

Applied Machine Learning

Neural Networks for Sequences

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Deep Neural Networks

- Neural Networks for **Tabular Data**
 - MLP
- Neural Networks for **Images**
 - CNN
- Neural Networks for **Sequences**
 - input is a sequence, the output is a sequence, or both are sequences
 - *e.g. machine translation, speech recognition, text classification, image captioning*

The interface shows a comparison between two sentences:

English	French
Lets learn how to translate a sentence that is a sequence of words	Apprenons à traduire une phrase qui est une séquence de mots.

At the top right, there are buttons for "Automatic" and "Glossary".

Learning objectives

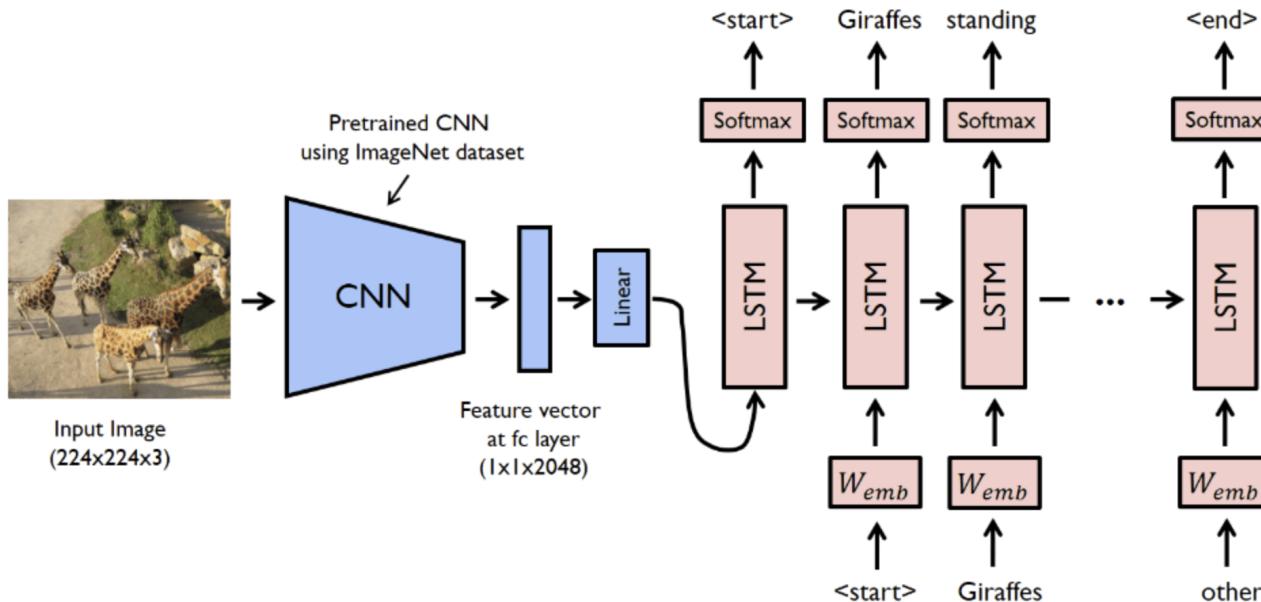
- Recurrent neural networks (RNNs)
 - 3 different models for different input/output
 - training with back propagation through time
- understand the attention mechanisms
- The architecture of transformer

Recurrent neural networks (RNNs)

- Vec2Seq (sequence generation)
- Seq2Vec (sequence classification)
- Seq2Seq (sequence translation)

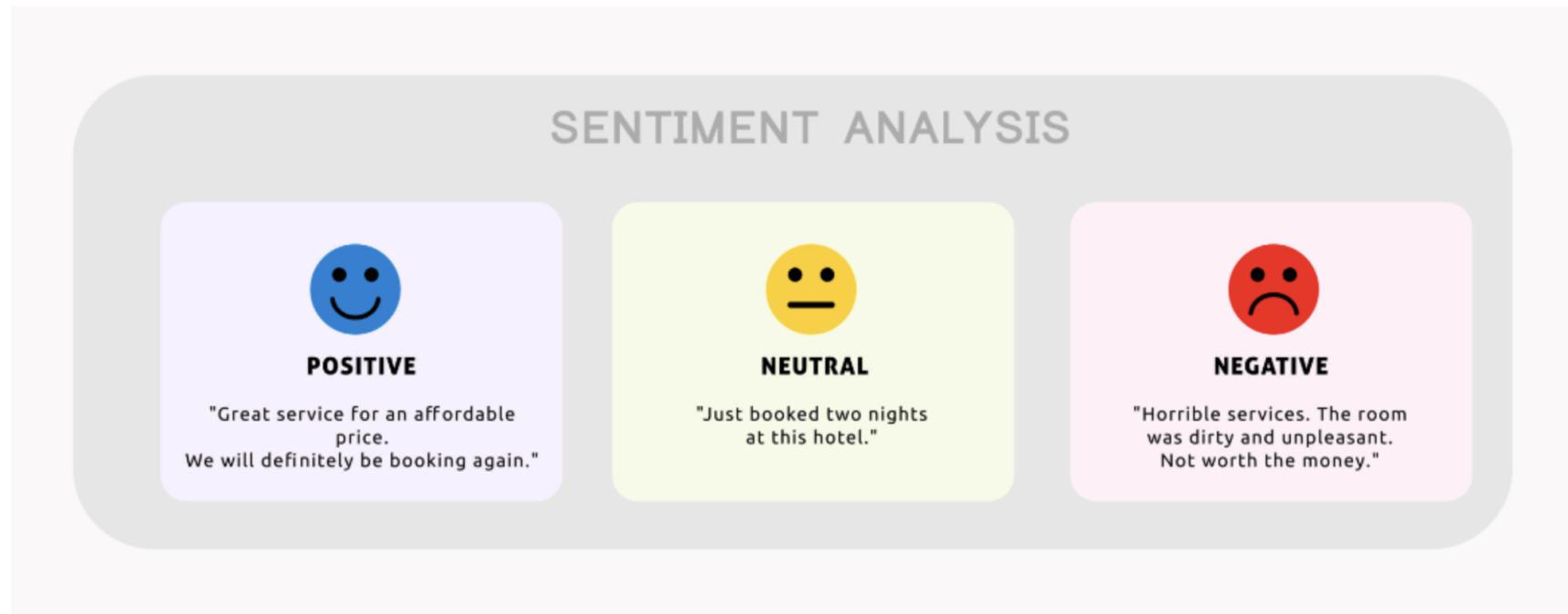
Vec2Seq (sequence generation)

Example : Caption generation



Seq2Vec (sequence classification)

Example : Sentiment classification



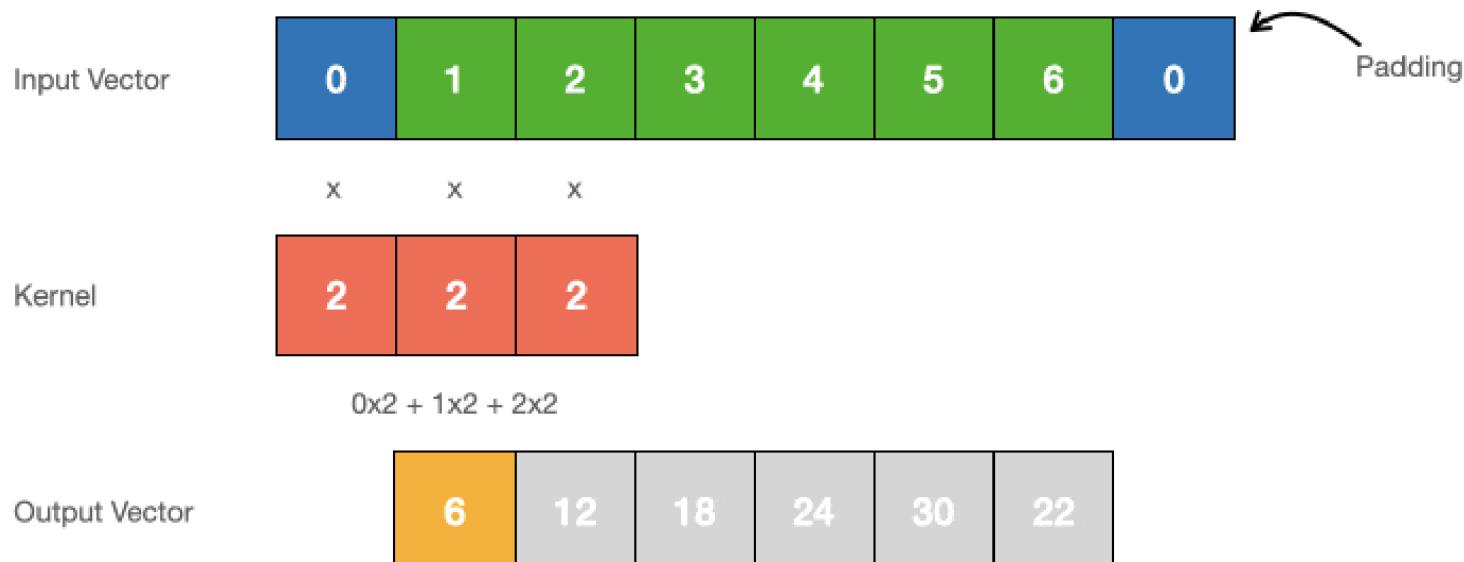
Seq2Seq (sequence translation)

Examples :

- Language translation (e.g. English to French)
- Language modelling (beginning of text to complete text)
- Protein folding (Sequence of amino acids to sequence of angles)
- Time series (e.g. stock price prediction, weather prediction)

Limitation of convolutions

We saw that convolutions can be used to process sequences



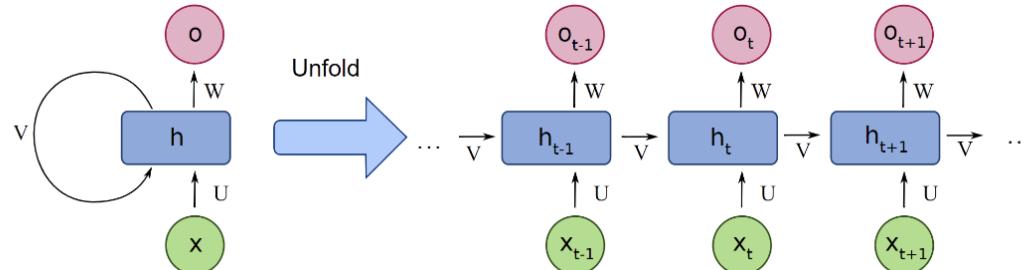
Cannot generate sequences of variable length

Generating sequences of variable length

The method we will look at works in the following way:

- Have a state that keeps track of past sequence information
- Have a special token <EOS> that indicates the end of sequence
- We can also have a <SOS> token that indicates the start of sequence

Recurrent neural network (RNN)



$$x_t \in \mathbb{R}^d, h_t \in \mathbb{R}^m, o_t \in \mathbb{R}^n$$

Matrix shapes: $U : m \times d, V : m \times m, W : n \times m$

RNN layer : $h_t = f(V \cdot h_{t-1} + U \cdot x_t + b_h)$

$$o_t = g(W \cdot h + b_o)$$

f is an activation function (tanh or ReLU)

Recurrent neural network (RNN)

$$h_t = \text{ReLU}(V \cdot h_{t-1} + U \cdot x_t + b_h)$$

$$o_t = (W \cdot h_t + b_o), \quad x_t \in \mathbb{R}^2, h_t \in \mathbb{R}^3, o_t \in \mathbb{R}^1$$

$$U = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ -1 & 0 \end{bmatrix}, V = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}, W = [1 \ 0 \ -1], b_h = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, b_o = 0$$

$$h_{t-1} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, x_t = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

What is h_t ?

Recurrent neural network (RNN)

$$h_t = \text{ReLU}(V \cdot h_{t-1} + U \cdot x_t + b_h)$$

$$o_t = (W \cdot h_t + b_o), \quad x_t \in \mathbb{R}^2, h_t \in \mathbb{R}^3, o_t \in \mathbb{R}^1$$

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$$h_{t-1} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, x_t = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad \text{What is } h_t? \quad h_t = \text{ReLU}(V \cdot h_{t-1} + U \cdot x_t)$$

Recurrent neural network (RNN)

$$h_t = \text{ReLU}(V \cdot h_{t-1} + U \cdot x_t + b_h)$$

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$$h_{t-1} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, x_t = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad \text{What is } h_t? \quad h_t = \text{ReLU} \left(\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} + U \cdot x_t \right)$$

Recurrent neural network (RNN)

$$h_t = \text{ReLU}(V \cdot h_{t-1} + U \cdot x_t + b_h)$$

$$o_t = (W \cdot h_t + b_o), \quad x_t \in \mathbb{R}^2, h_t \in \mathbb{R}^3, o_t \in \mathbb{R}^1$$

$$U = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ -1 & 0 \end{bmatrix}, V = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}, W = [1 \ 0 \ -1], b_h = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, b_o = 0$$

$$h_{t-1} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, x_t = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad \text{What is } h_t? \quad h_t = \text{ReLU} \left(\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} + \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix} \right)$$

Recurrent neural network (RNN)

$$h_t = \text{ReLU}(V \cdot h_{t-1} + U \cdot x_t + b_h)$$

$$o_t = (W \cdot h_t + b_o), \quad x_t \in \mathbb{R}^2, h_t \in \mathbb{R}^3, o_t \in \mathbb{R}^1$$

$$U = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ -1 & 0 \end{bmatrix}, V = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}, W = [1 \ 0 \ -1], b_h = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, b_o = 0$$

$$h_{t-1} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, x_t = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad \text{What is } o_t ? \quad o_t = W \cdot h_t = [1 \ 0 \ -1] \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} = 1$$

Recurrent neural networks (RNNs)

- Vec2Seq (sequence generation)

- output, $y_{1:T}$ is generated one token at a time
- at each step we sample y_t from the hidden state h_t and then feed it back to the model to get h_{t+1}

conditional generative model:

$$p(y_{1:T}|x) = \sum_{h_{1:T}} p(y_{1:T}, h_{1:T}|x) = \sum_{h_{1:T}} \prod_{t=1}^T p(y_t|h_t)p(h_t|h_{t-1}, y_{t-1}, x)$$

with the initial hidden state $p(h_1|h_0, y_0, x) = p(h_1|x)$

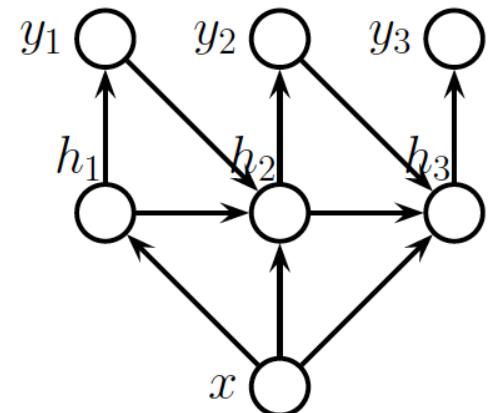
arbitrary-length sequence of vectors

$$f_\theta : \mathbb{R}^D \rightarrow \mathbb{R}^{N_\infty C}$$

D : input vector size

N_∞ : arbitrary-length sequence of vectors of length C

C : each output vector size



Recurrent neural networks (RNNs)

- Vec2Seq (sequence generation)

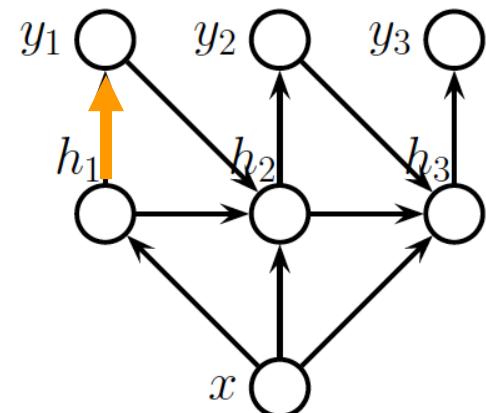
$$f_{\theta} : \mathbb{R}^D \rightarrow \mathbb{R}^{TC}$$

conditional generative model:

$$p(y_{1:T}|x) = \sum_{h_{1:T}} p(y_{1:T}, h_{1:T}|x) = \sum_{h_{1:T}} \prod_{t=1}^T p(y_t|h_t) p(h_t|h_{t-1}, y_{t-1}, x)$$

- real-valued output: $\hat{y}_t = W_{hy} h_t$
 $p(y_t|h_t) = \mathcal{N}(y_t|\hat{y}_t, \mathbf{I})$
- categorical output: $\hat{y}_t = \text{softmax}(W_{hy} h_t)$
 $p(y_t|h_t) = \text{Categorical}(y_t|\hat{y}_t)$

** per usual dropping bias terms for simplicity



Recurrent neural networks (RNNs)

- Vec2Seq (sequence generation)

$$f_{\theta} : \mathbb{R}^D \rightarrow \mathbb{R}^{TC}$$

conditional generative model:

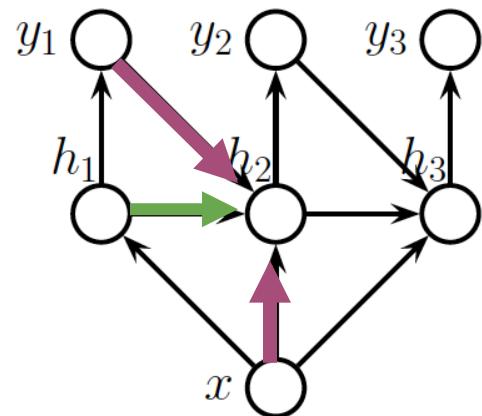
$$p(y_{1:T}|x) = \sum_{h_{1:T}} p(y_{1:T}, h_{1:T}|x) = \sum_{h_{1:T}} \prod_{t=1}^T p(y_t|h_t) p(h_t|h_{t-1}, y_{t-1}, x)$$

hidden state:

$$p(h_t|h_{t-1}, y_{t-1}, x) = \mathbb{I}(h_t = f(h_{t-1}, y_{t-1}, x))$$

input-to-hidden weights hidden-to-hidden weights

$$h_t = \varphi(W_{xh}[x; y_{t-1}] + W_{hh}h_{t-1})$$



Recurrent neural networks (RNNs)

- Vec2Seq (sequence generation)

$$f_{\theta} : \mathbb{R}^D \rightarrow \mathbb{R}^{TC}$$

model

$$\hat{y}_t = g(W_{hy} h_t)$$

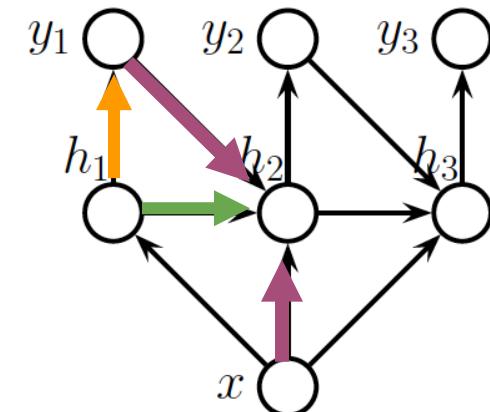
hidden-to-output weights

$$h_t = \varphi(W_{xh}[x; y_{t-1}] + W_{hh} h_{t-1})$$

input-to-hidden weights hidden-to-hidden weights

RNNs are powerful

- In theory can have unbounded memory and are as powerful as a [Turing machine](#)
- In practice, memory size is determined by the size of the latent space and strength of the parameters



Recurrent neural networks (RNNs)

- Vec2Seq (sequence generation)

conditional generative model:

$$p(y_{1:T}|x) = \sum_{h_{1:T}} p(y_{1:T}, h_{1:T}|x) = \sum_{h_{1:T}} \prod_{t=1}^T p(y_t|h_t) \textcolor{teal}{p(h_t|h_{t-1}, y_{t-1}, x)}$$

language modelling: generating sequences unconditionally (by setting $x = \emptyset$) which is learning joint probability distributions over sequences of discrete tokens, i.e., $p(y_1, \dots, y_T)$

Example:

character level RNN trained
on the book *The Time*

Machine by H. G. Wells (32,000
words and 170k character)

Output when given prefix

"the":

in his hand was a glitteringmetallic framework scarcely larger than a
small clock and verydelicately made there was ivory in it and the latter than s bettyre tat howhong s ie time thave
ler simk you a dimensions le ghat dionthat shall travel indifferently in any direction of space and timeas the driver
determinesfilby contented himself with laughterbut i have experimental verification said the time travellerit would
be remarkably convenient for the histo

Recurrent neural networks (RNNs)

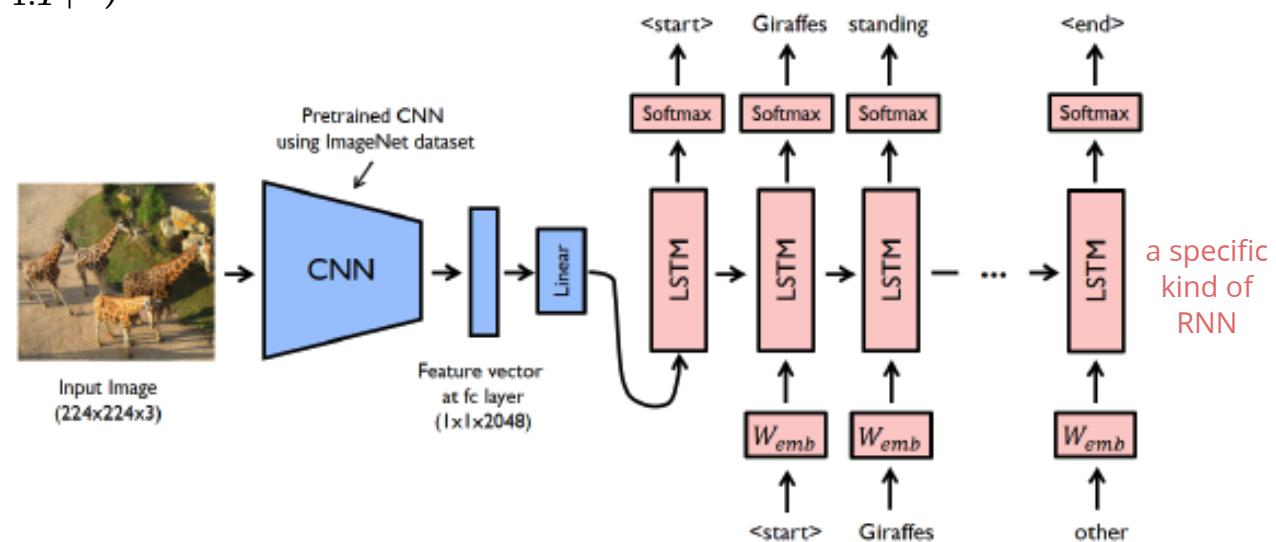
- Vec2Seq (sequence generation)

conditional generative model:

$$p(y_{1:T}|x) = \sum_{h_{1:T}} p(y_{1:T}, h_{1:T}|x)$$

Example:

CNN-RNN model for
image captioning
when x is embedding
by a CNN



See more [here](#)

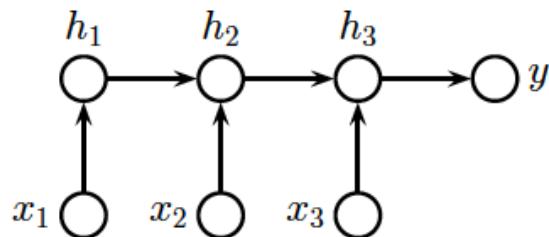
Recurrent neural networks (RNNs)

- Seq2Vec (sequence classification)
■ predict a single fixed-length output vector given a variable length sequence as input $y \in \{1, \dots, C\}$

use the final state:

$$\hat{y} = \text{softmax}(W h_T)$$

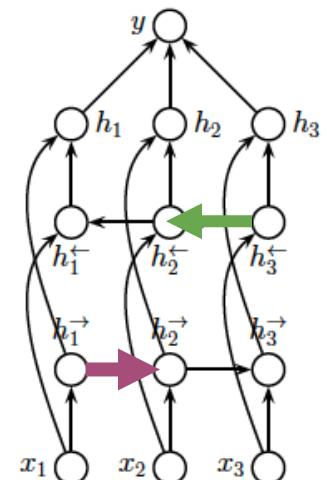
$$p(y|x_{1:T}) = \text{Categorical}(y|\hat{y})$$



Bi-directional RNN:

the hidden states of the RNN depend on the **past** and **future** context

gives better results



Recurrent neural networks (RNNs)

- Seq2Vec (sequence classification)
 - predict a single fixed-length output vector given a variable length sequence as input

$$h_t^{\rightarrow} = \varphi(W_{xh}^{\rightarrow} x_t + W_{hh}^{\rightarrow} h_{t-1}^{\rightarrow})$$

$$h_t^{\leftarrow} = \varphi(W_{xh}^{\leftarrow} x_t + W_{hh}^{\leftarrow} h_{t+1}^{\leftarrow})$$

$$h_t = [h_t^{\rightarrow}, h_t^{\leftarrow}]$$

$$\bar{h} = \frac{1}{T} \sum_{t=1}^T h_t$$

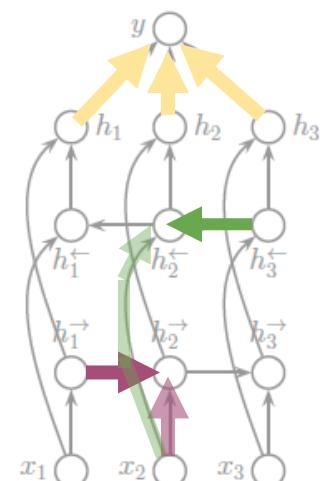
$$\hat{y} = \text{softmax}(W\bar{h})$$

$$p(y|x_{1:T}) = \text{Categorical}(y|\hat{y})$$

Bi-directional RNN:

the hidden states of the RNN depend on the **past** and **future** context

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Recurrent neural networks (RNNs)

- Seq2Vec (sequence classification)
 - predict a single fixed-length output vector given a variable length sequence as input

Example:

Sentiment classification with word level **bidirectional** LSTM trained on a subset of the Internet Movie Database (IMDB) reviews. (20k positive and 20k negative examples)

Prediction examples for two inputs:

'this movie is so great' \Rightarrow 'positive'
'this movie is so bad' \Rightarrow 'negative'



see the code [here](#), and read more [here](#)

Recurrent neural networks (RNNs)

- Seq2Seq (sequence translation)
 - aligned: $T = T'$
 - unaligned: $T \neq T'$
- $$f_\theta : \mathbb{R}^{TD} \rightarrow \mathbb{R}^{T'C}$$

Recurrent neural networks (RNNs)

- Seq2Seq (sequence translation)
 - aligned: $T = T'$

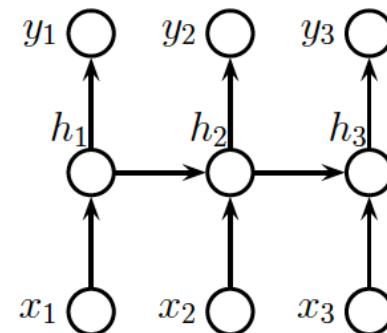
$$f_\theta : \mathbb{R}^{TD} \rightarrow \mathbb{R}^{TC}$$

modify the RNN as:

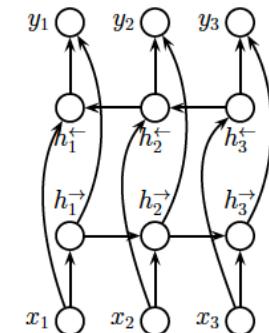
$$p(y_{1:T} | x_{1:T}) = \sum_{h_{1:T}} \prod_{t=1}^T p(y_t | h_t) \mathbb{I}(h_t = f(h_{t-1}, x_t))$$

initial state: $h_1 = f(h_0, x_1) = f_0(x_1)$

dense sequence labeling:
predict one label per location



Bi-directional



Recurrent neural networks (RNNs)

- Seq2Seq (sequence translation)
 - aligned: $T = T'$

$$f_\theta : \mathbb{R}^{TD} \rightarrow \mathbb{R}^{TC}$$

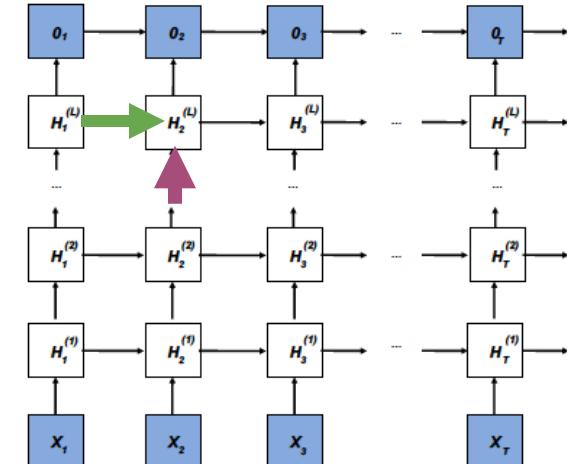
modify the RNN as:

$$p(y_{1:T} | x_{1:T}) = \sum_{h_{1:T}} \prod_{t=1}^T p(y_t | h_t) \mathbb{I}(h_t = f(h_{t-1}, x_t))$$

more depth to be more

$$h_t^l = \varphi_l \left(W_{xh}^l h_t^{l-1} + W_{hh}^l h_{t-1}^l \right)$$

$$y_t = W_{hy} h_t^L$$



Recurrent neural networks (RNNs)

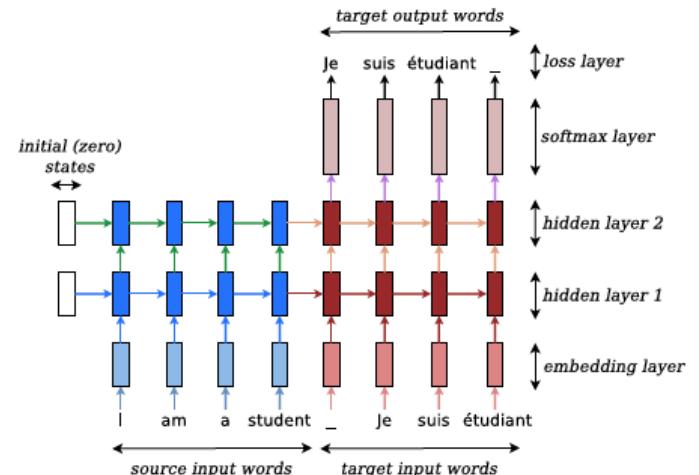
- Seq2Seq (sequence translation)
 - unaligned: $T \neq T'$

$$f_\theta : \mathbb{R}^{TD} \rightarrow \mathbb{R}^{T'C}$$

- **encode** the input sequence to get the context vector, the last state of an RNN, $c = f_e(x_{1:T})$
- generate the output sequence using an RNN **decoder**, $y_{1:T'} = f_d(c)$

see code [here](#)

Example: translating English to French



Training: Backpropagation through time (BPTT)

unroll the computation graph, then apply the backpropagation

Example:

model

$$h_t = W_{hx}x_t + W_{hh}h_{t-1}$$

$$\hat{y}_t = W_{hy}h_t$$

loss

$$L = \frac{1}{T} \sum_{t=1}^T \ell(y_t, \hat{y}_t)$$

derivatives

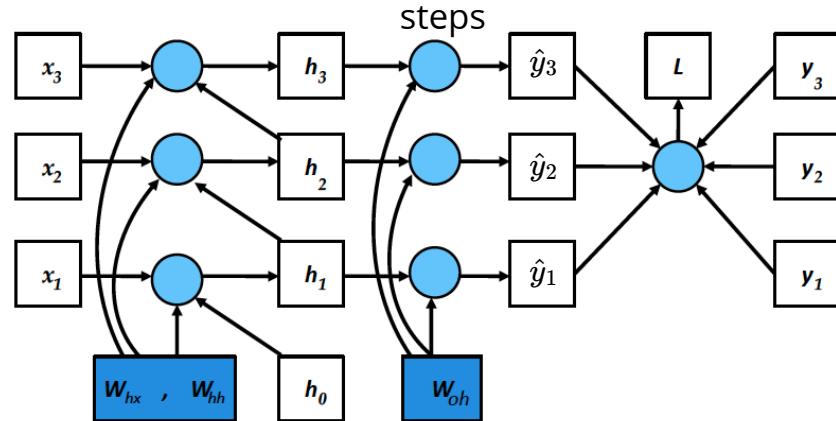
$$\frac{\partial L}{\partial W_{hx}}$$

$$\frac{\partial L}{\partial W_{hh}}$$

$$\frac{\partial L}{\partial W_{hy}}$$

Example:

An RNN unrolled (vertically) for 3 time steps



Training: Backpropagation through time (BPTT)

unroll the computation graph, then apply the backpropagation

Example:

model

$$h_t = W_{hx}x_t + W_{hh}h_{t-1} = f(x_t, h_{t-1}, w_h) \quad [\text{vec}(W_{hx}); \text{vec}(W_{hh})]$$

$$\hat{y}_t = W_{hy}h_t = g(h_t, w_y)$$

loss

$$L = \frac{1}{T} \sum_{t=1}^T \ell(y_t, \hat{y}_t) \quad \frac{\partial f(x_t, h_{t-1}, w_h)}{\partial w_h} + \frac{\partial f(x_t, h_{t-1}, w_h)}{\partial h_{t-1}} \frac{\partial h_{t-1}}{\partial w_h}$$

derivatives

$$\left. \begin{aligned} \frac{\partial L}{\partial W_{hx}} \\ \frac{\partial L}{\partial W_{hh}} \end{aligned} \right\} \frac{\partial L}{\partial w_h} = \frac{1}{T} \sum_{t=1}^T \frac{\partial \ell(y_t, \hat{y}_t)}{\partial w_h} = \frac{1}{T} \sum_{t=1}^T \frac{\partial \ell(y_t, \hat{y}_t)}{\partial \hat{y}_t} \frac{\partial g(h_t, w_y)}{\partial h_t} \frac{\partial h_t}{\partial w_h}$$

$\frac{\partial L}{\partial W_{hy}}$

expand this recursively

$$\frac{\partial h_t}{\partial w_h} = \frac{\partial f(x_t, h_{t-1}, w_h)}{\partial w_h} + \sum_{i=1}^{t-1} \left(\prod_{j=i+1}^t \frac{\partial f(x_j, h_{j-1}, w_h)}{\partial h_{j-1}} \right) \frac{\partial f(x_i, h_{i-1}, w_h)}{\partial w_h}$$

see code [here](#)

Gating and long term memory

Vanishing and exploding gradients

activations can decay or explode as we go forwards and backwards in time

RNN variations that circumvent this:

- Gated recurrent units (GRU)
 - learns when to update the hidden state, by using a gating unit
- Long short term memory (LSTM)
 - augments the hidden state with a memory cell

Limitations of RNNs

We saw that RNNs have some important limitations that result in suboptimal performance:

1. All the information about the past of a sequence is encoded in the hidden state
Result: Loss of context when processing long sequences
2. The sequence is processed one token at the time using the current token and past hidden-state
Result: Processing cannot be parallelized in time and is slow for long sequences

Attention

$$z = g(\mathbf{W} \mathbf{x})$$

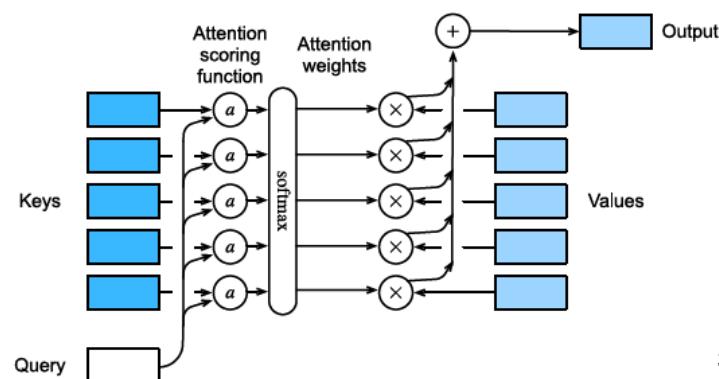
Instead of linear combination of the input activations, the model dynamically decides (in an input dependent way) which one to use based on how similar the input **query** vector $q \in \mathbb{R}^q$ is to a set of m **keys** $\mathbf{K} \in \mathbb{R}^{m \times k}$. If q is most similar to key i , then we use value v_i .

$$\text{Attn}(q, (k_1, v_1), \dots, (k_m, v_m)) = \text{Attn}(q, (k_{1:m}, v_{1:m})) = \sum_{i=1}^m \alpha_i(q, k_{1:m}) v_i \in \mathbb{R}^v$$

$$\alpha_i(q, k_{1:m}) = \text{softmax}_i([\mathbf{a}(q, k_1), \dots, \mathbf{a}(q, k_m)]) = \frac{\exp(\mathbf{a}(q, k_i))}{\sum_{j=1}^m \exp(\mathbf{a}(q, k_j))}$$

attention weight

The attention weights are computed from an attention score function $\mathbf{a}(q, k_i) \in \mathbb{R}$, which gives the similarity of query q to key k_i .



The Idea

The animal didn't cross the street because it was too tired .

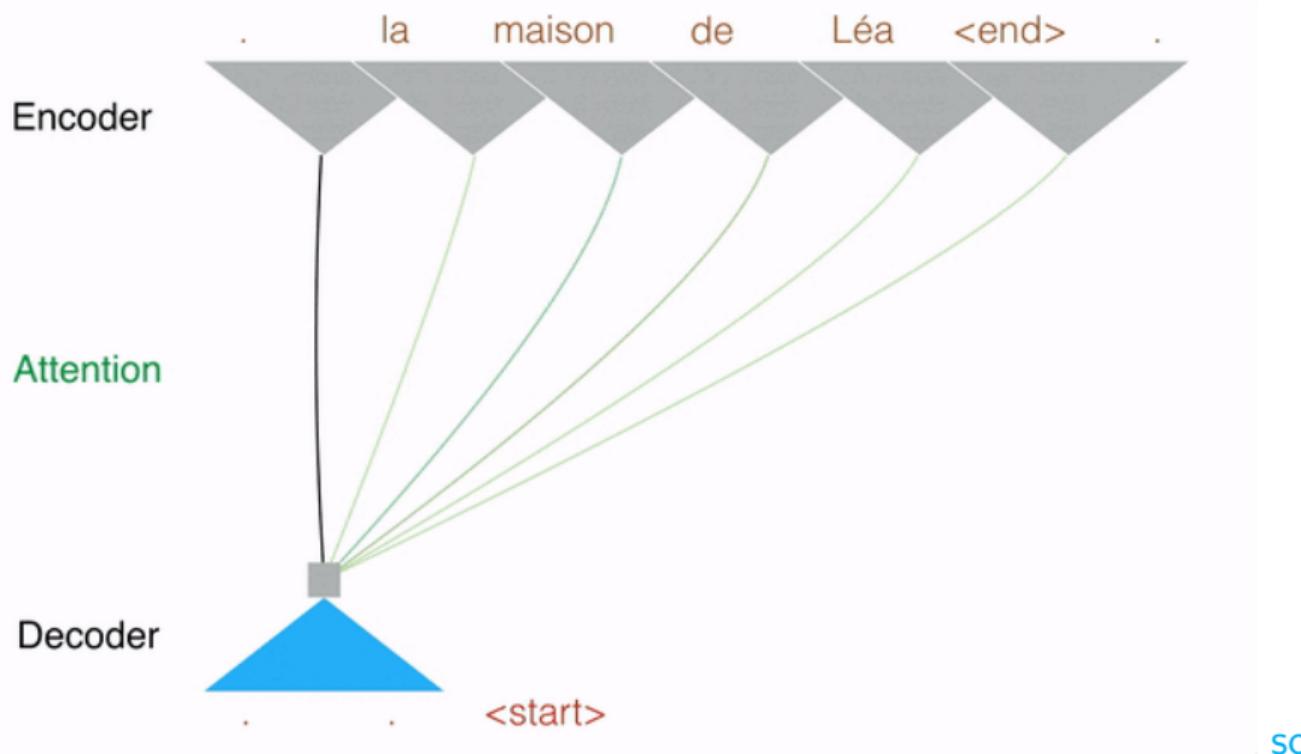
```
graph LR; A[The] --> B[animal]; B --> C[didn't]; C --> D[cross]; D --> E[the]; E --> F[street]; F --> G[because]; G --> H[it]; H -. "blue line" .-> I[was]; I --> J[too]; J --> K[tired]; K --> L[.]; H -. "light blue line" .-> M[cross]; M --> N[the]; N --> O[street]; O --> P[because]; P --> Q[it]; Q -. "blue line" .-> R[was]; R --> S[too]; S --> T[wide]; T --> U[.]
```

The animal didn't cross the street because it was too wide .

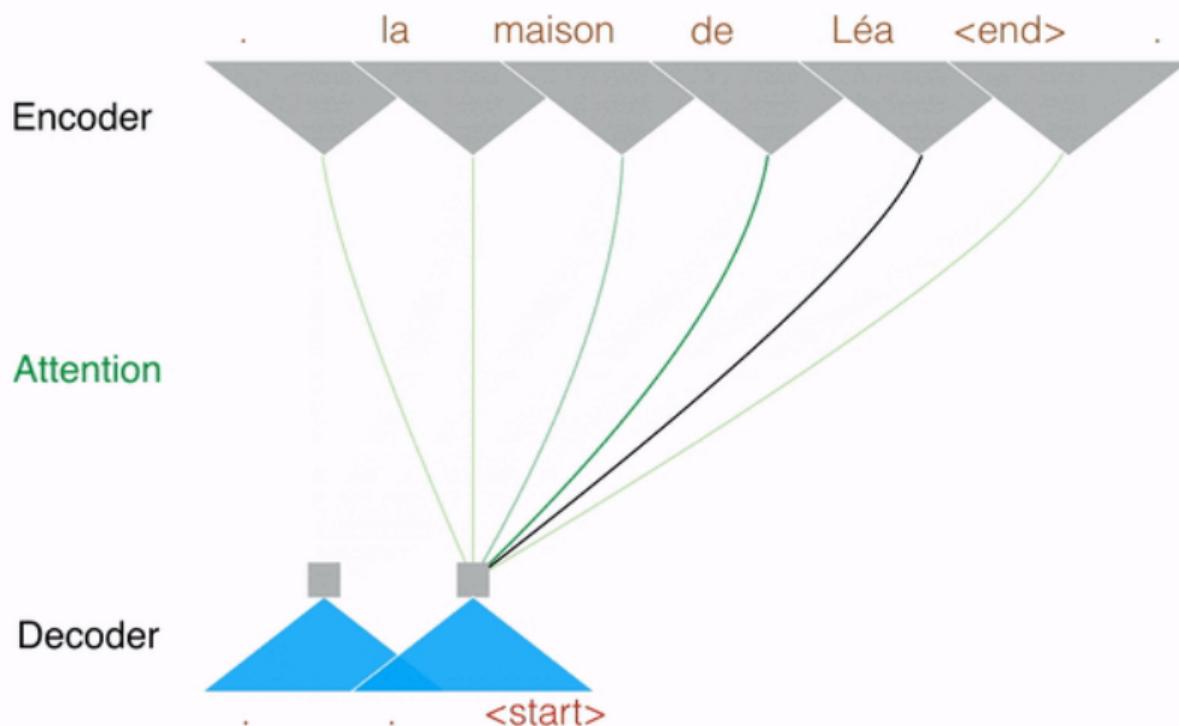
```
graph LR; A[The] --> B[animal]; B --> C[didn't]; C --> D[cross]; D --> E[the]; E --> F[street]; F --> G[because]; G --> H[it]; H -. "blue line" .-> I[was]; I --> J[too]; J --> K[wide]; K --> L[.]; H -. "light blue line" .-> M[cross]; M --> N[the]; N --> O[street]; O --> P[because]; P --> Q[it]; Q -. "blue line" .-> R[was]; R --> S[too]; S --> T[wide]; T --> U[.]
```

source

The Idea

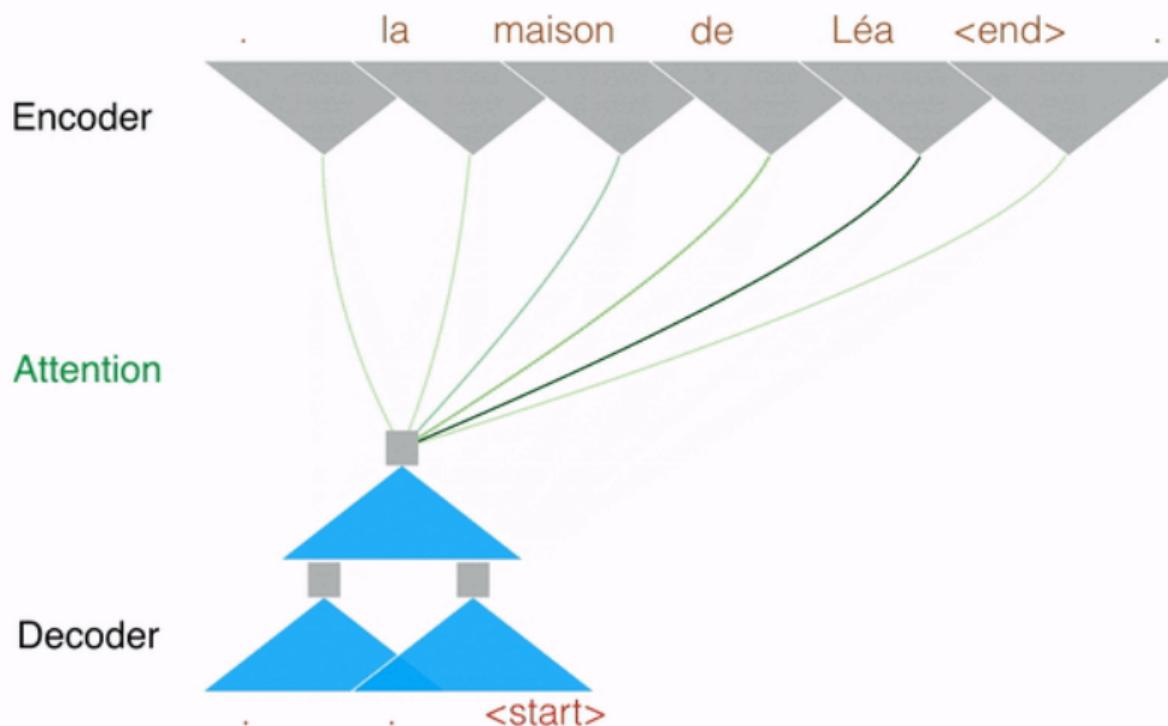


The Idea



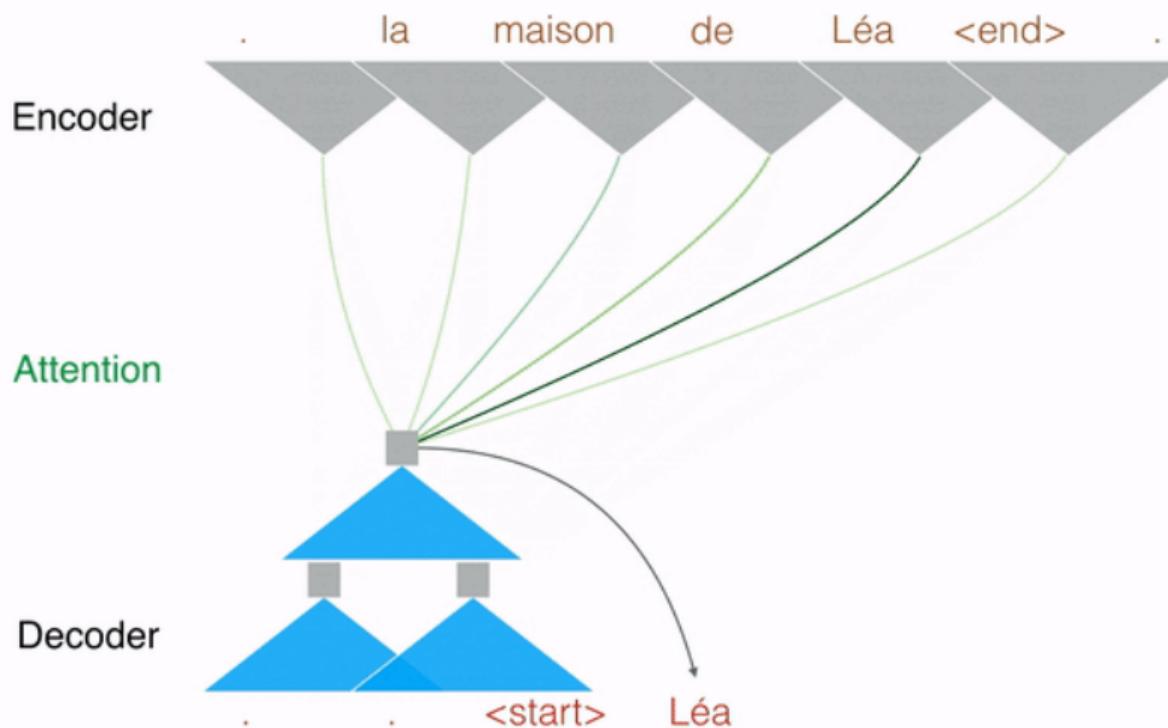
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The Idea



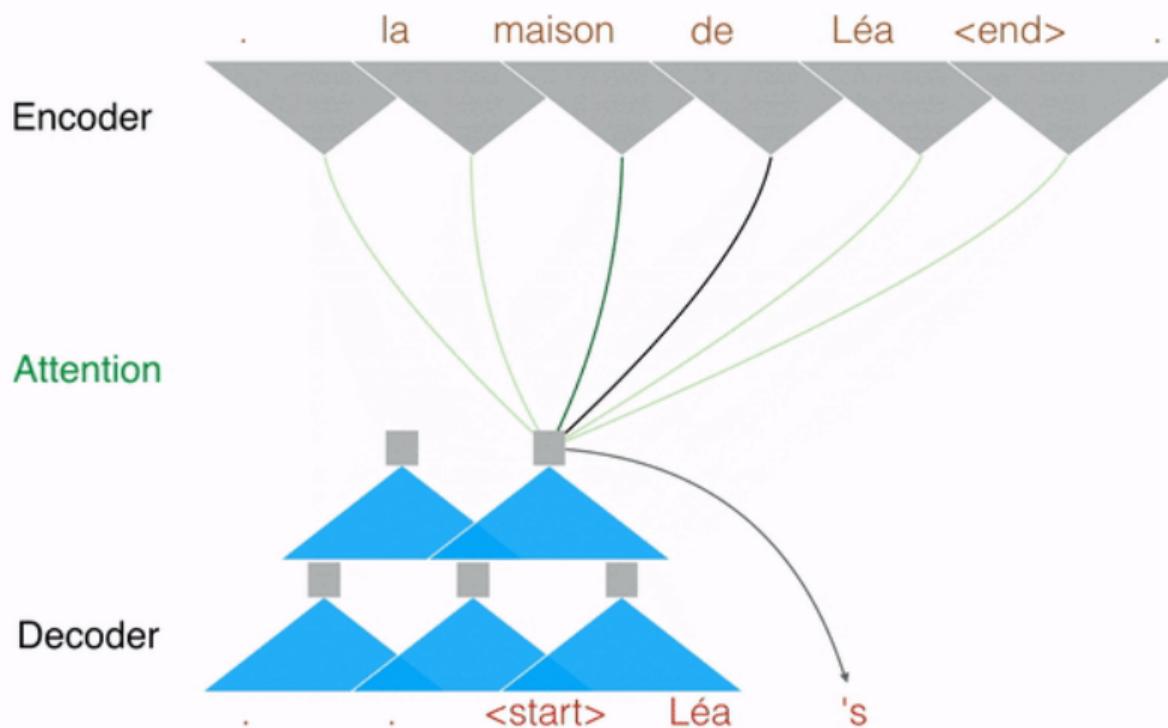
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The Idea



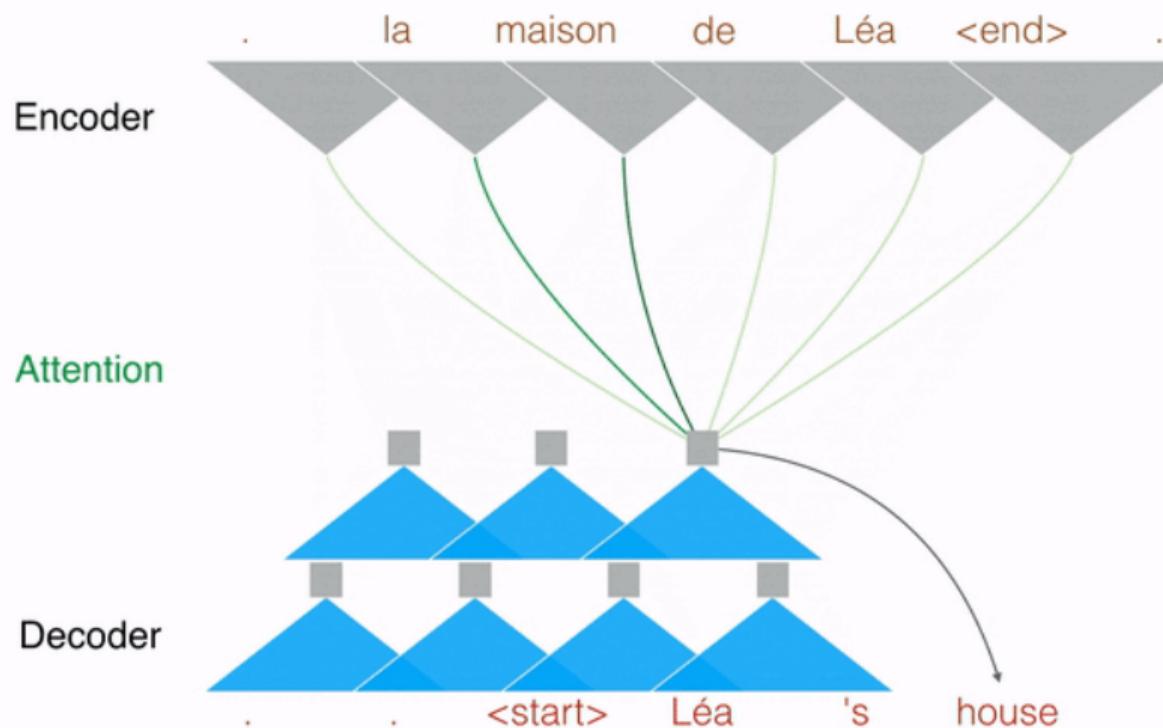
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The Idea



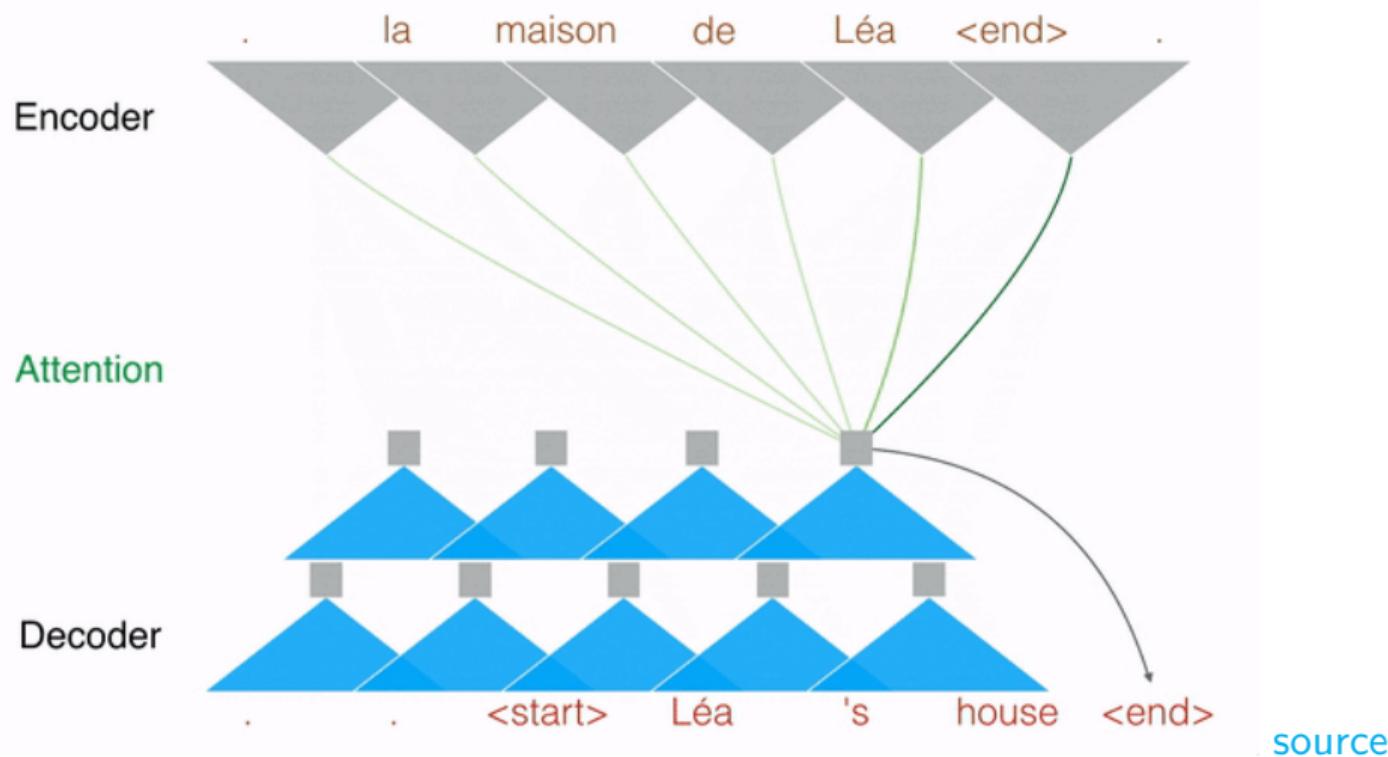
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The Idea

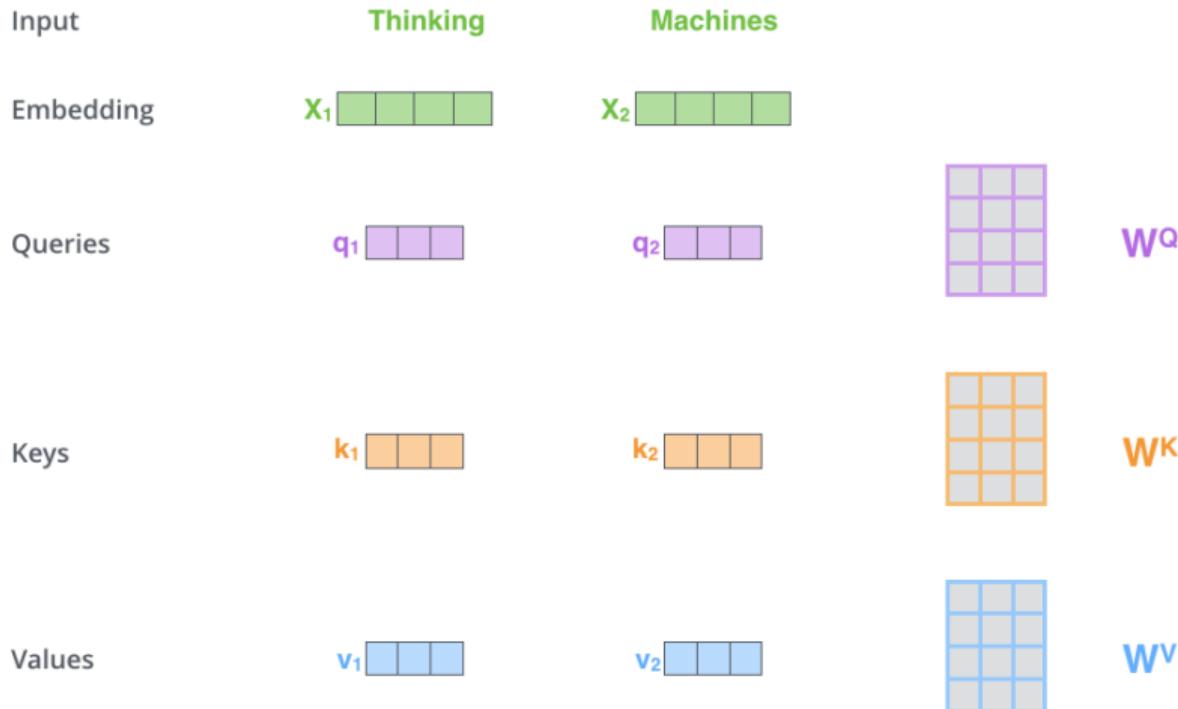


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The Idea

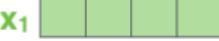


Attention Mechanism – High Level



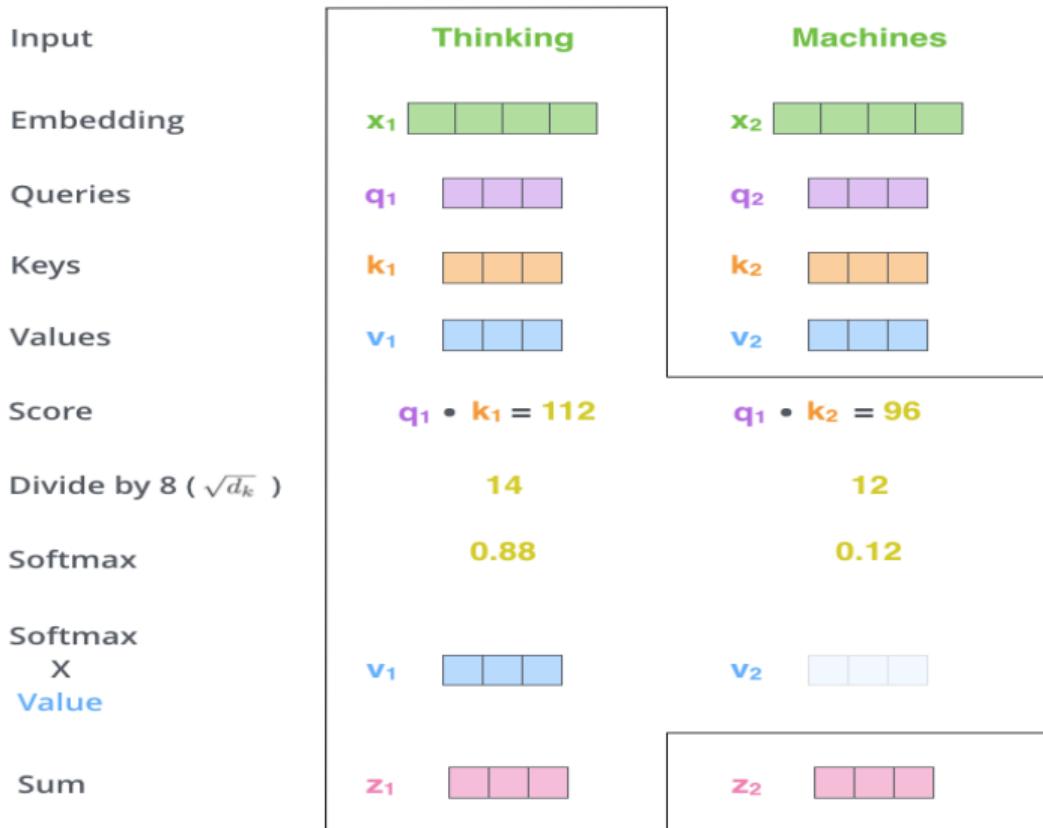
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Attention Mechanism – High Level

Input		
Embedding	x_1	
Queries	q_1	
Keys	k_1	
Values	v_1	
Score	$q_1 \cdot k_1 = 112$	$q_1 \cdot k_2 = 96$
Divide by 8 ($\sqrt{d_k}$)	14	12
Softmax	0.88	0.12

source

Attention Mechanism – High Level



Attention Mechanism – Math

Let $\{x_t \in \mathbb{R}^n | t \in \{1, \dots, T\}\}$ be a sequence of vectors being attended to, and $\{y_s \in \mathbb{R}^m | s \in \{1, \dots, S\}\}$ being a sequence of vectors doing the attending. Then we have that:

Attention Mechanism – Math

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Query vector: $q_s = \underbrace{W^Q}_{d \times m} \cdot y_s \in \mathbb{R}^d$.

Key vector: $k_t = \underbrace{W^K}_{d \times n} \cdot x_t \in \mathbb{R}^d$.

Value vector: $v_t = \underbrace{W^V}_{r \times n} \cdot x_t \in \mathbb{R}^r$.

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Value vector: $v_t = \underbrace{W^V}_{r \times n} \cdot x_t \in \mathbb{R}^r.$

The more q_s is aligned with k_t , the more the token at time s pays attention to the token at time t . The attention paid by the token at time s to the token at time t is

$$a_{st} = \frac{\exp(q_s \cdot k_t / \sqrt{d})}{\sum_{i=1}^T \exp(q_s \cdot k_i / \sqrt{d})}$$

Attention Mechanism – Math

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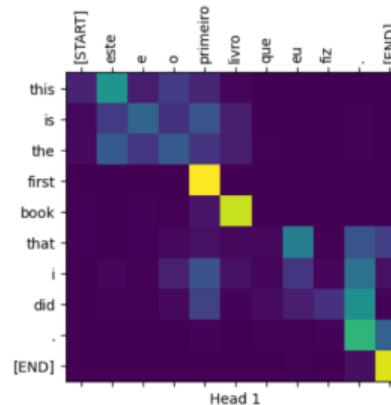
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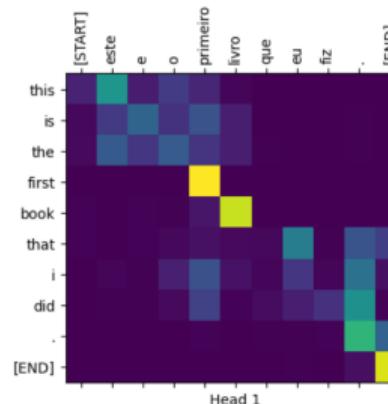
Key vector: $k_t = \underbrace{W^K}_{d \times n} \cdot x_t \in \mathbb{R}^d$.

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$$a_{st} = \frac{\exp(q_s \cdot k_t / \sqrt{d})}{\sum_{i=1}^T \exp(q_s \cdot k_i / \sqrt{d})}$$

$$z_s = \sum_{t=1}^T a_{st} v_t$$

The more q_s is aligned with k_t , the more the token at time s pays attention to the token at time t . The attention paid by the token at time s to the token at time t is



Attention Mechanism – Math

$$\underbrace{X}_{T \times n} = \begin{bmatrix} x_1 \\ \cdots \\ x_T \end{bmatrix}, \quad \underbrace{Y}_{S \times m} = \begin{bmatrix} y_1 \\ \cdots \\ y_S \end{bmatrix}, \quad \underbrace{Z}_{S \times r} = \begin{bmatrix} z_1 \\ \cdots \\ z_S \end{bmatrix},$$

Attention Mechanism – Math

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$$\underbrace{Q}_{S \times d} = Y \cdot W^{Q^\top} = \begin{bmatrix} q_1 \\ \cdots \\ q_S \end{bmatrix}, \quad \underbrace{K}_{T \times d} = X \cdot W^{K^\top} = \begin{bmatrix} k_1 \\ \cdots \\ k_T \end{bmatrix}, \quad \underbrace{V}_{T \times r} = X \cdot W^{V^\top} = \begin{bmatrix} v_1 \\ \cdots \\ v_T \end{bmatrix}$$

Attention Mechanism – Math

$$\underbrace{X}_{T \times n} = \begin{bmatrix} x_1 \\ \vdots \\ x_T \end{bmatrix}, \quad \underbrace{Y}_{S \times m} = \begin{bmatrix} y_1 \\ \vdots \\ y_S \end{bmatrix}, \quad \underbrace{Z}_{S \times r} = \begin{bmatrix} z_1 \\ \vdots \\ z_S \end{bmatrix},$$

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$$\underbrace{A}_{S \times T} = \text{softmax}_{\text{dim}=T}(Q \cdot K^\top / \sqrt{d}), \quad \underbrace{Z}_{S \times r} = A \cdot V$$

Attention Mechanism – Math

$$\underbrace{X}_{T \times n} = \begin{bmatrix} x_1 \\ \vdots \\ x_T \end{bmatrix}, \quad \underbrace{Y}_{S \times m} = \begin{bmatrix} y_1 \\ \vdots \\ y_S \end{bmatrix}, \quad \underbrace{Z}_{S \times r} = \begin{bmatrix} z_1 \\ \vdots \\ z_S \end{bmatrix},$$

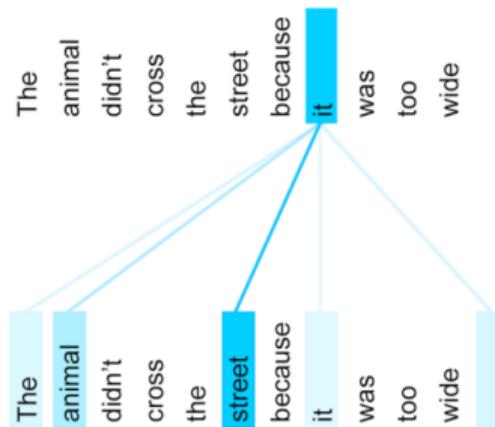
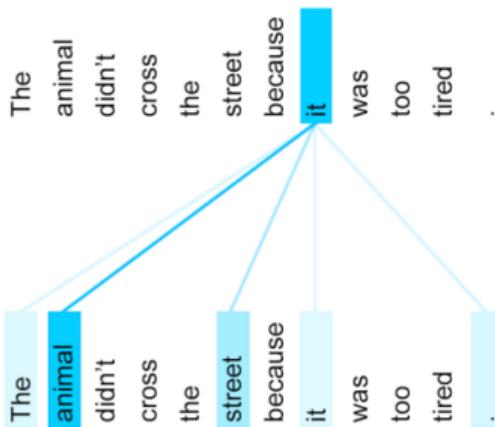
$$\underbrace{Q}_{S \times d} = Y \cdot W^{Q^\top} = \begin{bmatrix} q_1 \\ \vdots \\ q_S \end{bmatrix}, \quad \underbrace{K}_{T \times d} = X \cdot W^{K^\top} = \begin{bmatrix} k_1 \\ \vdots \\ k_T \end{bmatrix}, \quad \underbrace{V}_{T \times r} = X \cdot W^{V^\top} = \begin{bmatrix} v_1 \\ \vdots \\ v_T \end{bmatrix}$$

$$\underbrace{A}_{S \times T} = \text{softmax}_{\text{dim}=T}(Q \cdot K^\top / \sqrt{d}), \quad \underbrace{Z}_{S \times r} = A \cdot V$$

$$\begin{array}{c} \textcolor{violet}{Q} \\ \textcolor{orange}{K}^\top \\ \textcolor{blue}{V} \end{array} \quad \begin{array}{c} \textcolor{pink}{Z} \\ \text{softmax} \left(\frac{\textcolor{purple}{\begin{array}{|c|c|c|}\hline & & \\ \hline & & \\ \hline & & \\ \hline \end{array}} \times \textcolor{orange}{\begin{array}{|c|c|}\hline & \\ \hline & \\ \hline & \\ \hline \end{array}}}{\sqrt{d}} \right) \textcolor{blue}{\begin{array}{|c|c|c|}\hline & & \\ \hline & & \\ \hline & & \\ \hline \end{array}} \end{array}$$

Self-Attention

If the sequence $\{x_t \in \mathbb{R}^n | t \in \{1, \dots, T\}\}$ being attended to, is the same as the sequence $\{y_s \in \mathbb{R}^m | s \in \{1, \dots, S\}\}$ doing the attending, i.e. if $X = Y$, we call it **SELF-ATTENTION.**



Attention Mechanism – Example

$$x_t = \left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \right\}, \quad y = \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}.$$

$$W^K = \mathbb{I}, \quad , W^V = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \end{bmatrix}, \quad W^Q = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & -1 \end{bmatrix}.$$

$$z =$$

Attention Mechanism – Example

$$x_t = \left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \right\}, \quad y = \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}.$$

$$W^K = \mathbb{I}, \quad , \quad W^V = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \end{bmatrix}, \quad W^Q = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & -1 \end{bmatrix}.$$

$$k_t = \left\{ \mathbb{I} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad \mathbb{I} \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \quad \mathbb{I} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \right\} = \left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \right\}$$

Attention Mechanism – Example

$$x_t = \left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \right\}, \quad y = \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}.$$

$$k_t = \left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \right\}, \quad W^V = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \end{bmatrix}, \quad W^Q = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & -1 \end{bmatrix}.$$

$$v_t =$$

Attention Mechanism – Example

$$x_t = \left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \right\}, \quad y = \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}.$$

$$k_t = \left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \right\}, \quad W^V = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \end{bmatrix}, \quad W^Q = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & -1 \end{bmatrix}.$$

$$v_t = \left\{ W^V \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad W^V \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \quad W^V \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \right\}$$

Attention Mechanism – Example

$$x_t = \left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \right\}, \quad y = \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}.$$

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$$v_t = \left\{ \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad W^V \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \quad W^V \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \right\}$$

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Attention Mechanism – Example

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$$v_t = \left\{ \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \quad \begin{bmatrix} 1 \\ 0 \end{bmatrix} \right\}$$

Attention Mechanism – Example

$$x_t = \left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \right\}, \quad y = \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}.$$

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$$\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & -1 \end{bmatrix}.$$

$$q =$$

Attention Mechanism – Example

$$x_t = \left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \right\}, \quad y = \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}.$$

$$k_t = \left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \right\}, \quad v_t = \left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \right\}, \quad W^Q = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & -1 \end{bmatrix}.$$
$$q = W^Q y = \begin{bmatrix} -1 \\ 1 \\ 0 \\ 1 \end{bmatrix}$$

Attention Mechanism – Example

$$x_t = \left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \right\}, \quad y = \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}.$$

$$k_t = \left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \right\}, \quad v_t = \left\{ \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \quad \begin{bmatrix} 1 \\ 0 \end{bmatrix} \right\}, \quad q = \begin{bmatrix} -1 \\ 1 \\ 0 \\ 1 \end{bmatrix}.$$

$$q \cdot k_t =$$

Attention Mechanism – Example

$$x_t = \left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \right\}, \quad y = \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}.$$

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$$q \cdot k_t = [-1, 1, -1]$$

Attention Mechanism – Example

$$x_t = \left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \right\}, \quad y = \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}.$$

$$k_t = \left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \right\}, \quad v_t = \left\{ \begin{bmatrix} 1 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \right\}, \quad q = \begin{bmatrix} -1 \\ 1 \\ 0 \\ 1 \end{bmatrix}.$$

$$q \cdot k_t = [-1, 1, -1], \quad \text{softmax}(q \cdot k_t / \sqrt{d}) = \frac{[e^{-1/2}, e^{+1/2}, e^{-1/2}]}{e^{-1/2} + e^{+1/2} + e^{-1/2}}$$

Attention Mechanism – Example

$$x_t = \left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \right\}, \quad y = \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}.$$

$$k_t = \left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \right\}, \quad v_t = \left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \right\}, \quad q = \begin{bmatrix} -1 \\ 1 \\ 0 \\ 1 \end{bmatrix}.$$

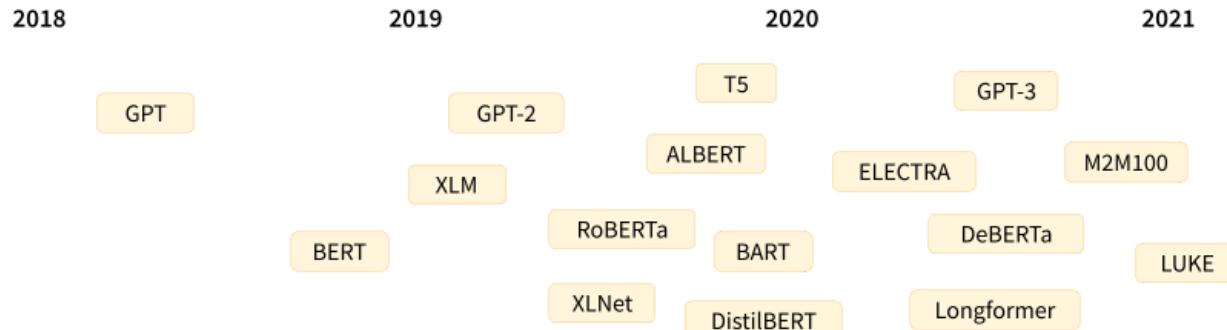
$$\text{softmax}(q \cdot k_t / \sqrt{d}) = \frac{[e^{-1/2}, e^{+1/2}, e^{-1/2}]}{e^{-1/2} + e^{+1/2} + e^{-1/2}}$$

$$z = \frac{e^{-1/2} \begin{bmatrix} 1 \\ 0 \end{bmatrix} + e^{+1/2} \begin{bmatrix} 0 \\ 1 \end{bmatrix} + e^{-1/2} \begin{bmatrix} 1 \\ 0 \end{bmatrix}}{e^{-1/2} + e^{+1/2} + e^{-1/2}} = \begin{bmatrix} 2e^{-1/2} \\ e^{+1/2} \end{bmatrix} / (2e^{-1/2} + e^{+1/2})$$

Transformers

a seq2seq model which uses attention in the encoder as well as the decoder, thus eliminating the need for RNNs

- Self-attention
- Multi-headed attention
- Positional encoding



read more [here](#)

Transformers: self-attention

given a sequence of input tokens x_1, \dots, x_n , generate a sequence of outputs of the same size with:

$$y_i = \text{Attn}(x_i, (x_1, x_1), \dots, (x_n, x_n))$$

query $\in \mathbb{R}^d$ (key, value)s

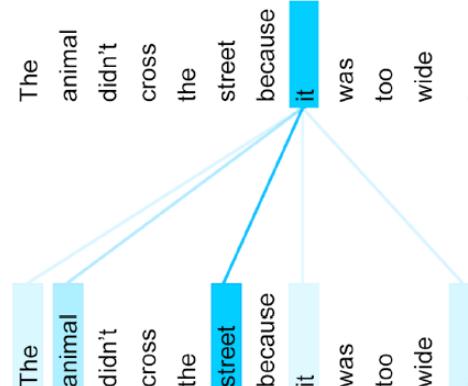
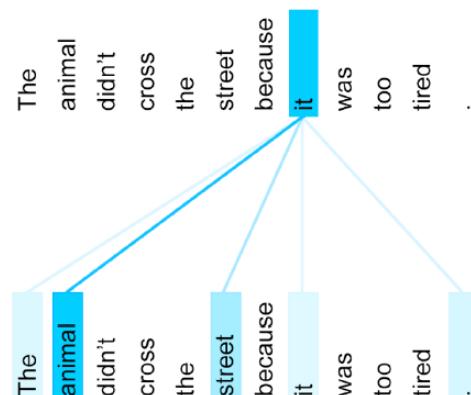
for decoder we set $x_i = y_{i-1}$ and $n = i - 1$

this gives improved representations of context

Example:

coreference resolution:

encoder self-attention for the word "it" differs depending on the input context which is important in translation, e.g. what pronoun to use in French



Transformers: positional encoding

attention is permutation invariant, and hence ignores the input word ordering. To overcome this, we can concatenate the word embeddings with a positional embedding so that the model knows what **order the words** occur in

$$p_{i,2j} = \sin\left(\frac{i}{10000^{2j/d}}\right)$$

$$p_{i,2j+1} = \cos\left(\frac{i}{10000^{2j/d}}\right)$$

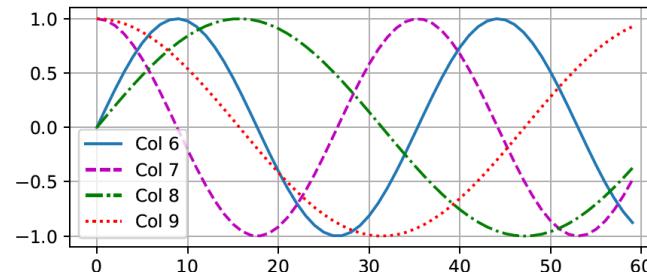
$$\text{POS}(\text{Embed}(X)) = X + P$$

$\in \mathbb{R}^{n \times d}$
 $\in \mathbb{R}^{n \times d}$

```
0 in binary is 000
1 in binary is 001
2 in binary is 010
3 in binary is 011
4 in binary is 100
5 in binary is 101
6 in binary is 110
7 in binary is 111
```

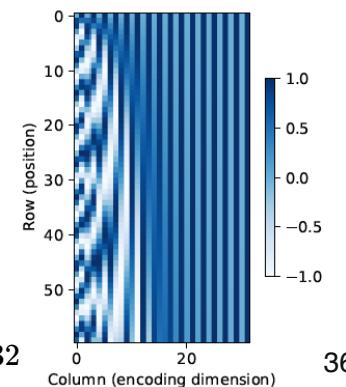
lower columns have higher frequencies

read more [here](#)



Example:

$n = 60, d = 32$



Transformers: putting it all together

Attention Is All You Need

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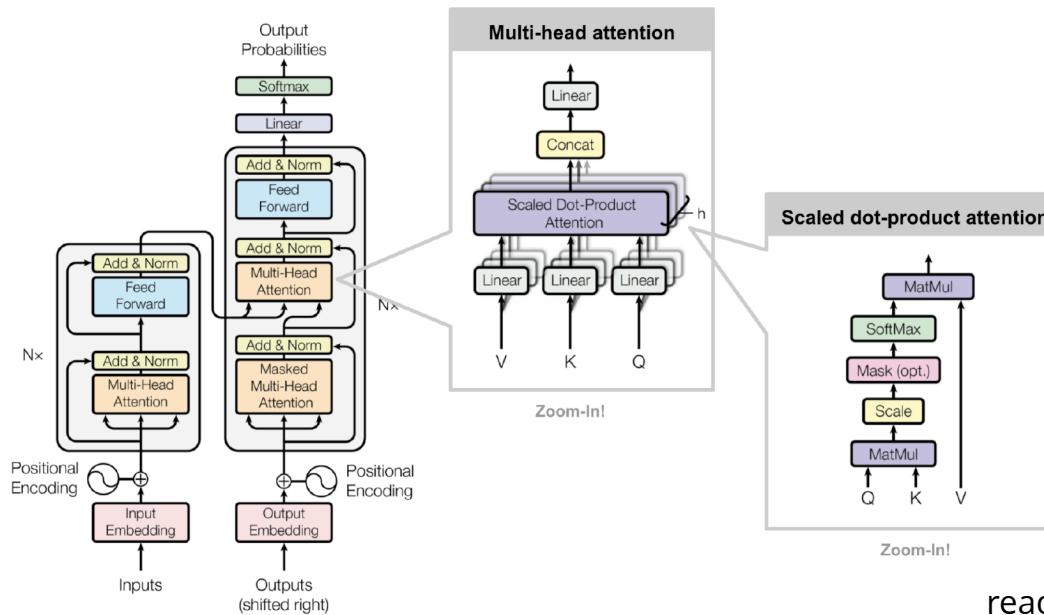
Abstract

The dominant sequence transduction models are based on complex recurrent or convolutional neural networks that include an encoder and a decoder. The best performing models also connect the encoder and decoder through an attention mechanism. We propose a new simple network architecture, the Transformer, based solely on attention mechanisms, dispensing with recurrence and convolutions entirely. Experiments on two machine translation tasks show these models to be superior in quality while being more parallelizable and requiring significantly less time to train. Our model achieves 28.4 BLEU on the WMT 2014 English-to-German translation task, improving over the existing best results, including ensembles, by over 2 BLEU. On the WMT 2014 English-to-French translation task,

read more [here](#), see the code [here](#)

Transformers: putting it all together

A transformer is a seq2seq model that uses self-attention for the encoder and decoder rather than an RNN. The encoder uses a series of encoder blocks, each of which uses multi-headed attention, residual connections, and layer normalization



read more [here](#), see the code [here](#)

Language models

- **ELMo** (Embeddings from Language Model)
 - RNN based, trained unsupervised to minimize the negative log likelihood of the input sentence,
i.e. $y_t = x_{t-1}$
- **BERT** (Bidirectional Encoder Representations from Transformers)
 - Transformer-based: map a modified version of a sequence back to the unmodified form and
compute the loss at the masked locations: **fill-in-the-blank** :

Let's make [MASK] chicken! [SEP] It [MASK] great with orange sauce

- **GPT** (Generative Pre-training Transformer)
 - uses a masked transformer as the decoder, see an open-source model [here](#) (20 billion parameters)

Generative Pre-trained Transformer (GPT)

Model	Architecture	Parameters	Training data	Release date	Training cost
GPT-1	12-level, 12-headed Transformer decoder (no encoder).	117 million	BookCorpus: 4.5 GB of text, from 7000 unpublished books.	June 11, 2018	30 days on 8 P600 GPUs, or 1 petaFLOP/s-day.
GPT-2	GPT-1, but with modified normalization	1.5 billion	WebText: 40 GB of text, 8 million documents, from 45 million webpages upvoted on Reddit.	February 14, 2019 (initial/limited version) and November 5, 2019 (full version)	"tens of petaflop/s-day", or 1.5e21 FLOP.
GPT-3	GPT-2, but with modification to allow larger scaling	175 billion	499 billion tokens of CommonCrawl (570 GB), WebText, English Wikipedia, book corpora (Books1 and Books2).	May 28, 2020	3640 petaflop/s-day.
GPT-3.5	Undisclosed	175 billion	Undisclosed	March 15, 2022	Undisclosed
GPT-4	Trained with both text prediction and RLHF.	Estimated 1.7 trillion.	Undisclosed	March 14, 2023	Undisclosed. Estimated 2.1×10^{12} FLOP.

Summary

- Recurrent neural networks (RNNs)
 - Vec2Seq (sequence generation)
 - Seq2Vec (sequence classification)
 - Seq2Seq (sequence translation)
 - training with back propagation through time
- attention mechanisms, self-attention and multi-headed attention
- The architecture of transformer
- language models with transformer