Encoder-Decoder Models
Attention. “The” transformer model.

Venelin Kovatchev

Lecturer in Computer Science

v.o.kovatchev@bham.ac.uk

Outline

- Quick recap
- Encoder-decoder networks
- Attention
- Original transformer

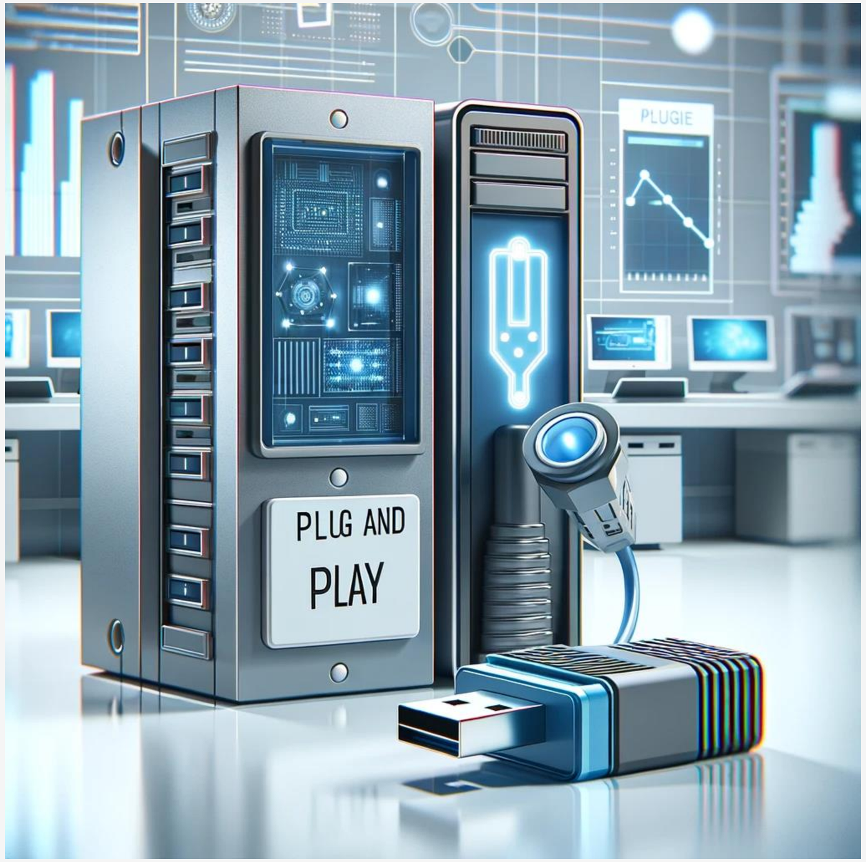
Quick recap:
End-to-end neural networks

What are end-to-end models

- Task specific models
- Map directly from input to output
- No feature engineering
- Trained via backpropagation
  - Data and compute expensive

What are some advantages of end-to-end

- Better performance
- Simpler pipeline
- Changing the problem formulation
  - The task is defined by the data and the metrics
- Making NLP more accessible
  - Plug and play



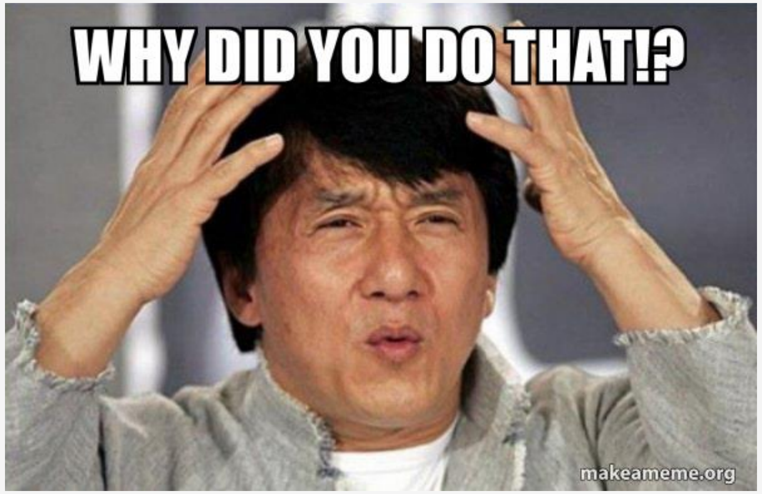
Challenges with going end to end

- My take on key challenges
    - Computational and data cost
    - Dependency on data and task formulation
    - Explainability and Interpretability
    - Bias, guarantees, and robustness

Explainability and Interpretability

- Interpreting feature-based models
  - Feature values (“v1agra”) + weights = prediction (“spam”)

- Interpreting end-to-end neural networks
  - Feature values (300d dense vector)
  - weights (input, forget, output gates)
  - different types of nonlinearity

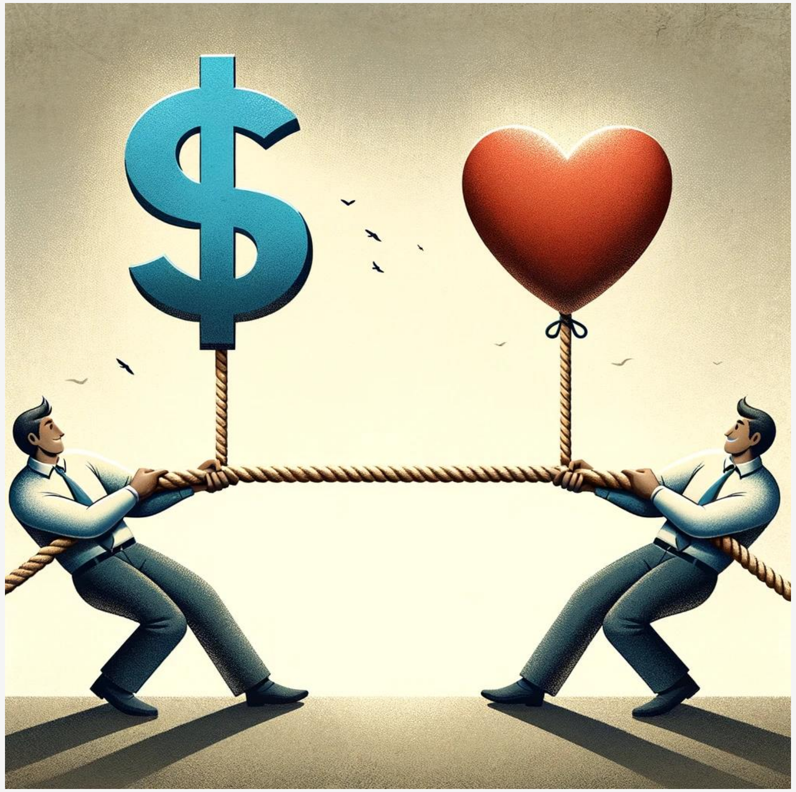


Explainability and Interpretability

- Provide a (valid) justification for the model behavior
- Provide a faithful explanation of the model behavior
- Provide an explanation that is useful for a human
  - To assess the model
  - To learn how to perform the task
  - In a Human-Computer collaboration

Bias, Guarantees, and Robustness

- An end-to-end neural network finds the (mathematically) optimal solution to a formally defined problem
- Sometimes the optimal solution can lead to undesired behavior
  - bias with respect to race, gender, religion, sexual orientation
  - “shortcuts” to solving tasks
- How do we guarantee the model is consistent and bias-free?
  - Evaluation and algorithmic fairness
- How do we know if the algorithm is safe from adversarial attacks?



What networks do we know so far

- Feed forward networks (FFN)
- Recurrent neural networks (RNN) (+ LSTM, GRU)
- Convolutional neural networks (CNN)

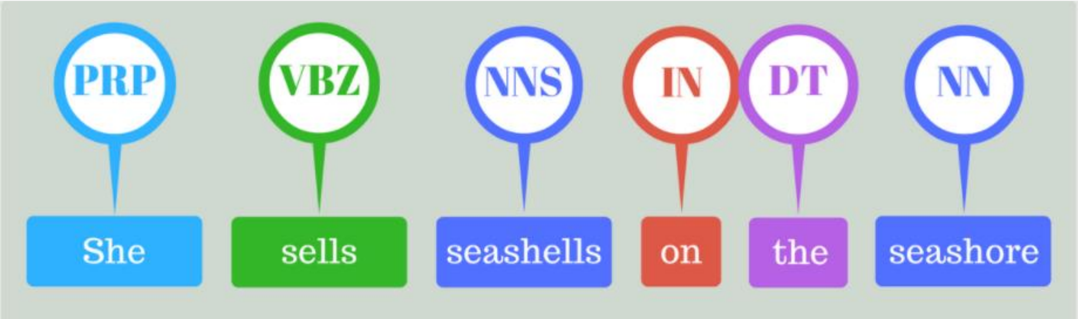
- Pop quiz: are these networks for supervised or unsupervised NLP?

Encoder-Decoder Models

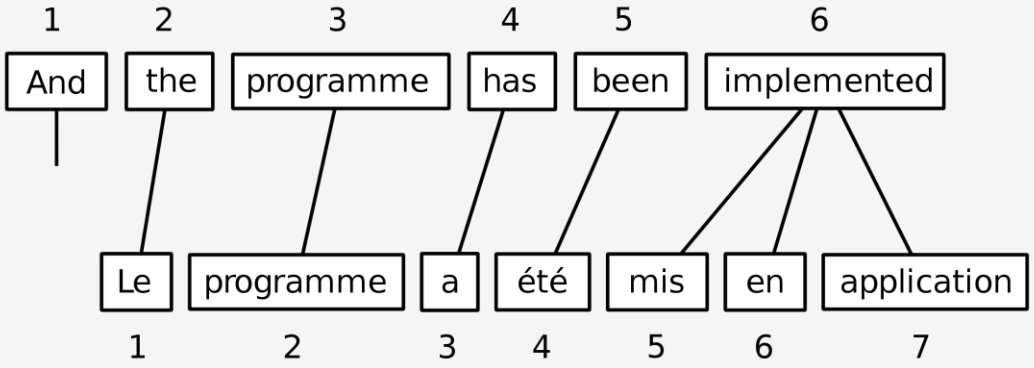
Input and output in NLP tasks

- What is the input and output of the following tasks
  - Sentiment analysis
  - Automated fact checking
  - Clustering documents based on topic
  - Machine translation
- How many possible outputs does each of those tasks have?

Sequence labeling vs sequence-to-sequence



- Consider the following two tasks
- What is similar between them?
- What is different?
- How would you approach each of them?

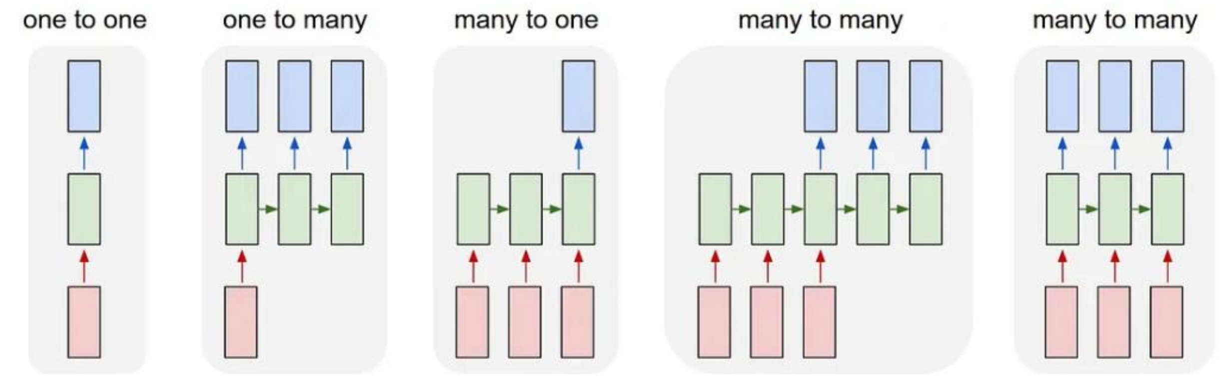


Key differences

- Same length vs different length
- One-to-one alignment vs no one-to-one alignment
- Local dependencies vs long-distance dependencies
    - Within the output
    - Between the input and the output

Different task formulations

- Which of the following images corresponds to:
  - FFN
  - RNN for text classification
  - Machine translation
  - Image captioning
  - Sequence labeling



The Unreasonable Effectiveness of Recurrent Neural Networks by Andrej Karpathy

Encoder decoder

- We use a model family called encoder-decoder
- Simple idea
  - Encoder "represents" the source (e.g., English)
  - Decoder "generates" the target (e.g., German)
- Can you suggest tasks that can use encoder-decoder?

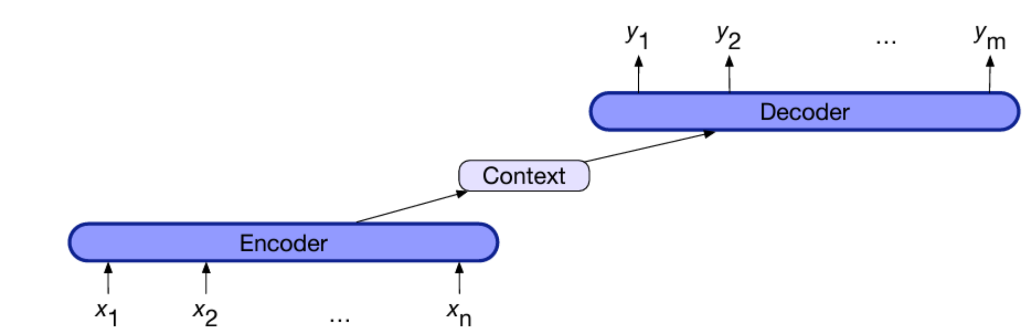


Fig 9.16

Usage of encoder decoder

- General usage of encoder decoder
  - Mapping between data of different format, size, and structure
  - Encoder-decoder vs sequence-to-sequence
- Examples for tasks that can use encoder-decoder:
  - Machine translation
  - Text summarization
  - Question answering
  - Image captioning

How do we implement encoder-decoder?

- Can you propose a way to implement enc-dec model with what we know so far?

- How do we encode the input?

- How do we decode the output?

Single RNN as encoder decoder

- Let's consider a single RNN for the task

- Add a separator between the two texts:
  - [sentence] [in] [English] [SEP] [sentence] [in] [German]

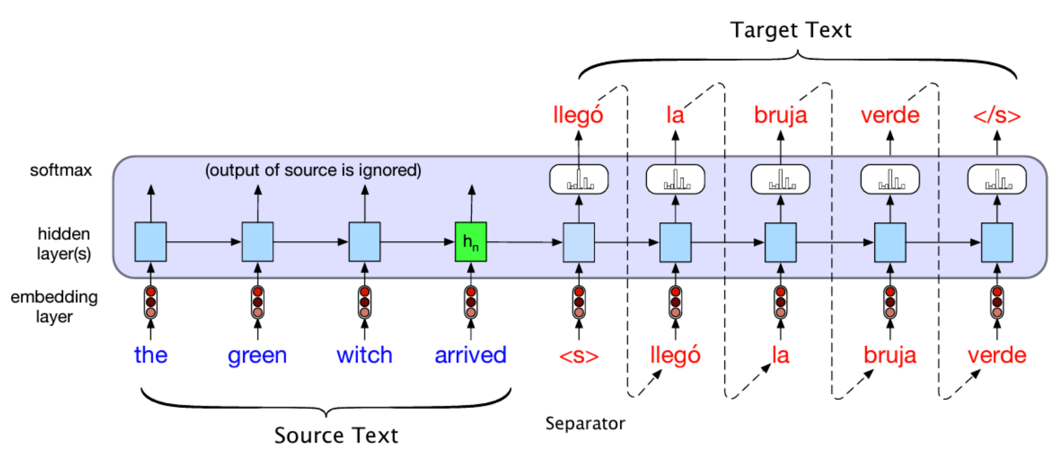
- The hidden state at SEP will contain all the information about the first sentence

Conditional generation

- How does a traditional language model generate text?
- How does an encoder-decoder RNN generate text?
- Does that concept look familiar?

A single RNN as encoder-decoder

- Consider using the following model
  - We use “English” as a “prompt”
  - Hidden state at <s> “encodes” the text
  - We generate Spanish step by step from x and h



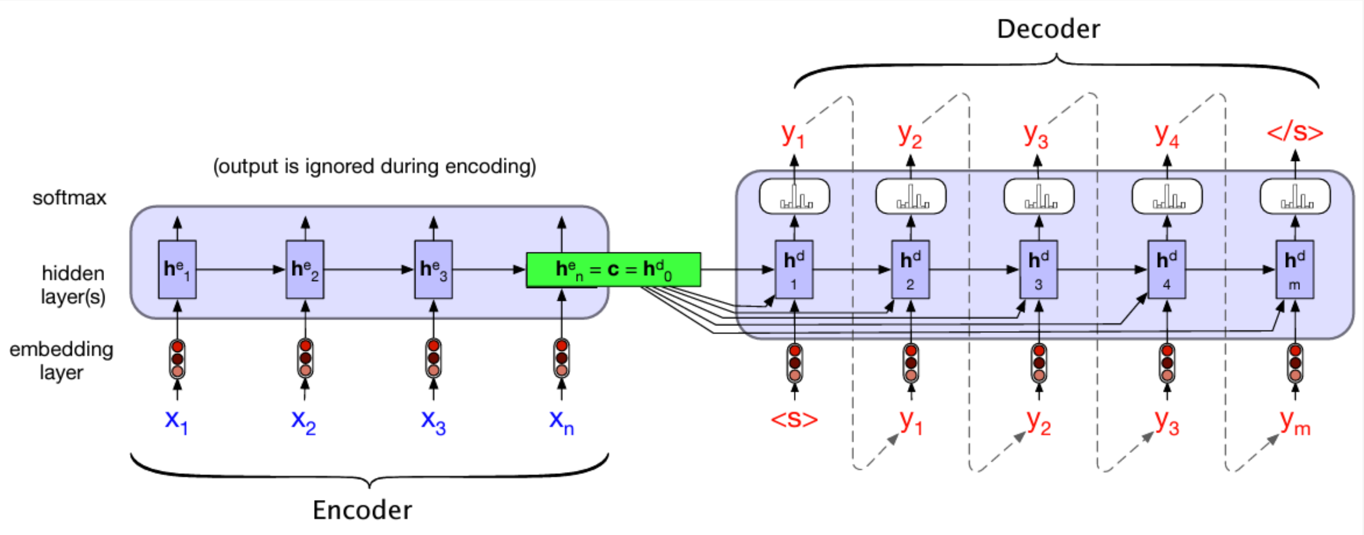
- What would be some problems with this model?
  - What if the task was text captioning?

Using separate RNNs for encoder and decoder

- Train two models
- Pass the context at every step

$$\mathbf{h}_t^d = g(\hat{y}_{t-1}, \mathbf{h}_{t-1}^d, \mathbf{c})$$

- Can you point a potential problem?
  - What could improve this architecture?



- What is the purpose of the encoder?
  - Should it be able to generate?

Formal representation of RNN based decoder

- The context is the last h of the encoder
- The hidden stage at step 0 is just the context
- For every step after 0, we use both h and c
- We use the hidden state to predict y at time t

$$
\begin{aligned}
\mathbf{c} &= \mathbf{h}_n^e \\
\mathbf{h}_0^d &= \mathbf{c} \\
\mathbf{h}_t^d &= g(\hat{y}_{t-1}, \mathbf{h}_{t-1}^d, \mathbf{c}) \\
\mathbf{z}_t &= f(\mathbf{h}_t^d) \\
y_t &= \text{softmax}(\mathbf{z}_t)
\end{aligned}
$$

- Why is there a “y” at the calculation of the hidden state h_t^d?

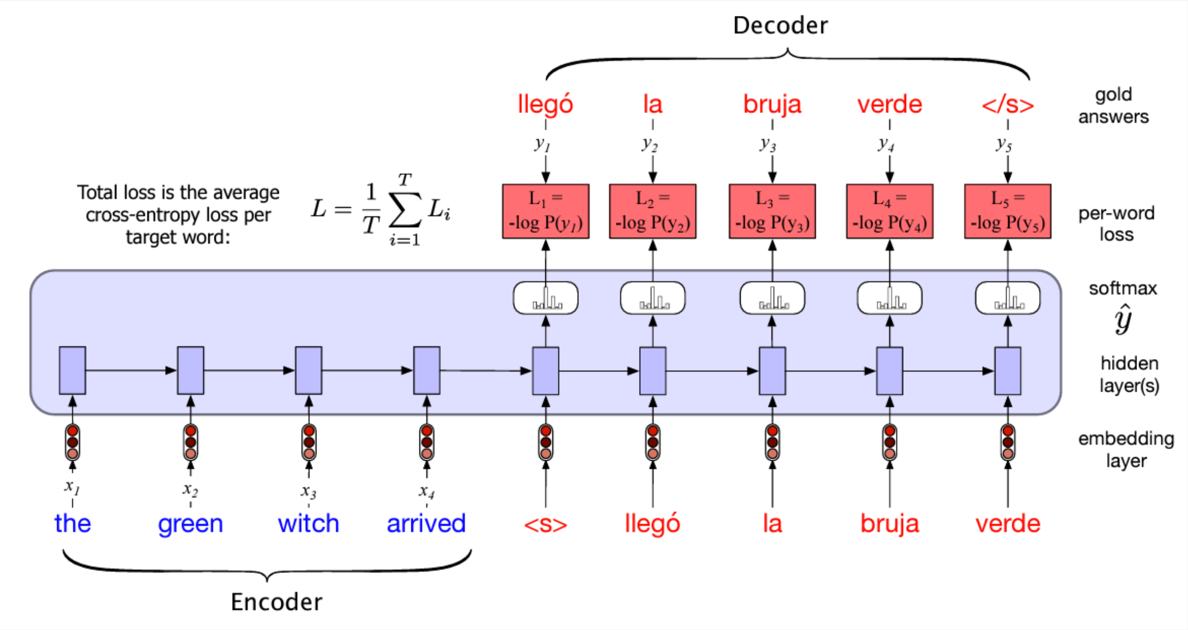
Training encoder-decoder models

- Models are trained end-to-end

- Encoder is trained through hidden layers

- Decoder is trained through teacher forcing

    - Remember "teacher forcing"?



Why are encoder-decoder models important?

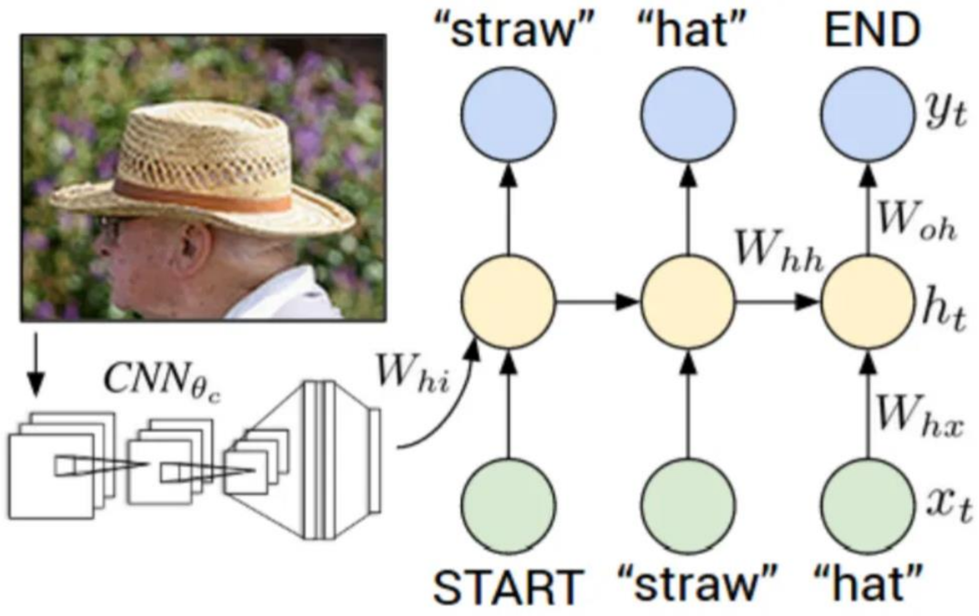
- Instant improvement on machine translation
  - Google Translate switching to NMT

- Key concepts reused (and giving raise to) Attention and Transformers

- Bridging the gap between modalities

Encoder decoder across modalities: image captioning

- The encoder and decoder “talk” via the context
- They don’t have to be the same type of model
- The modalities don’t have to match
  - Speech to text
  - Image to text



Deep Visual-Semantic Alignments for Generating Image Descriptions

Attention

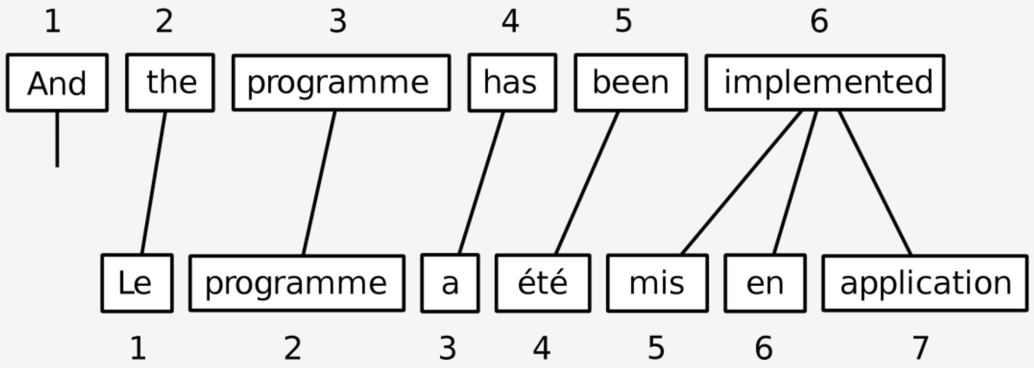
A bottleneck of RNNs

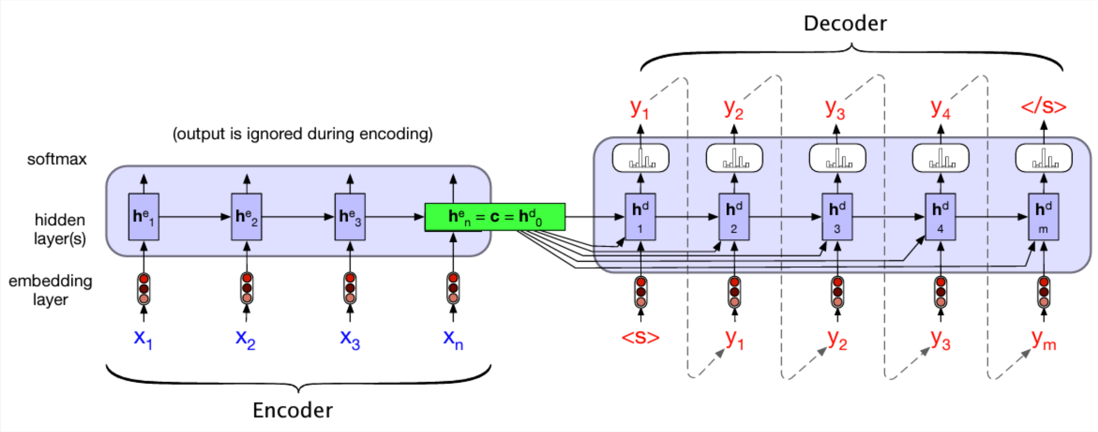
- Consider the problem of MT and an encoder-decoder solution

- The “context” is the information from the input that we need to generate the target

- To generate word y_t, we use the prior information for $y_1 - y_{(t-1)}$ and the same c

- Should c be the same for every word?



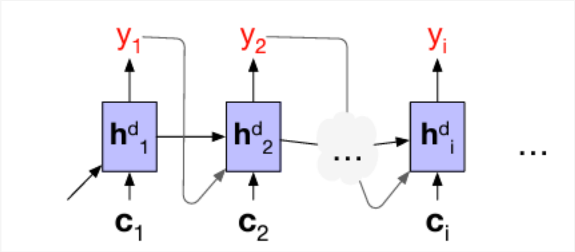


Attention – intuition and restrictions

- Intuition: each token in the target should use a “personalized” context
- Access all the hidden states in the encoder
  - Still needs to have a fixed length, regardless of variable input length
- Any ideas how we can do that?

Attention – basic implementation

- Weighted sum of all encoder hidden states
  - Calculated separately at each decoder step
  - Using the hidden state at (t-1)



- Dot product attention
  - Calculate the similarity between $h_{(t-1)}$ and each encoder state h^e
  - Use the similarity scores to calculate the weighted sum

Dot product attention (formally)

- Scoring function: $$\text{score}(\mathbf{h}^d_{i-1}, \mathbf{h}^e_j) = \mathbf{h}^d_{i-1} \cdot \mathbf{h}^e_j$$

- Weight vector: $$\begin{aligned} \alpha_{ij} &= \text{softmax}(\text{score}(\mathbf{h}^d_{i-1}, \mathbf{h}^e_j)) \\ &= \frac{\exp(\text{score}(\mathbf{h}^d_{i-1}, \mathbf{h}^e_j))}{\sum_k \exp(\text{score}(\mathbf{h}^d_{i-1}, \mathbf{h}^e_k))} \end{aligned}$$

- Personalized context: $$\mathbf{c}_i = \sum_j \alpha_{ij}\, \mathbf{h}^e_j$$

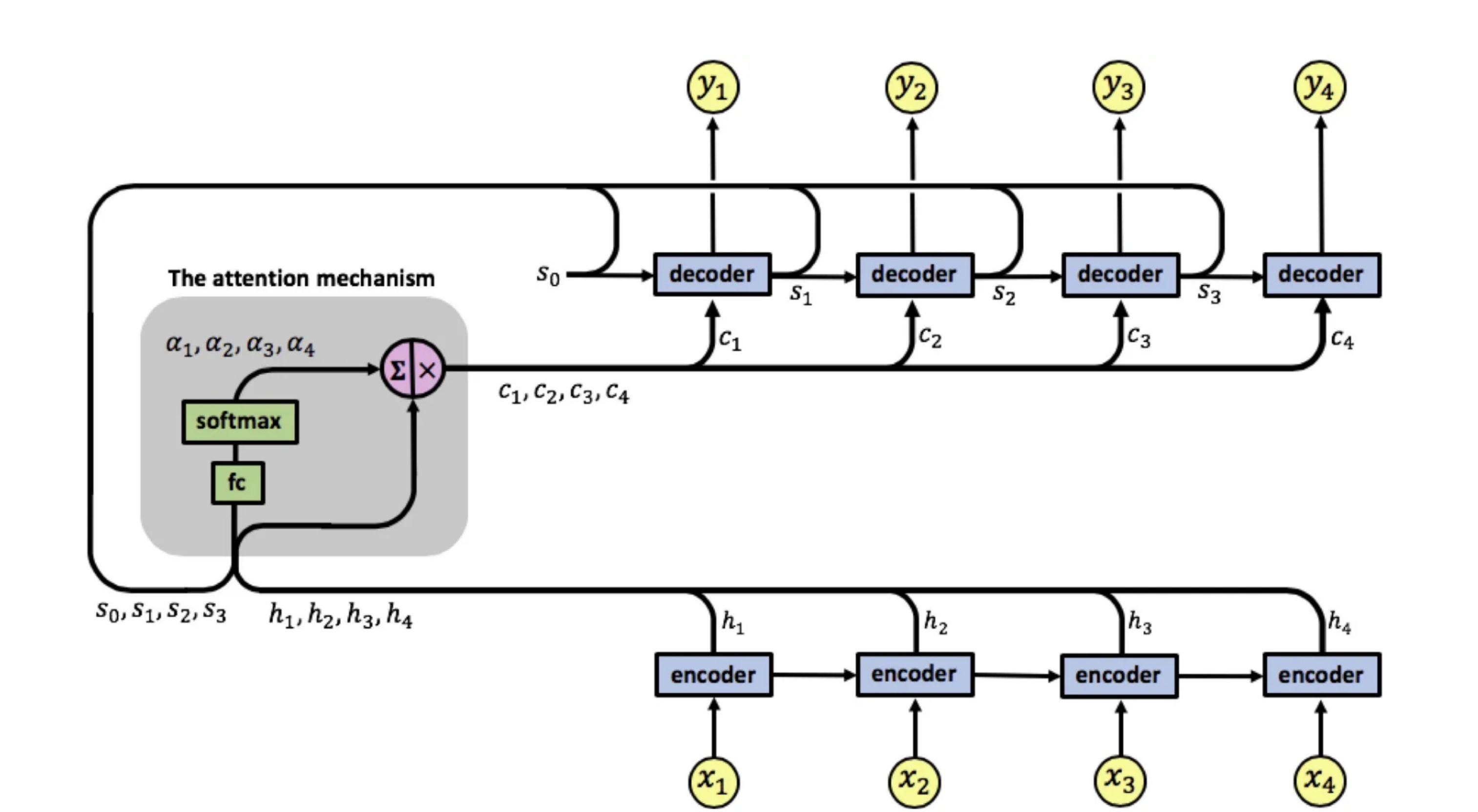
- More complex scoring functions:

$$\text{score}(\mathbf{h}^d_{i-1}, \mathbf{h}^e_j) = \mathbf{h}^d_{t-1} \mathbf{W}_s \mathbf{h}^e_j$$

Visualization of RNN with attention

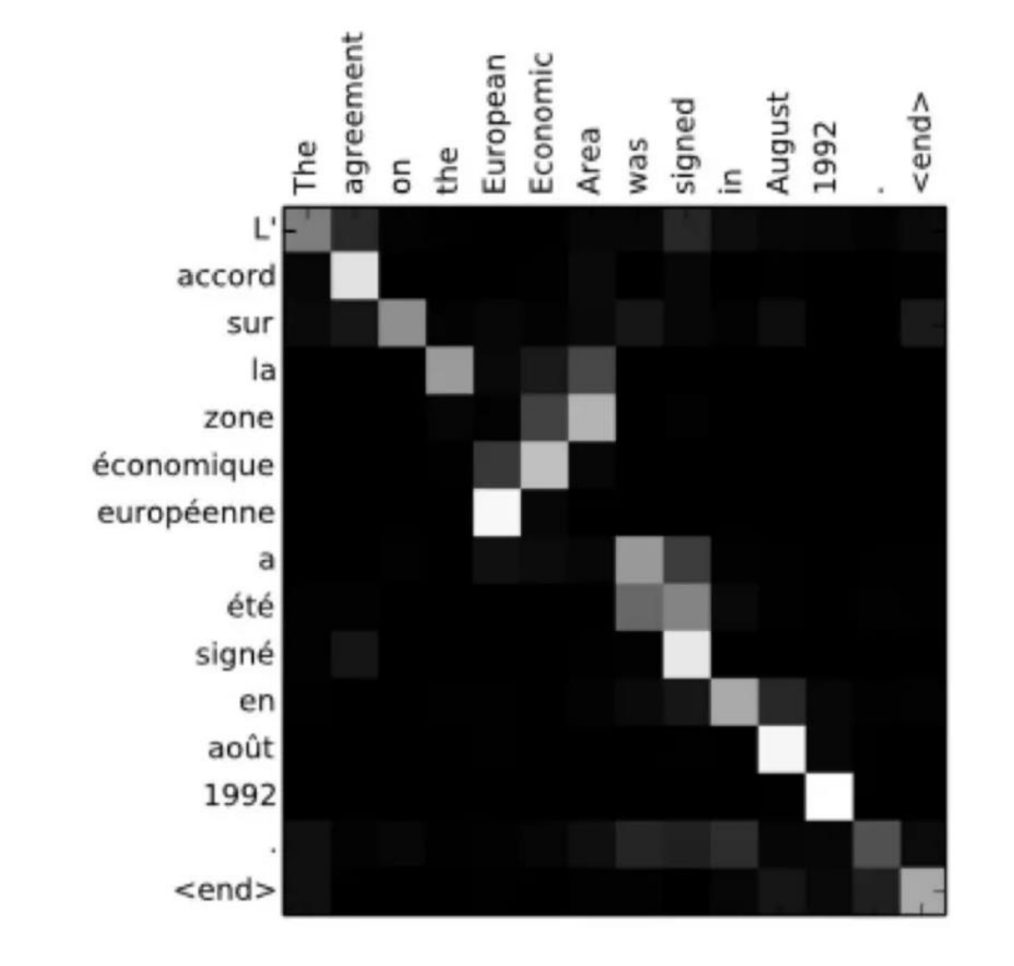
- RNN with attention

- Attention is learned via a simple FFN



Visualizing attention

- Linear weights are interpretable
- We can see which word is more important
- Can we use attention for explainability?



Attention is all you need
The original Transformer

Training vs Finetuning

- Simple end-to-end models are trained for a single task
- Word embeddings can be reused, compositionality is learned
- Transfer learning has limited capabilities
  - From similarity to inference
  - From emotion to sentiment

Need for powerful transfer learning models

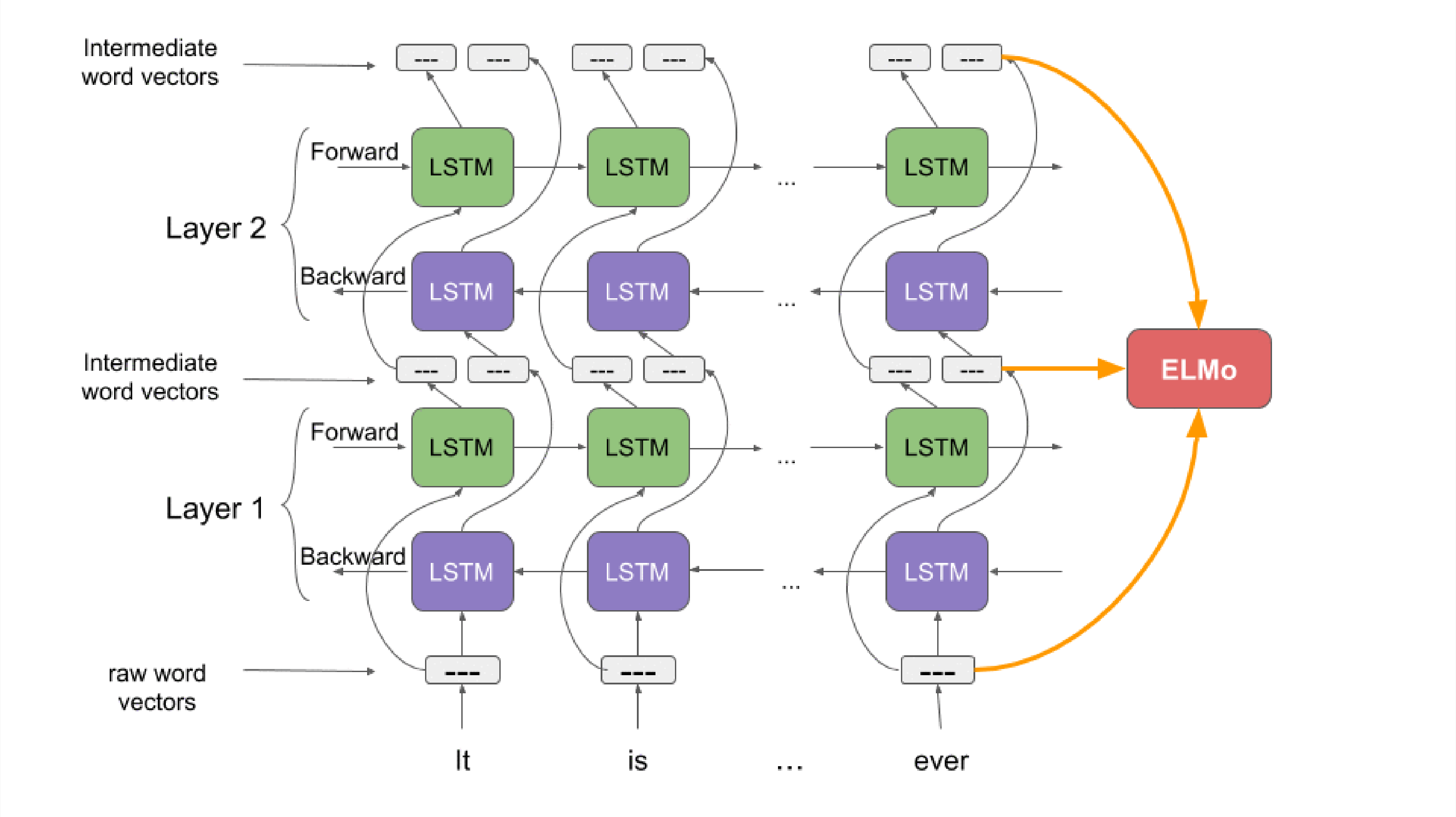
- Generic representation framework
  - Represent (contextual) word meaning
  - Represent interactions between words
  - Capture different types of meaning and interactions
- Easy to adapt to new tasks with minimal adjustment
- Looks familiar?
  - Many of the problems and RQs remain the same, just the context changes

Look back at ELMO

- ELMO embeddings meet most of those expectations
  - In-context meaning
  - Interactions between words
  - Deep representation capturing different relations
  - Task specific weight learning
- Pop quiz: how did ELMO embeddings work?

Elmo architecture

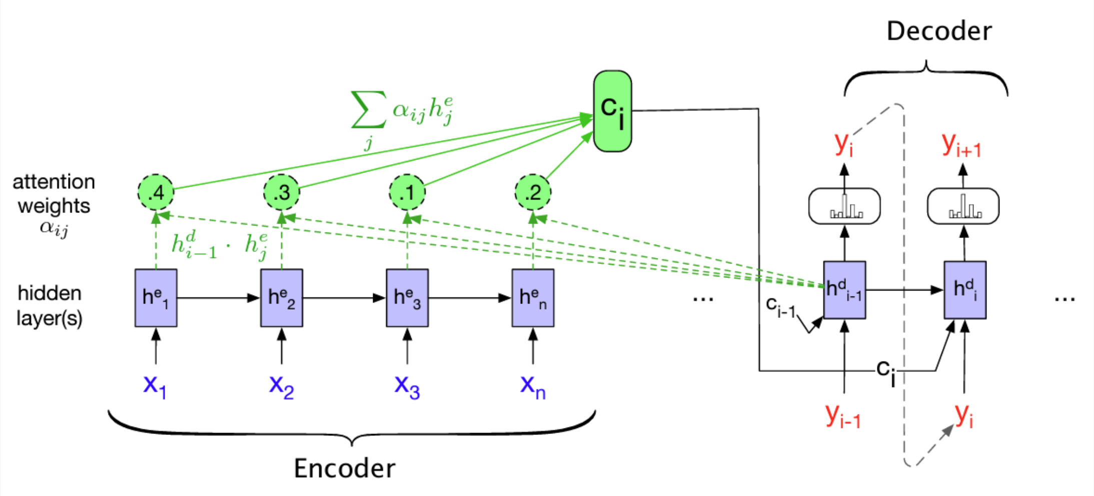
- How can we improve over that?



Self attention

- Attention works better than RNN/LSTM for encoder-decoder models

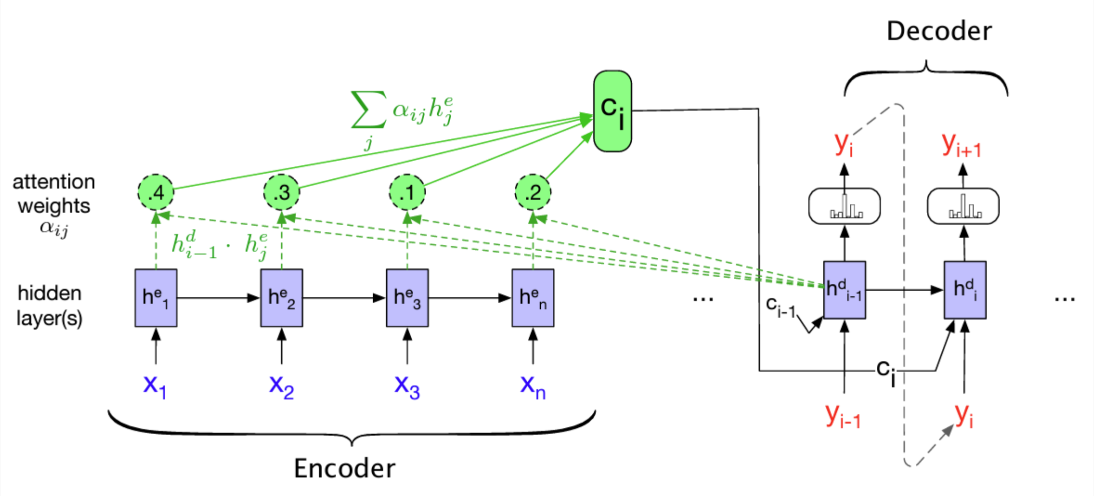
- Can we use attention for a standalone network?

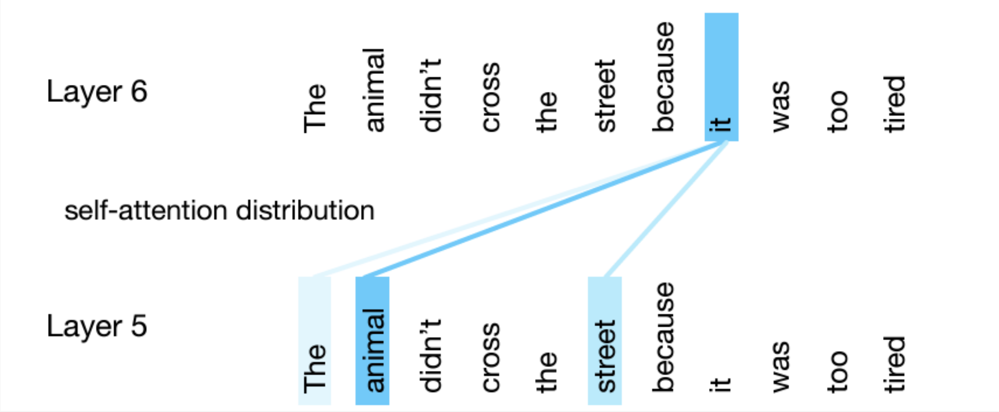


Self attention (2)

- Self attention is a key concept in building transformers

- It applies the same approach as attention in encoder-decoder, but on itself

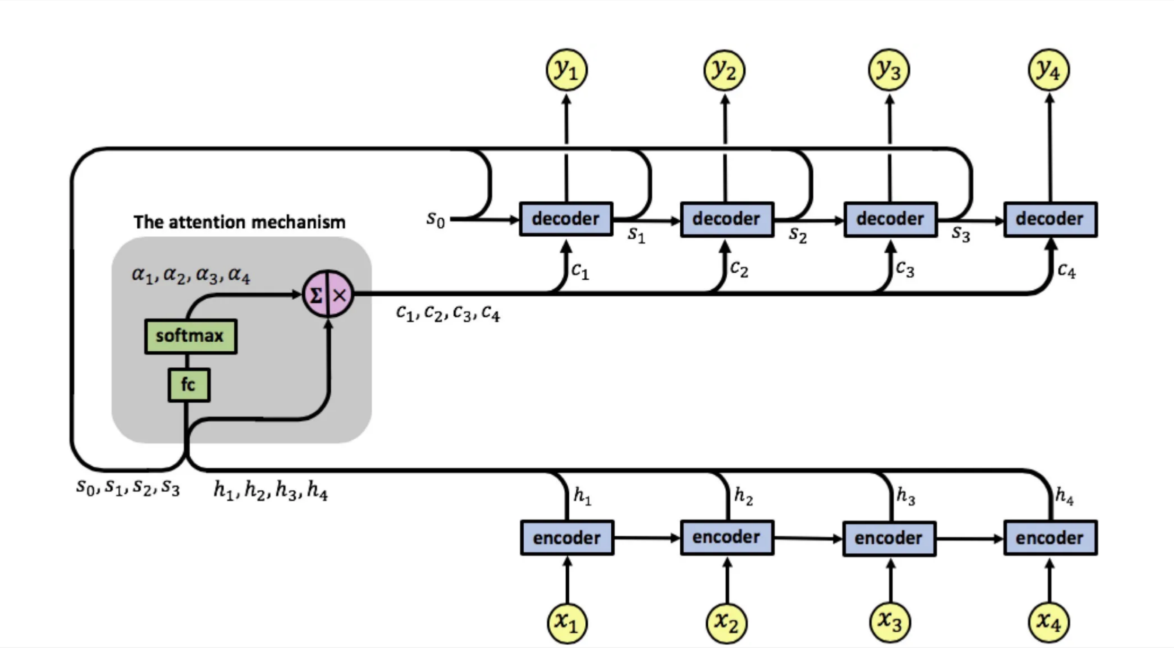




Causal attention vs bidirectional attention

- In encoder-decoder attention, the attention is the weighted sum of all hidden states of the encoder

- Which hidden states do we use in self attention?
  - Why?



Causal self attention

- Causal self-attention is used in models like GPT
- Two key properties
  - Only calculated using words in one direction (left for european languages)
  - Each representation at a layer L is calculated independently of the others
- How does this compare to RNNs and LSTMs?
  - Why are these two properties important?

Pop quiz

- Can a transformer model process infinite input?

- Can an RNN be (natively) parallelized?

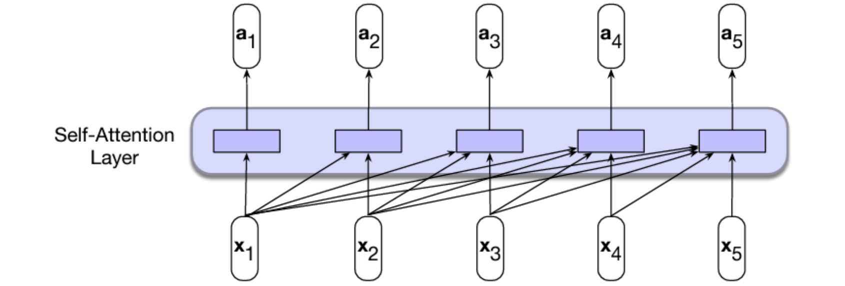
Causal self attention (intuition)

- Similar to RNNs, we have a 1:1 input-output mapping
- Same basic approach as original attention
  - Dot product + softmax + weighted sum

$$\text{score}(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{x}_i \cdot \mathbf{x}_j$$

$$\begin{aligned} \alpha_{ij} &= \text{softmax}(\text{score}(\mathbf{x}_i, \mathbf{x}_j)) \ \forall j \le i \\ &= \frac{\exp(\text{score}(\mathbf{x}_i, \mathbf{x}_j))}{\sum_{k=1}^{i} \exp(\text{score}(\mathbf{x}_i, \mathbf{x}_k))} \ \forall j \le i \end{aligned}$$

$$\mathbf{a}_i = \sum_{j \le i} \alpha_{ij} \mathbf{x}_j$$



  - Which is the most similar token to x_3? What is the input to the first hidden layer?

Decomposing input vectors

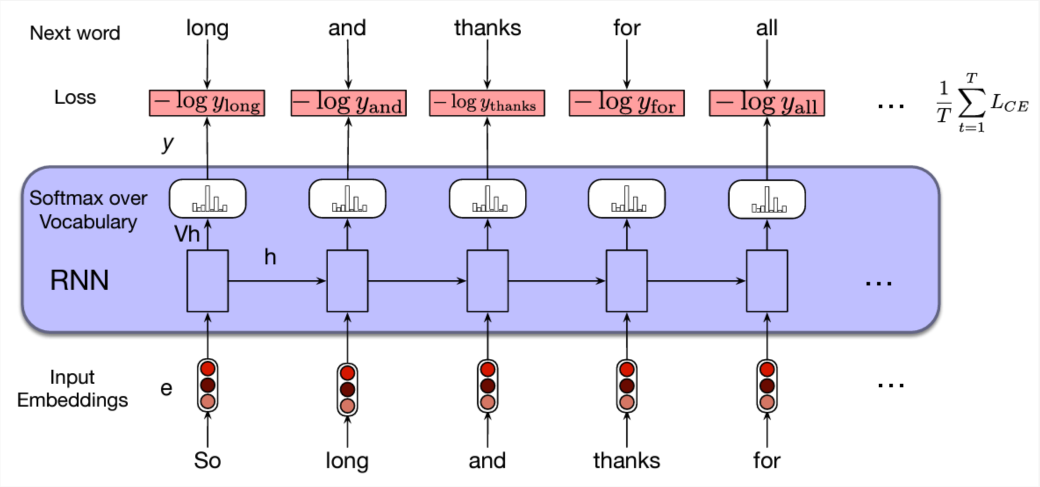
- We can use simple attention
- Transformers introduce query, key, value
- What are they, why do we need them and how do we use them?
  - The “dictionary” analogy
  - A semantic explanation, grounded in NLP

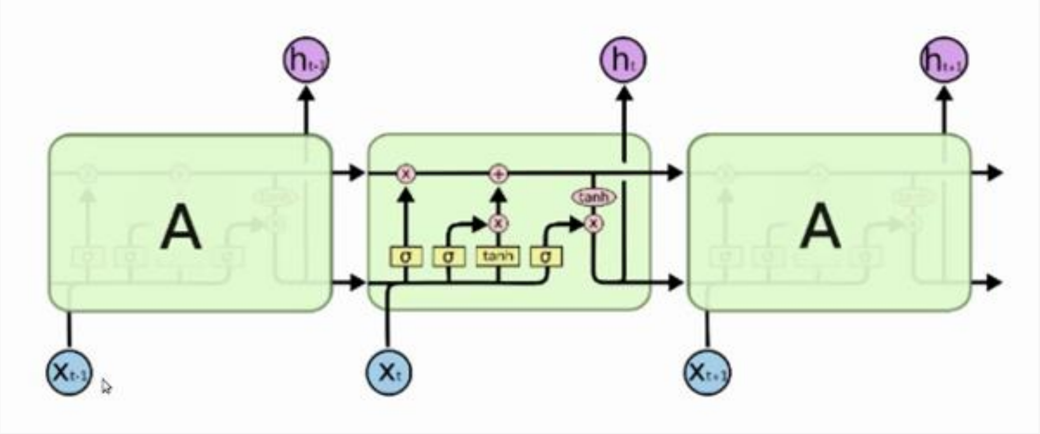
The LSTM and RNN

- What is the difference between LSTM and RNN?

- Why do we need that “evolution”?

- Break a single hidden state into two + gates
    - Filtering and specialization





Compositionality of meaning

- Consider the following phrases
  - “A black dog”
  - “A house for my dog”

- What is the meaning of the dog in each phrase?

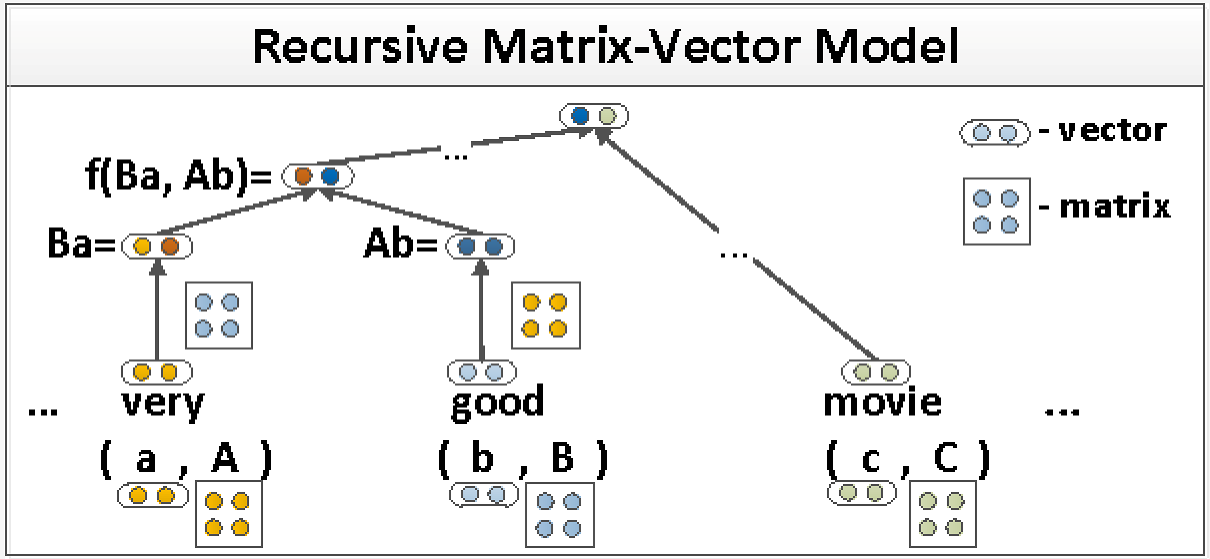
- Where is the dog in the second picture?

Compositionality of meaning (2)

- What about “A house for my black dog”?
  - Does “dog” change the meaning of “house”?
  - Does “house” change the meaning of “dog”?
  - Does “dog” change the meaning of “black”?
  - Does “black change the meaning of “dog”?
- Meaning compositionality can be asymmetrical!

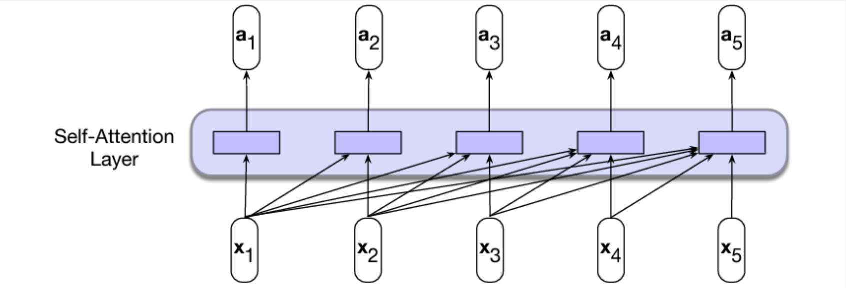
Different aspects of meaning compositionality

- Meaning compositionality is not a simple addition
- Words “behave” differently in different context
- Socher’s Vector-Matrix representation
  - Vector for the head, matrix for the complement
- Pop quiz: what would be the vector and what would be the matrix in “black dog”?



How to model asymmetric compositionality in attention?

- Self attention (that we have seen) has 1:1 correspondence
- Dot product attention is commutative
  - a · b = b · a
  - score(“black”, ”dog”) = score(“dog”, “black”)



- Pop quiz: would “black” have the same importance on “dog” as “dog” would have on “black”?

The query, key, value

- We project the input vector x to three vectors that serve different purpose: “query”, “key”, and “value”
- Two vector operations in the original attention:
  - “Score”: for indexes i and j, calculate how important is x_j for x_i: score(x_i, x_j)
  - “Scale”: for index i, calculate the hidden state h_i as a weighted sum of x_1 … x_i: $h_i = \sum_{j \leq i} \alpha_{ij} x_j$
- Each input vector x can three different roles
  - Argument 1 in score() [“dog” in score(“dog”, ”black”)] -> **query**
  - Argument 2 in score() [“dog” in score(“black”, “dog”)] -> **key**
  - The **value** used in scale to calculate the hidden state

Query, Key, Value (formally)

- We learn three different matrices (W^Q, W^K, W^V)
- Every input vector x_i is projected to three different representations
  - $q_i = x_i W^Q$; $k_i = x_i W^K$; $v_i = x_i W^V$
- The new formula for score: $\text{score}(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{q}_i \cdot \mathbf{k}_j$
- The new formula for calculating weights: $\mathbf{a}_i = \sum_{j \leq i} \alpha_{ij} \mathbf{v}_j$
- Pop quiz: which token will have the most impact on x_3?

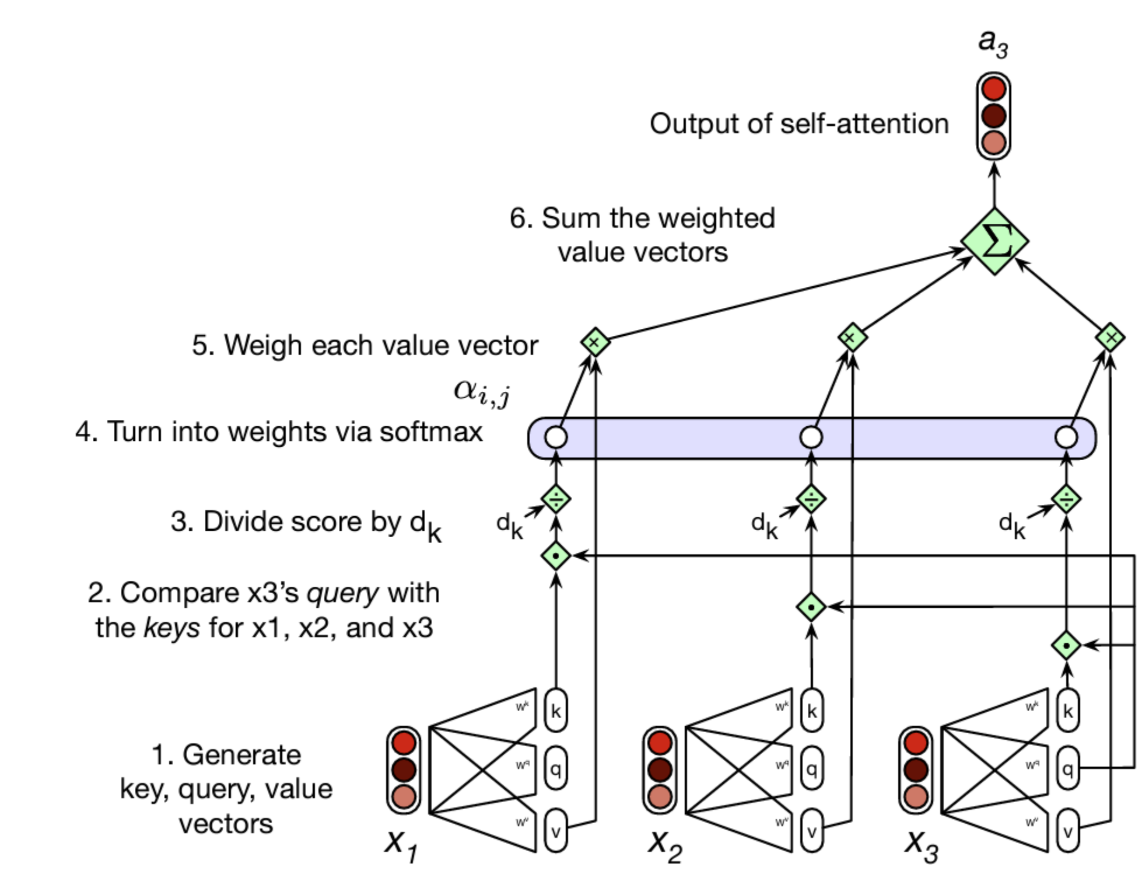
The transformer self attention

1. $\mathbf{q}_i = \mathbf{x}_i \mathbf{W}^{\mathbf{Q}}; \mathbf{k}_i = \mathbf{x}_i \mathbf{W}^{\mathbf{K}}; \mathbf{v}_i = \mathbf{x}_i \mathbf{W}^{\mathbf{V}}$

2. and 3. $\text{score}(\mathbf{x}_i, \mathbf{x}_j) = \frac{\mathbf{q}_i \cdot \mathbf{k}_j}{\sqrt{d_k}}$

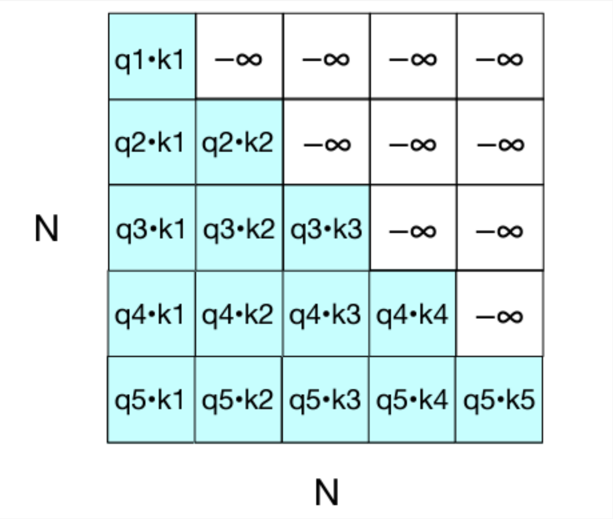
4. $\alpha_{ij} = \text{softmax}(\text{score}(\mathbf{x}_i, \mathbf{x}_j)) \ \forall j \leq i$

5. and 6. $\mathbf{a}_i = \sum_{j \leq i} \alpha_{ij} \mathbf{v}_j$



Parallelizing and masking the future

- Calculating hidden state h_t is independent of $h_{(t-1)}$
- We can compute all hidden states in a single operation
  - $Q = XW^Q$; $K = XW^K$; $V = XW^V$
  - $A = \text{SelfAttention}(Q,K,V) = \text{softmax}(\frac{QK^T}{\sqrt{d_k}})V$
- Can you see a problem for causal self attention?



- Pop quiz: What is the complexity of the self-attention w.r.t. length of the input?

Multiheaded self-attention

- Instead of using a single self attention, we can use multiple
  - Each "head" has its own weights W^Q, W^K, W^V
  - The outputs of all heads are concatenated and projected to input dimensions
- Formally:

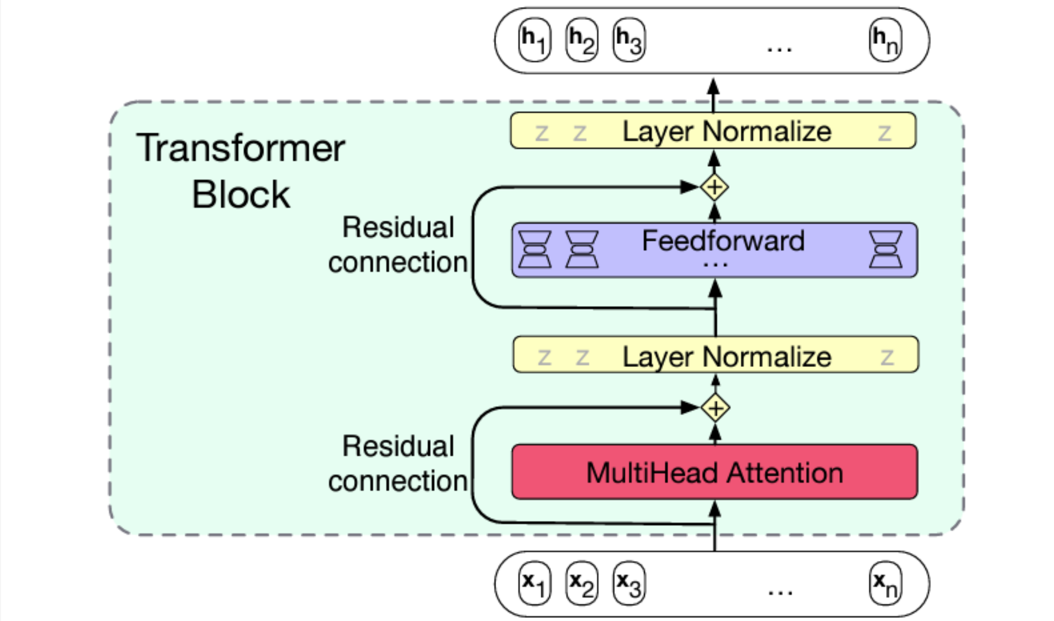
$$\mathbf{Q} = \mathbf{X}\mathbf{W}_i^Q \; ; \; \mathbf{K} = \mathbf{X}\mathbf{W}_i^K \; ; \; \mathbf{V} = \mathbf{X}\mathbf{W}_i^V$$

$$\mathbf{head}_i = \text{SelfAttention}(\mathbf{Q}, \mathbf{K}, \mathbf{V})$$

$$\mathbf{A} = \text{MultiHeadAttention}(\mathbf{X}) = (\mathbf{head}_1 \oplus \mathbf{head}_2 \ldots \oplus \mathbf{head}_h)\mathbf{W}^O$$

The transformer block

- Residual connection
  - Copy the input of a layer to its output
- Layer normalize
  - Rescale each x vector to 0-mean with STD=1
- Feedforward
  - Apply the same fully connected FFN to each x

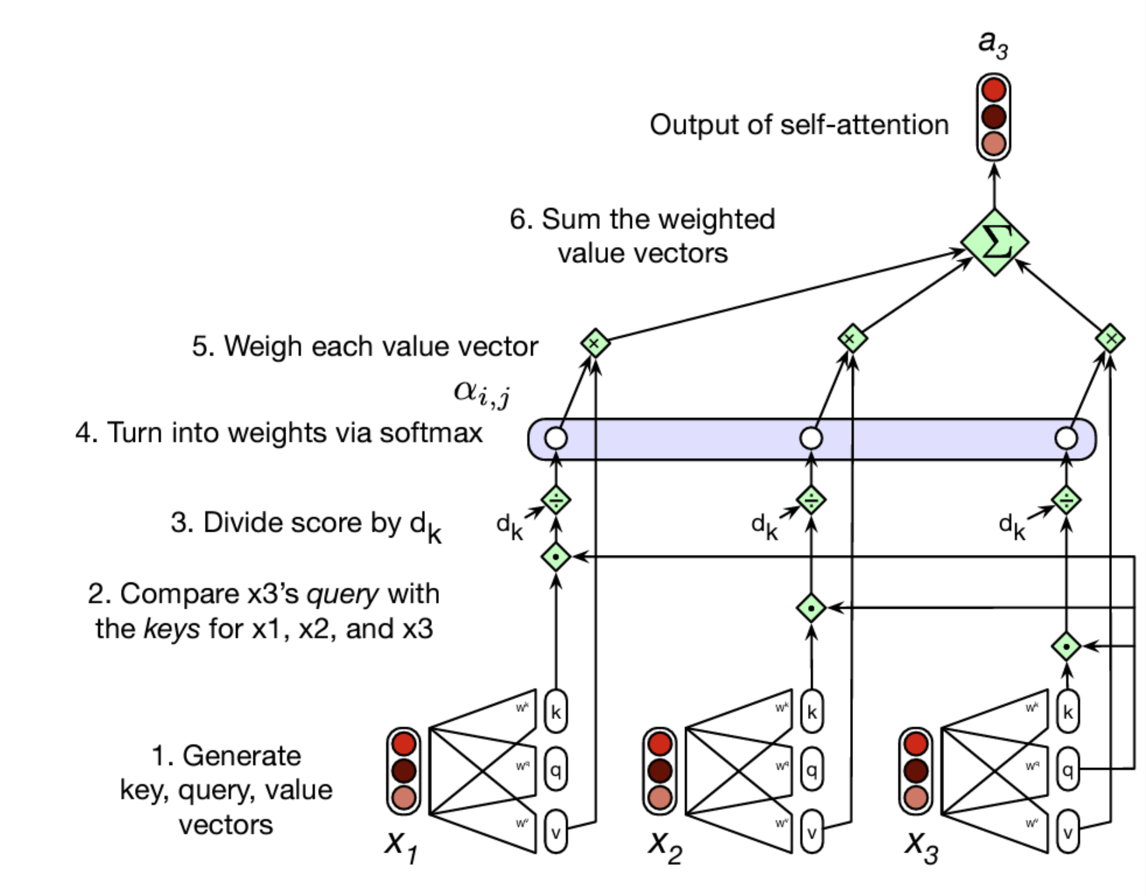


The transformer block (formally)

- Simplified representation
  - O = LayerNorm(X + MultiHeadAttention(X))
  - H = LayerNorm(O + FFN(O))
- You can change the order of operations in some implementaitons

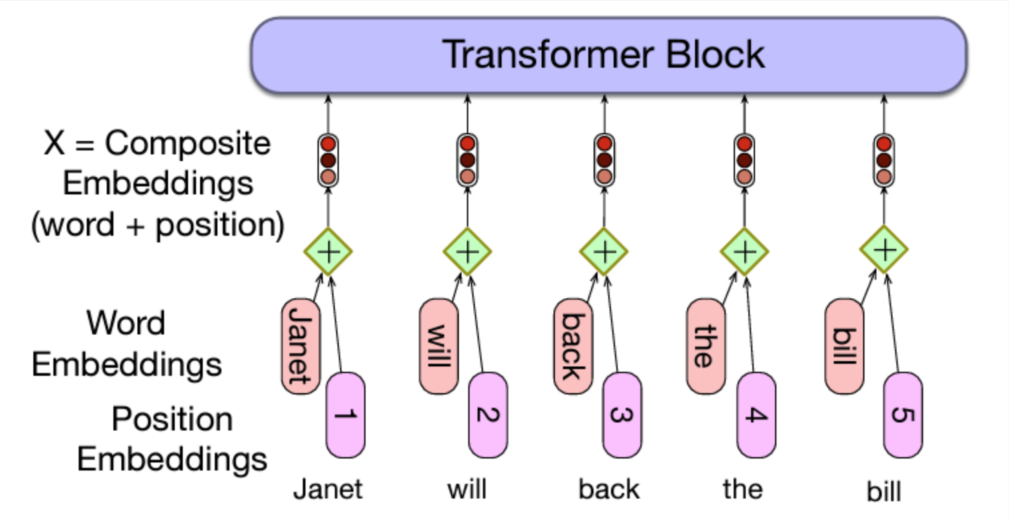
Does transformer consider word order?

- Consider an autoregressive transformer
- Does it handle long-distance dependencies?
- Does it handle word order?
    - Does the position of x1 and x2 matter?



Encoding the Input. Positional Embeddings.

- Semantic embeddings
  - One-hot encoding maps to a row in a matrix
- Positional embeddings
  - One embedding for each position
  - Learnable; Same dimension as semantic
- Add semantic and positional embeddings



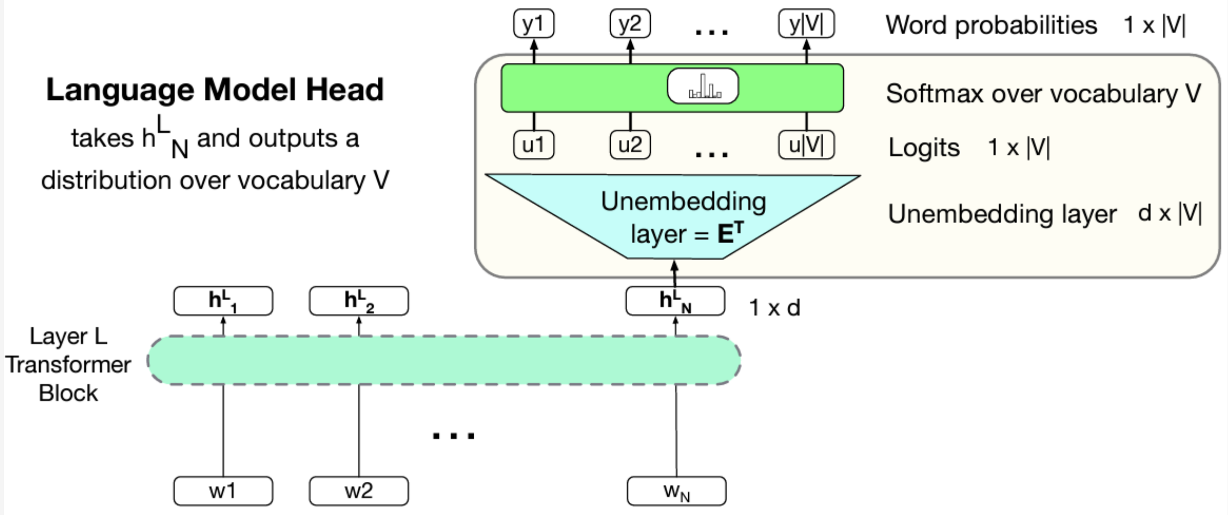
- Alternative techniques: use functions (sine/cosine); calculate relative positional embeddings

Classification layer: The “Head” of the model

- How did we train word2vec?
  - How did we reduce the computational cost?
- The concept of transfer learning
  - Train on one objective
  - Reuse the model on another task
  - We keep the stacked transformer blocks, change the “head”

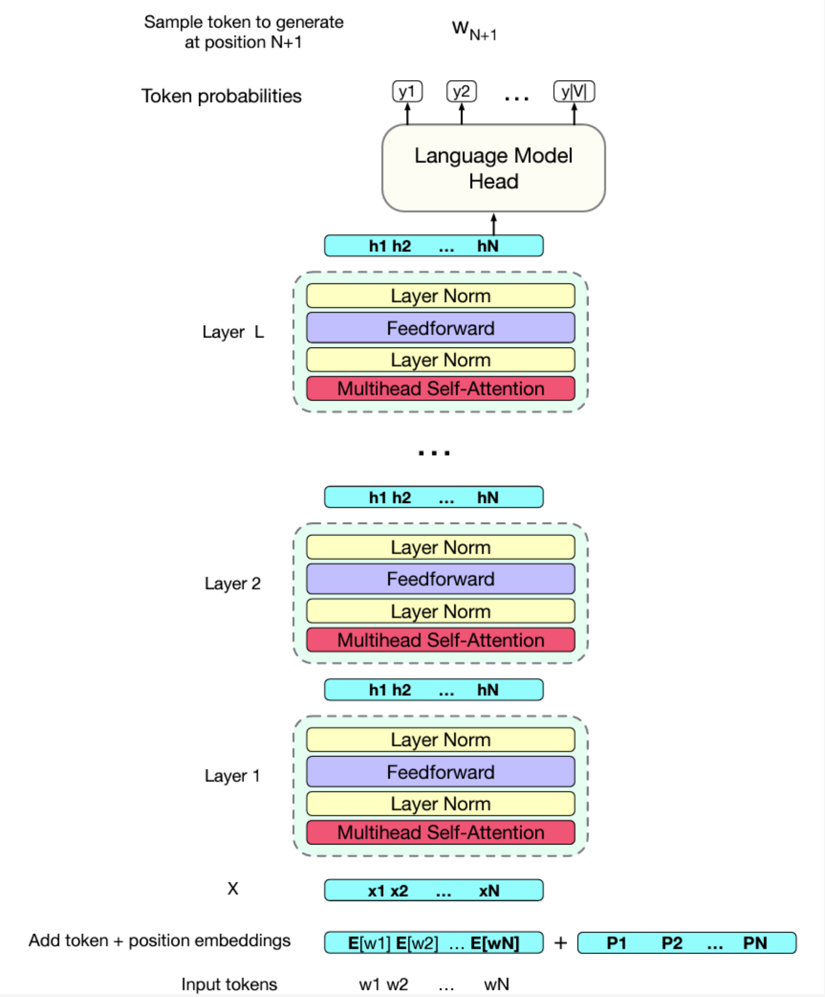
Language modeling head

- Language modeling
  - Efficient for learning representations
  - Self-supervised
- Project h_N to vocabulary size
  - Do we know any computational tricks for that?
  - What would h_N^L look like?



A final transformer representation for LM

- Token + positional embedding
- Multiple stacked transformer blocks
- A classification head
  - Language modeling with weight tying and sampling



Conclusions

Encoder decoder models

- Dealing with tasks where input and output are mismatched
  - Different length
  - No 1 to 1 alignment
- We use one model to encode the input (image, text in English)
- We use another model to generate text in target language
- Simple encoder decoder is based on RNNs/LSTMs

Attention

- RNNs have problems with long-distance dependencies
- Decoding from a single hidden state is restricted
- Attention uses all hidden states and compares current decoder state
  - Dot product attention

Transformers

- Self attention builds upon the attention from encoder-decoder
- Query, Key, Value project the input based on its function
- Multiheaded attention stacks multiple self attentions

Transfer learning

- The goal of transformers – learn contextual (and text) representations and reuse
- The head of the transformer determines the task
- Multiple problems can be framed as classification or generation