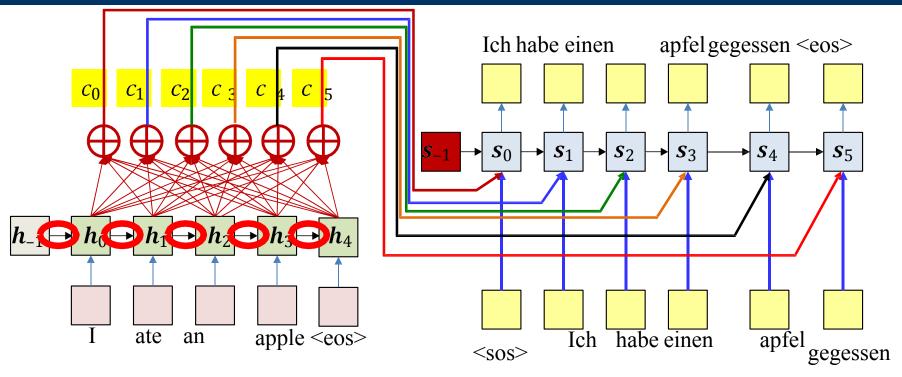




- Encoder recurrently produces hidden representations of input word sequence
- Decoder recurrently generates output word sequence
  - For each output word the decoder uses a weighted average of the hidden input representations as input "context", along with the recurrent hidden state and the previous output word

#### Recap: Attention Models





- Problem: Because of the recurrence, the hidden representation for any word is also influenced by *all* preceding words
  - The decoder is actually paying attention to the sequence, and not just the word
- If the decoder is automatically figuring out which words of the input to attend to at each time, is recurrence in the input even necessary?

# Impact of Attention



Improves translation accuracy

Helps handle longer sequences

Interpretable: shows what the model is focusing on

Forms the foundation of **Transformer models** 

#### Led to development of:

- Bahdanau Attention (Additive, 2014)
- Luong Attention (Multiplicative, 2015)
- ► Self-Attention and Transformers (2017+)

# Seq2Seq vs Seq2Seq + Attention



Aspect	Basic Seq2Seq	With Attention
Memory	Single vector (fixed)	Multiple encoder states (dynamic)
Long Sequences	Poor performance	Good performance
Interpretability	Low	High (via attention weights)
Use Cases	Short/medium sequences	Longer, complex tasks

# Applications of Seq2Seq + Attention



- Machine Translation
- ► Text Summarization
- Chatbots and Dialog Systems
- Speech Recognition
- Question Answering
- Video Captioning
- DNA Sequence Modeling

#### Limitations



- ► Still sequential not fully parallelizable
- Attention adds computational cost
- ► Hard to interpret in large-scale models
- ► Might struggle with very long-range dependencies in huge contexts

#### **Future Directions**



- ► Transformers: Fully attention-based, no recurrence
- ► Efficient Attention Models: Longformer, Reformer, Linformer
- ► Multimodal Attention: Vision + Text
- Memory-Augmented Models
- ▶ Structured Attention: Parses, syntax, and alignment bias

Attention paved the way for GPT, BERT, and LLMs

# Summary



- Seq2Seq enables mapping input to output sequences of variable lengths
- ▶ Bottleneck: Fixed-size context vector limits learning capacity
- ▶ Attention: Improves performance by giving adaptive access to input states
- ightharpoonup Attention ightharpoonup Transformer ightharpoonup LLMs
- Still evolving: From additive attention to self-attention and beyond

#### References



#### These slides have been adapted from

- Younes Mourri & Lukasz Kaiser, <u>Natural Language Processcing</u> <u>Specialization, DeepLearning.Ai</u>
- Bhiksha Raj & Rita Singh, <u>11-785 Introduction to Deep</u> <u>Learning, CMU</u>

#### References



#### **Foundational Papers:**

- Sutskever et al. (2014). Sequence to Sequence Learning with Neural Networks. NeurIPS.
- ▶ Bahdanau et al. (2014). Neural Machine Translation by Jointly Learning to Align and Translate.
- Luong et al. (2015). Effective Approaches to Attention-based Neural Machine Translation.
- ▶ Vaswani et al. (2017). Attention Is All You Need (Transformer).
- Chan et al. (2016). Listen, Attend and Spell (Speech recognition).

#### References



#### Courses & Tutorials:

- ► Stanford CS224n: Lecture 9 (Attention)
- DeepLearning.ai NLP Specialization (Coursera)
- ► Harvard NLP Annotated Transformer: http://nlp.seas.harvard.edu/2018/04/03/attention.html
- ► Jay Alammar's blog: "The Illustrated Transformer"