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



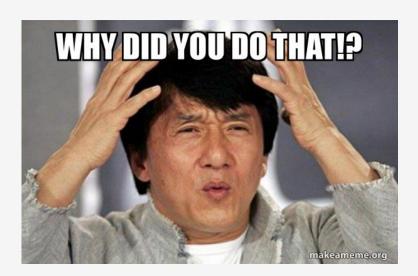
Challenges with going end to end

- 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



- 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?

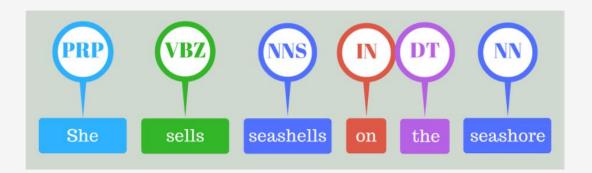
Sequence labeling vs sequence-to-sequence

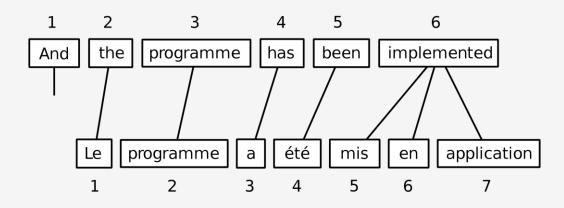
Consider the following two tasks

What is similar between them?

What is different?

How would you approach each of them?





Key differences

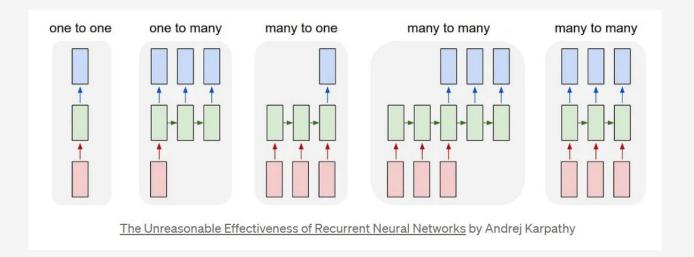
Same length vs different length

• 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

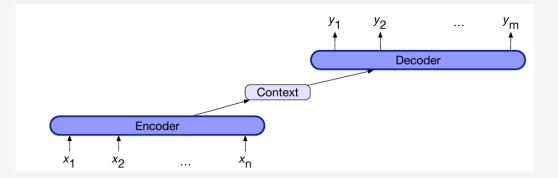


Encoder decoder

• We use a model family called encoder-decoder

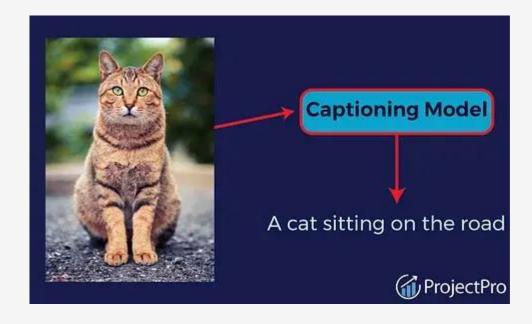
- Simple idea
 - Encoder "represents" the source (e.g., English)
 - Decoder "generates" the target (e.g., German)

Can you suggest tasks that can use encoder-decoder?



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
- softmax
 hidden layer(s)
 embedding layer

 the green witch arrived separator

 Source Text

 Separator

Target Text

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

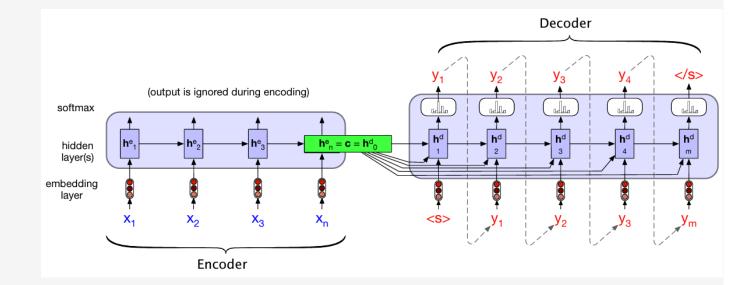
Using separate RNNs for encoder and decoder

- 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

• Why is there a "y" at the calculation of the hidden state h_t^d ?

$$\mathbf{c} = \mathbf{h}_{n}^{e}$$

$$\mathbf{h}_{0}^{d} = \mathbf{c}$$

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

$$\mathbf{z}_{t} = f(\mathbf{h}_{t}^{d})$$

$$\mathbf{y}_{t} = \operatorname{softmax}(\mathbf{z}_{t})$$
Use the value from the previous state:
$$\mathbf{z}_{t} = \mathbf{h}_{n}^{e}$$

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

$$\mathbf{z}_{t} = \mathbf{f}(\mathbf{h}_{t}^{d})$$

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Training encoder-decoder models

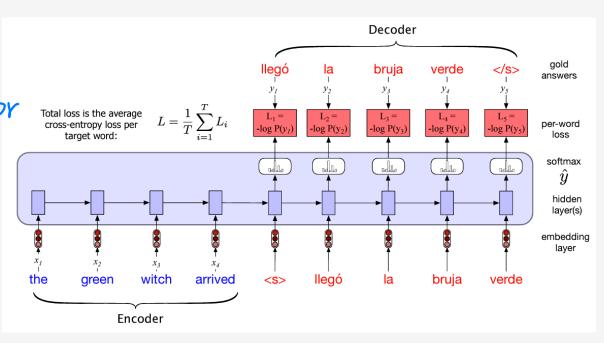
Models are trained end-to-end

- Encoder is trained through hidden layers

 if you get a word, calculate the error

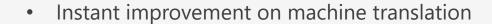
 and mitigate them
- Decoder is trained through teacher forcing
 - Remember "teacher forcing"?





incorrect.

Why are encoder-decoder models important?



Google Translate switching to NMT

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

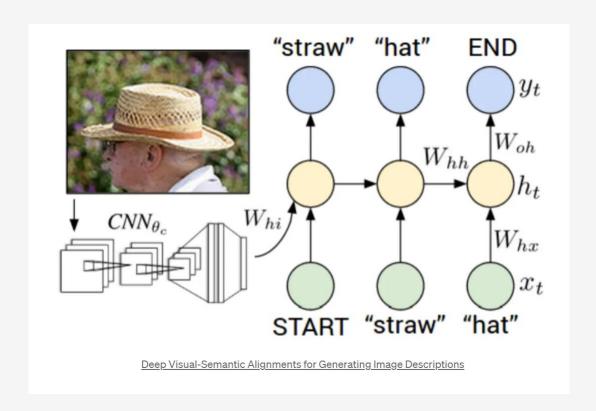
• Bridging the gap between modalities

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



Attention

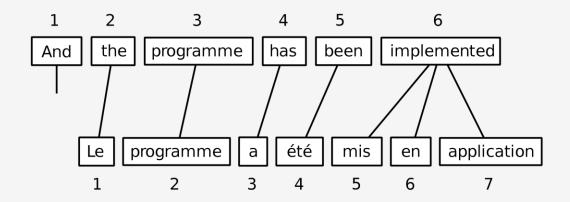
A bottleneck of RNNs

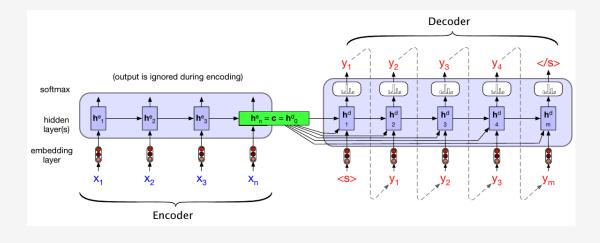
 Consider the problem of MT and an encoderdecoder solution

• 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

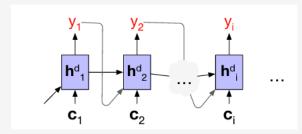
• Still needs to have a fixed length, regardless of variable input length

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:

$$\operatorname{score}(\mathbf{h}_{i-1}^d, \mathbf{h}_j^e) \ = \ \mathbf{h}_{i-1}^d \cdot \mathbf{h}_j^e$$

• Weight vector:

$$\alpha_{ij} = \operatorname{softmax}(\operatorname{score}(\mathbf{h}_{i-1}^d, \mathbf{h}_j^e))$$

$$= \frac{\exp(\operatorname{score}(\mathbf{h}_{i-1}^d, \mathbf{h}_j^e))}{\sum_k \exp(\operatorname{score}(\mathbf{h}_{i-1}^d, \mathbf{h}_k^e))}$$

• Personalized context:

$$\mathbf{c}_i \ = \ \sum_j lpha_{ij} \, \mathbf{h}^e_j$$

More complex scoring functions:

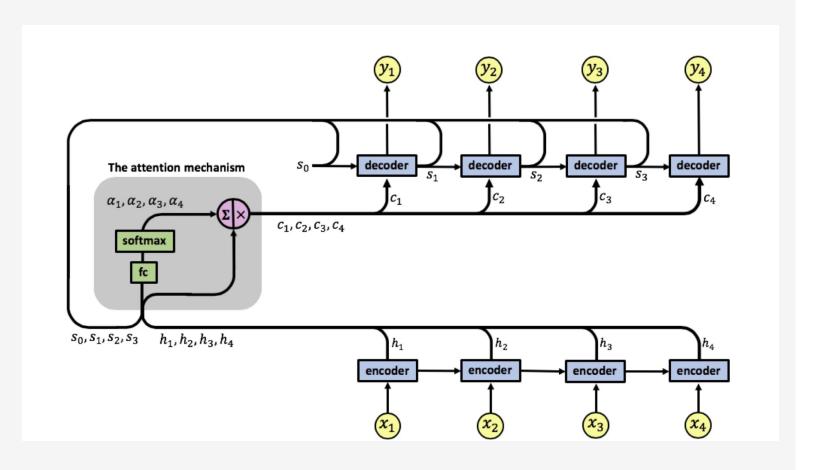
$$score(\mathbf{h}_{i-1}^d, \mathbf{h}_{j}^e) = \mathbf{h}_{t-1}^d \mathbf{W}_s \mathbf{h}_{j}^e$$

we don't use softmax

Visualization of RNN with attention

RNN with attention

• Attention is learned via a simple FFN

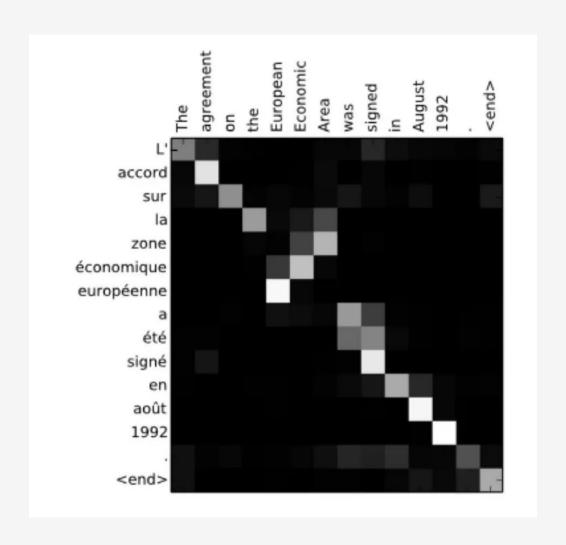


Visualizing attention

• 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

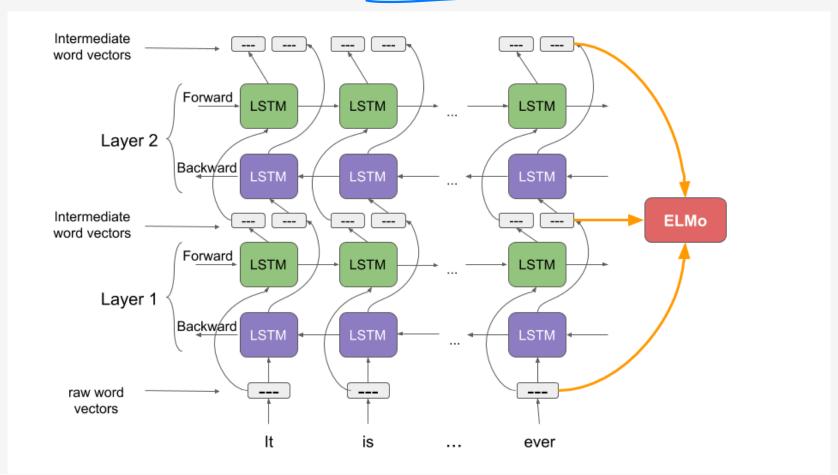
- ELMO embeddings meet most of those expectations
 - In-context meaning
 - Interactions between words
 - Deep representation capturing different relations
 - Task specific weight learning

• Pop quiz: how did ELMO embeddings work?

Elmo architecture

How can we improve over that?

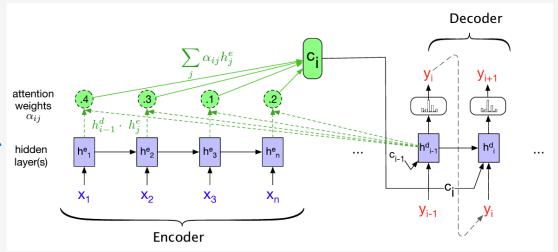
using Attention



Self attention

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

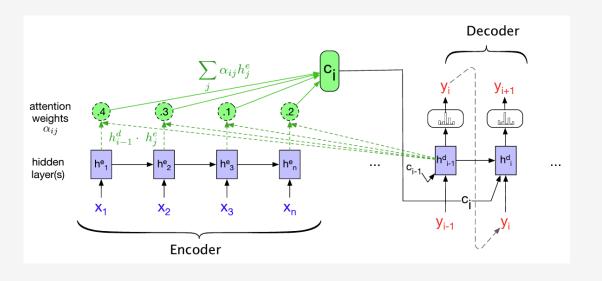
Can we use attention for a standalone network?

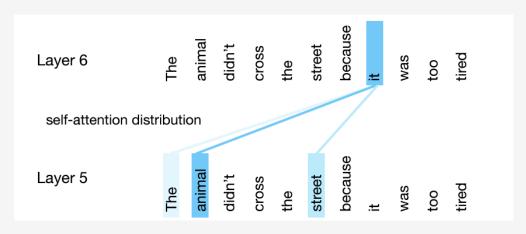


Self attention (2)

Self attention is a key concept in building transformers

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





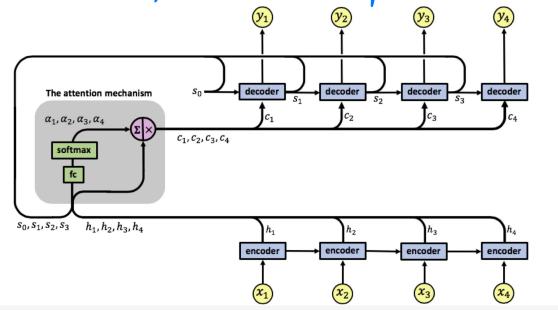
Causal attention vs bidirectional attention

[more used for classification.

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

RNN can't handle long sequence (they do, but compare to LSTM)

- Which hidden states do we use in self attention?
 - Why?
 - . bidirectional attention Cannor look into the future



-> time efficiency is not a problem

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?

RNN has to compute hidden State sequentially.

Pop quiz

• Can a transformer model process infinite input?

Və

• Can an RNN be (natively) parallelized?

No

Causal self attention (intuition)

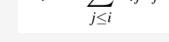
- Similar to RNNs, we have a 1:1 input-output mapping
- Same basic approach as original attention
 - Dot product + softmax + weighted sum

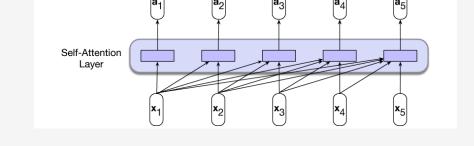
$$score(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{x}_i \cdot \mathbf{x}_j$$

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

$$= \frac{\exp(\operatorname{score}(\mathbf{x}_i, \mathbf{x}_j))}{\sum_{k=1}^{i} \exp(\operatorname{score}(\mathbf{x}_i, \mathbf{x}_k))} \ \forall j \leq i$$

$$\mathbf{a}_i = \sum_{j \leq i} lpha_{ij} \mathbf{x}_j$$

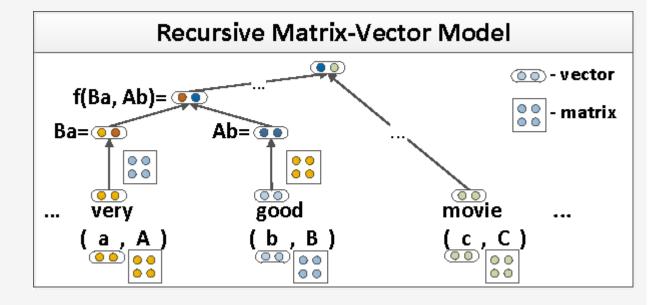




Which is the most similar token to x_3 ? What is the input to the first hidden layer?

The query, key, value

- You can use a simple dot-product attention
- Transformers introduce the "query, key, value" concepts
- The key ideas:
 - Tokens have different roles
 - Meaning has different aspects
- Consider the following phrases:
 - "The dog is happy"
 - "The toy of the dog"



The query, key, value (2)

- Attention has two key computations
 - Calculate relative weight between vector x_i , and every other vector x_j : score(x_i , x_j)
 - Weighted sum of each vector x_j based on its relative importance to x_i :

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

- Three roles a token has in self attention.
 - The query: the vector for x_i when x_i is the first element of score(), when we calculate a_i
 - The key: the vector for x_j when x_j is the second element of score(), when we calculate a_i
 - The value: the vector that we use for the scaling and the weighted sum
- Two vectors that define the interactions; One vector that contains the "substance"

The complex nature of meaning and meaning compositionality

• Simple semantic representations assume meaning is static and can be defined with a single function

- Modern algorithms (implicitly) account for complexity of meaning:
 - Vector-Matrix operators in early compositionality
 - Separation between long- and short-term memory (different gates)
 - Deep (contextual) representations
 - Query, Key, Value

Query, Key, Value (formally)

- We learn three different matrices (WQ, WK, WV)
- Every input vector xi 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: $score(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{q}_i \cdot \mathbf{k}_j$
- The new formula for calculating weights: $\mathbf{a}_i = \sum_{j \leq i} \alpha_{ij} \mathbf{v}$

• 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.
$$\operatorname{score}(\mathbf{x}_i, \mathbf{x}_j) = \frac{\mathbf{q}_i \cdot \mathbf{k}_j}{\sqrt{d_k}}$$

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

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

