Lecture 15:

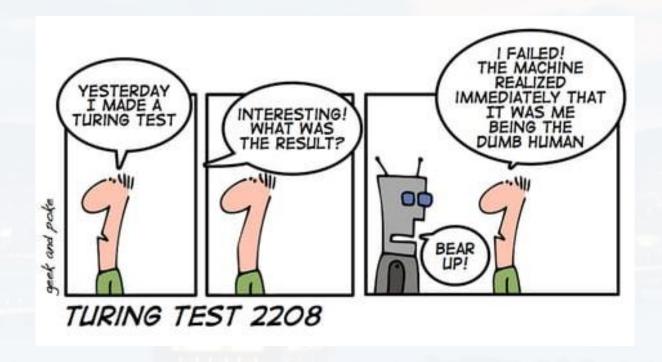
Language Models and Transformer



Markus Hohle
University California, Berkeley

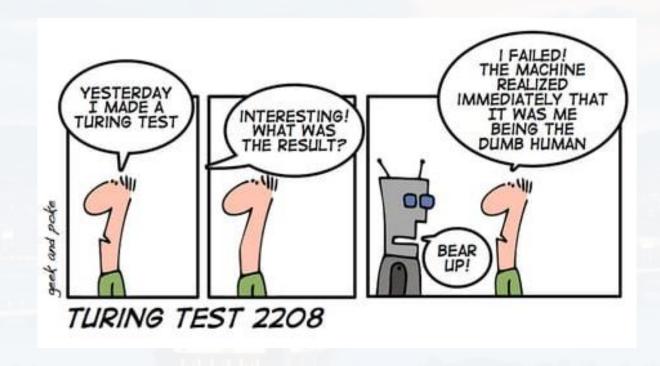
Machine Learning Algorithms
MSSE 277B, 3 Units
Fall 2024

Outline



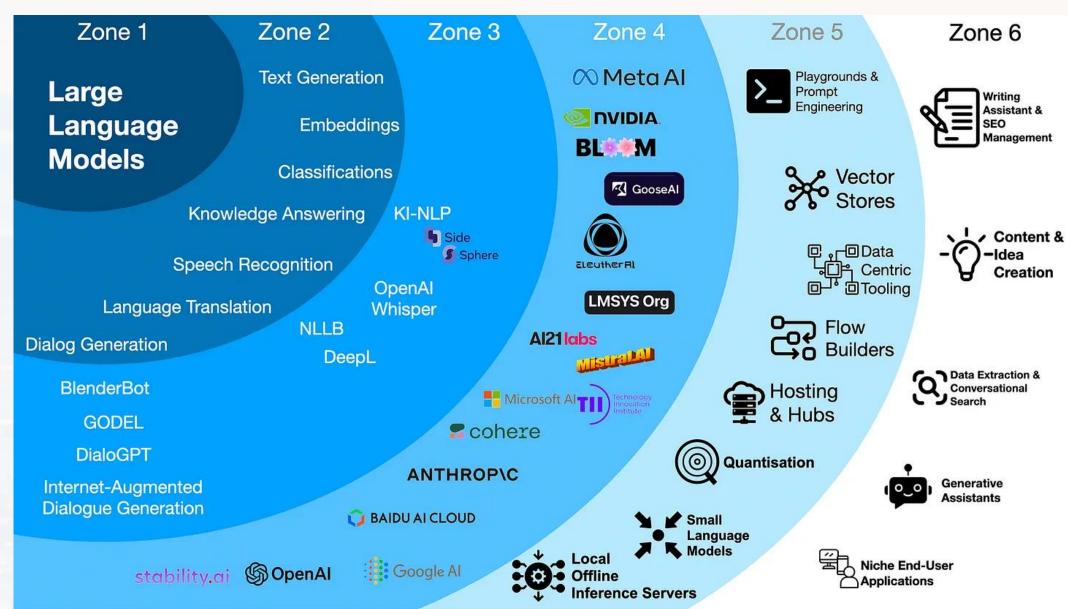
- Introduction
- Bigram and MAP
- Positional Encoding
- Word Embedding
- Attention
- Transformer Architecture

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corpus: (large, representative) data set containing sequences of a language

token: individual, independent entity of a language

alphabet/vocabulary: set of tokens

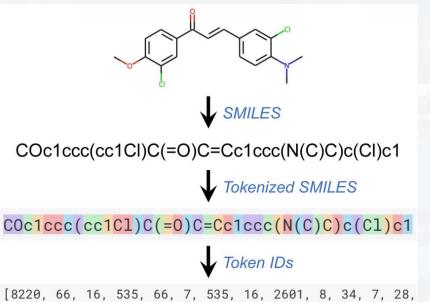
token	size of <i>alphabet</i>
- letters in a word	- 10 ²
- words in a sentence	$-10^4 \dots 10^6$
(upper/lower case, cases, gender, tenses, conjugations)	
- amino a <mark>cids in a protein sequence</mark>	- 21
- nucleotides in a DNA/RNA sequence	- 4
- motifs in a DNA/RNA sequence	- 10 ⁴

corpus: (large, representative) data set containing sequences of a language

token: individual, independent entity of a language

alphabet/vocabulary: set of tokens

tokenization



token: - single atom vs...

- ...functional group

34, 8, 66, 7, 2601, 8, 66, 16]

46, 8, 34, 28, 34, 66, 16, 535, 66, 7, 45, 7, 34, 8,

DOI:10.1039/D3SC04610A

corpus: (large, representative) data set containing sequences of a language

token: individual, independent entity of a language

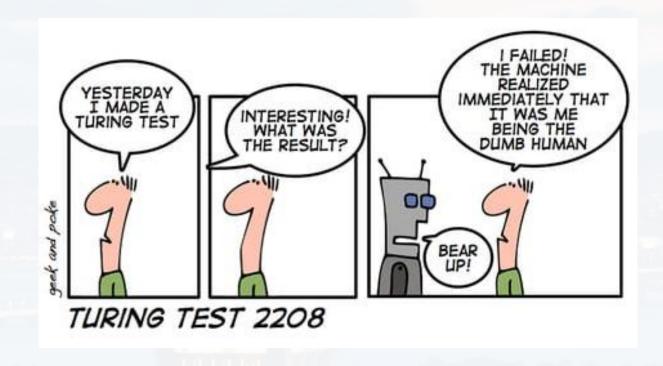
alphabet/vocabulary: set of tokens

note: language models don't know grammar as we do, but they don't need to anyway...

three things make context (details: see later):

- word embedding (relation between similar/different token)
- positional encoding (location of token in a sequence)
- **attention** (relation between token within a sequence)

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$$X_1 X_2 X_3 X_4 X_5 \dots X_n$$

sequence of *n* **token** *X*

actually:

$$P(X_1 X_2 X_3 X_4 X_5 \dots X_n) = P(X_n | X_{n-1} \dots X_1) P(X_{n-1} | X_{n-2} \dots X_1) \dots P(X_1)$$

bigram (1st order Markov Chain, see e.g. first WhatsApp versions):

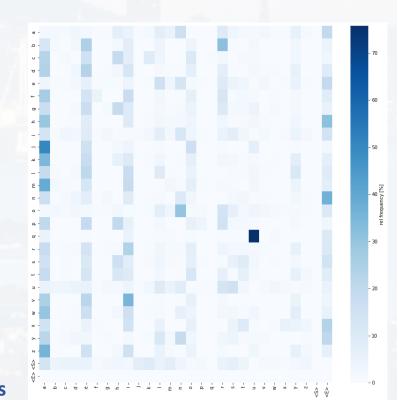
$$P(X_1 X_2 X_3 X_4 X_5 \dots X_n) = P(X_n | X_{n-1}) P(X_{n-1} | X_{n-2}) \dots P(X_1)$$



P(i/j): that token **i** is generated after token **j**

→ N x N transition matrix from frequencies

→ "bigram" = "two words"



bigram (1st order Markov Chain):

let's build our own bigram model: generate new names based on a corpus of names

```
In [15]: words[0:12]
Out[15]:
['emma',
  'olivia',
  'ava',
  'isabella',
  'sophia',
  'charlotte',
  'mia',
  'amelia',
  'harper',
  'evelyn',
  'abigail',
  'emily']
```

see Andrej Karpathy's GitHub repository

$$P(X_1 X_2 X_3 X_4 X_5 \dots X_n) = P(X_n | X_{n-1}) P(X_{n-1} | X_{n-2}) \dots P(X_1)$$

we only need to count how often a letter is followed by another

we also need to indicate when a name has started and ended

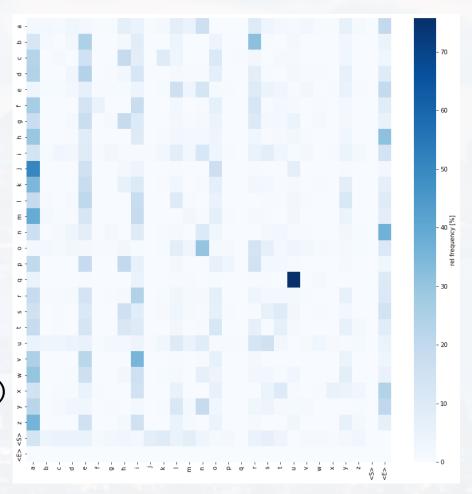
→ alphabet: 26 letters + the two special "letters"

let's create a dictionary first (will help for counting):

bigram (1st order Markov Chain):

let's build our own bigram model: generate new names based on a corpus of names

- 1) dictionary first (will help for counting)
- 2) count how often letter *i* is followed by letter *j*
 - → bigram matrix **N**
- 3) normalize **N** accordingly
- 4) begin with a start token
- 5) draw a letter randomly based on **N**, using
 - np.argmax(np.random.multinomial(1,p))
- 6) if next token is stop token \rightarrow stop



bigram (1st order Markov Chain):

let's build our own bigram model: **generate new names** based on a corpus of names check out **Bigram.ipynb**

B.SampleNames(15) vs totally random **B.SampleNames(15, False)**

some names are gibberish

some names sound real

some names are real

```
In [295]: B.SampleNames(15)
keesa
ann
ja
jon
nma
malynojana
sall
daha
dryah
lzaxi
tyunusthun
jorrwro
ja
asoow
```

```
In [296]: B.SampleNames(15,False)

mtkgy
yufexhviovmorhqvikbbbjxebpxwurejaqlzzuwuanxmmomhr<S>uhb
xlmusadjfdzxadaotd
ik<S>vdtydvxevtaselkykcfbamceprtvl
zyr<S>inzoerobzwuovx
eg<S>pbdvikf<S>tomcnkfsjay<S>rikatnaykizszcivpds<S>zj
kh<S>y<S>ualzugqgakakeubjbasc
bblupnibtqmyl<S>vyobf
kybs
rznjgpmlo
tnhoxuckkjjzbwmj<S>vshkycicf<S>kowskphy
rxodh
jvswmzw
jzpcfnpcg
```

Note, there is no conceptual difference between applying our model to *letters in a word* vs *words in a sentence*

caveats:

- the bigram model derives $P(X_n)$ from **observed** frequencies \rightarrow essentially **MLE** (problematic if a letter hasn't appeared in the sequence yet $\rightarrow P(X_n)$ assumed to be zero!)

Nsam =
$$N/np.sum(N+0.0001)$$
, axis = 1, keepdims = True)
S_bi += $np.sum(-N[:,i]*np.log(N[:,i]+1e-16))$

- can we implement something that is closer to:

$$P(X_1 X_2 X_3 X_4 X_5 \dots X_n) = P(X_n | X_{n-1} \dots X_1) P(X_{n-1} | X_{n-2} \dots X_1) \dots P(X_1) ?$$

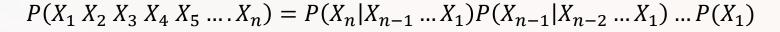
binomial process

$$q-1$$
 q \downarrow

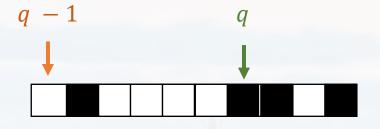
$$P(k|n,q) = \binom{n}{k} q^k (1-q)^{n-k}$$

$$q = ?$$





Bayesian
Parameter
Estimation*)



$$P(k|n,q) = \binom{n}{k} q^k (1-q)^{n-k} \qquad q = ?$$

likelihood function (here: binomial)

$$P(q|data|set) = \frac{P(data|set|q)P(q)|prior(\sim P(X_n|X_{n-1}...X_1))}{P(data|set)|evidence|(const|wrt|q)}$$

$$= \frac{1}{\int_0^1 P(q|data \ set)dq} (1-q)^{n-k} q^k$$

$$q = const$$

before 1st data point
(max entropy!)

$$= \frac{q^{k+\alpha-1}(1-q)^{n-k+\beta-1}}{\int_0^1 q^{k+\alpha-1}(1-q)^{n-k+\beta-1} dq}$$

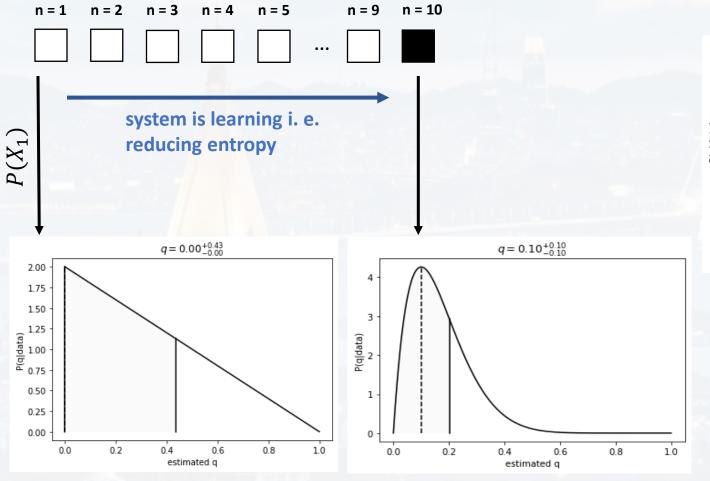
q =conjugate prior after n^{th} data point

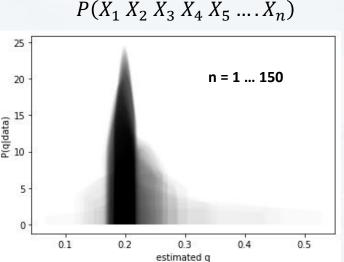


$$P(X_1 X_2 X_3 X_4 X_5 \dots X_n) = P(X_n | X_{n-1} \dots X_1) P(X_{n-1} | X_{n-2} \dots X_1) \dots P(X_1)$$

$$P(k|n,q) = \binom{n}{k} q^k (1-q)^{n-k}$$
 $q = ?$

Bayesian
Parameter
Estimation*)







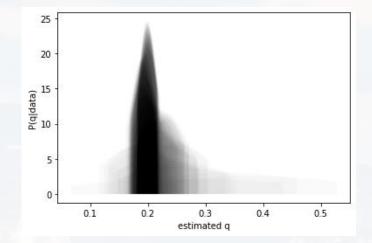
$$P(X_1 X_2 X_3 X_4 X_5 \dots X_n) = P(X_n | X_{n-1} \dots X_1) P(X_{n-1} | X_{n-2} \dots X_1) \dots P(X_1)$$

$$P(k|n,q) = \binom{n}{k} q^k (1-q)^{n-k}$$

BayesianParameterEstimation*)

$$P(q|data set) = \frac{q^{k+\alpha-1}(1-q)^{n-k+\beta-1}}{\int_0^1 q^{k+\alpha-1}(1-q)^{n-k+\beta-1} dq}$$

Beta function



more general, we want to learn the probability $P_j(a)$ of letter a at position j $q \rightarrow P_j(a)$

- → multinomial problem
- → conjugate prior is the **Dirichlet distribution**

$$P(sequence) \sim \prod_{j} \prod_{a} P(a)_{j}^{\alpha(a)-1}$$

equivalent to what was P(q|data|set) earlier

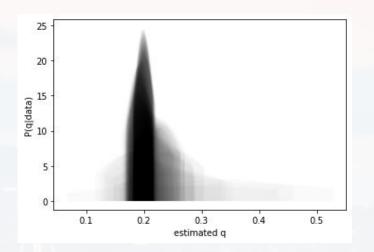
$$P(X_1 X_2 X_3 X_4 X_5 \dots X_n) = P(X_n | X_{n-1} \dots X_1) P(X_{n-1} | X_{n-2} \dots X_1) \dots P(X_1)$$

Dirichlet distribution

$$P(sequence) \sim \prod_{j} \prod_{a} P(a)_{j}^{\alpha(a)-1}$$

note: $\sum_{i=1}^{n} P(a)_{j} = 1$

 \rightarrow N – dim simplex



note:

- we don't need to extract P(a) from the maximum of the pdf given by the BPE posterior
- we can directly derive the maximum of P(a) from P(sequence) given the constrain $\sum_{over\ all\ a} P(a)_j = 1$ (Lagrangian multipliers)
- Maximum a-posteriori (MAP) approach → see XXmotif (Siebert & Soeding, 2016)



$$P(X_1 X_2 X_3 X_4 X_5 \dots X_n) = P(X_n | X_{n-1} \dots X_1) P(X_{n-1} | X_{n-2} \dots X_1) \dots P(X_1)$$

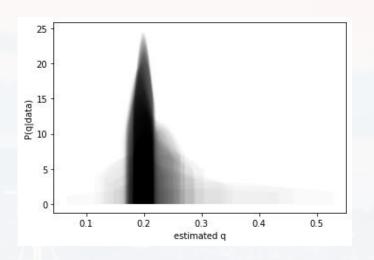
Dirichlet distribution

$$P(sequence) \sim \prod_{j} \prod_{a} P(a)_{j}^{\alpha(a)-1}$$

note:

$$\sum_{i} P(a)_j = 1$$

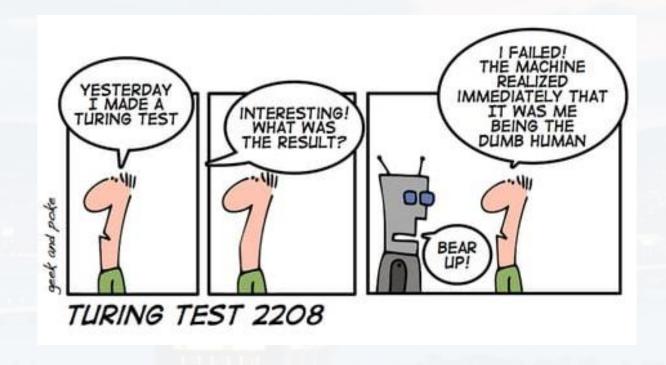
 \rightarrow N – dim simplex



Maximum a-posteriori (MAP)

- XXmotif (Siebert & Soeding, 2016) significantly outperformed PWMs
- it struggled however with related motifs which where physically located far apart from each other
- → solution see later: attention
- → older solutions: LSTMs

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three things make context:

- **positional encoding** (location of token in a sequence)
- word embedding (relation between similar/different token)
- **attention** (relation between token within a sequence)

"The cat jumped on the roof."

order matters!:

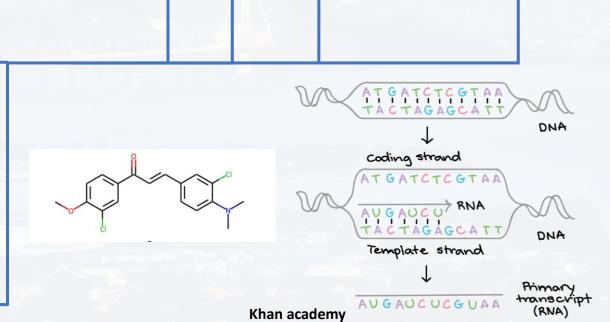
1st: article

2nd: noun/subject

3rd: verb

4th: noun/object (in English)

→ positional encoding



goal: find a positional encoding that is

- reasonably simple
- independent from the length of the sequence
- somehow normalized

one idea: n-bit binary encoding position code ← 8bit i.e. eight dimensions depending on dimensions (bit) → different frequencies bit frequency 1/2 1/4 Does that look familiar? 1/8 → *like* Fourier Series

even dimensions:
$$E(p, 2k) = \sin\left(\frac{p}{10,000^{\frac{2k}{d}}}\right)$$

odd dimensions:
$$E(p, 2k + 1) = \cos\left(\frac{p}{10,000^{2k/d}}\right)$$

p: position in sequence

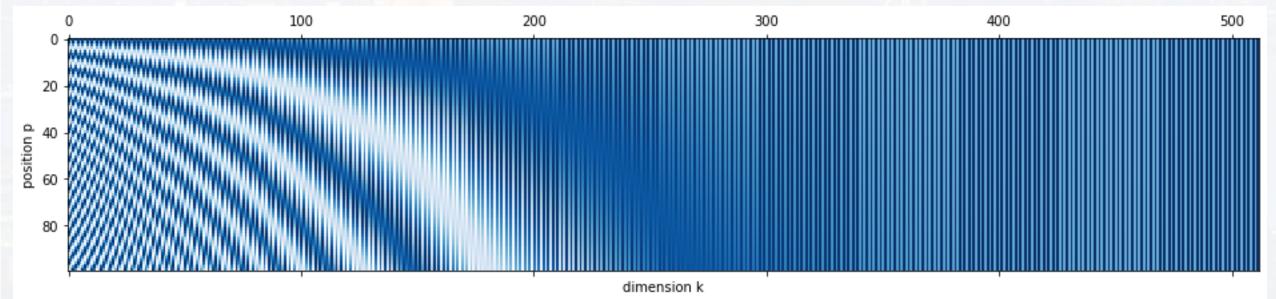
k: dimension index

d: number of dimensions

10,000: an arbitrary number

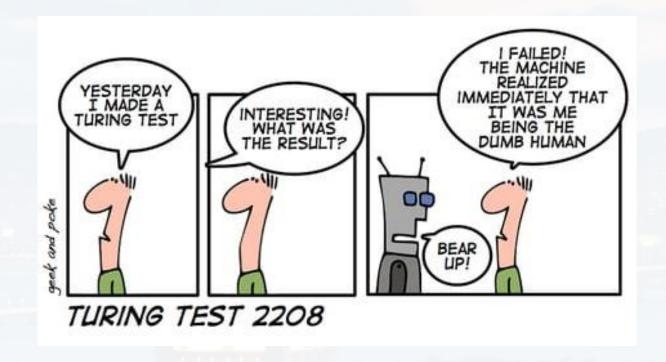
run PlotPositionEncoding.py

more info here



Vaswani et al., 2017

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three things make context:

- positional encoding (location of token in a sequence)
- word embedding (relation between similar/different token)
- attention (relation between token within a sequence)

problem: turning token (words/letters) into numbers

single letters:

ACGT

one – hot works perfectly (four different token)

abcd...

- lower/upper case, special characters (50 different token), one – hot is fine too

words:

actual words

 $-10^4 \dots 10^6$ (upper/lower case, cases, gender, tenses, conjugations)

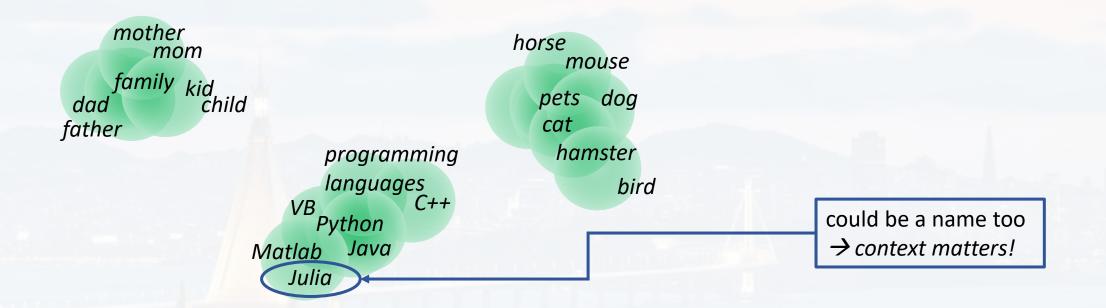
→ one – hot doesn't work (matrices would be too large)

→ some words have a **similar meaning**, should be **close** in parameter space

(cluster)



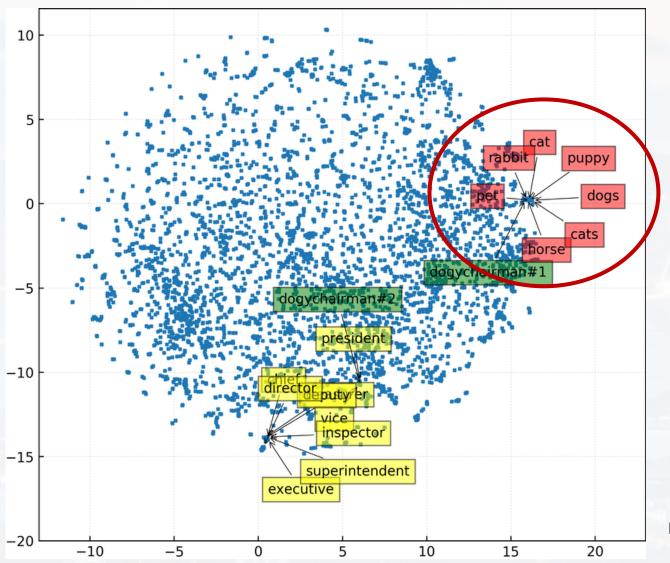
words with a **similar meaning** should form **cluster**



- embedding, instead of one hot encoding
- from experience: N = 30 300 dim vector for each token (which is a lot less than 10^4 ... 10^6) is sufficient
- as a result: token with **similar meaning are close** in the vector space!



words with a **similar meaning** should form **cluster**



"Joint Learning of Sense and Word Embeddings"

M Alsuhaibani & D Bollegala



common training set: recorded speeches from the European Parliament:

...It seems absolutely disgraceful that we pass legislation and do not adhere to it ourselves. Mrs Lynne, you are quite right and I shall check whether this has actually not been done. I shall also refer the matter to the College of Quaestors, and I am certain that they will be keen to ensure that we comply with the regulations we ourselves vote on.

Madam President, Mrs Díez González and I had tabled questions on certain opinions of the Vice-President, Mrs de Palacio, which appeared in a Spanish newspaper.

The competent services have not included them in the agenda on the grounds that they had been answered in a pievious part-session.

I would ask that they reconsider, since this is not the case....

words of similar meaning should appear in similar environment

→ target token within a window

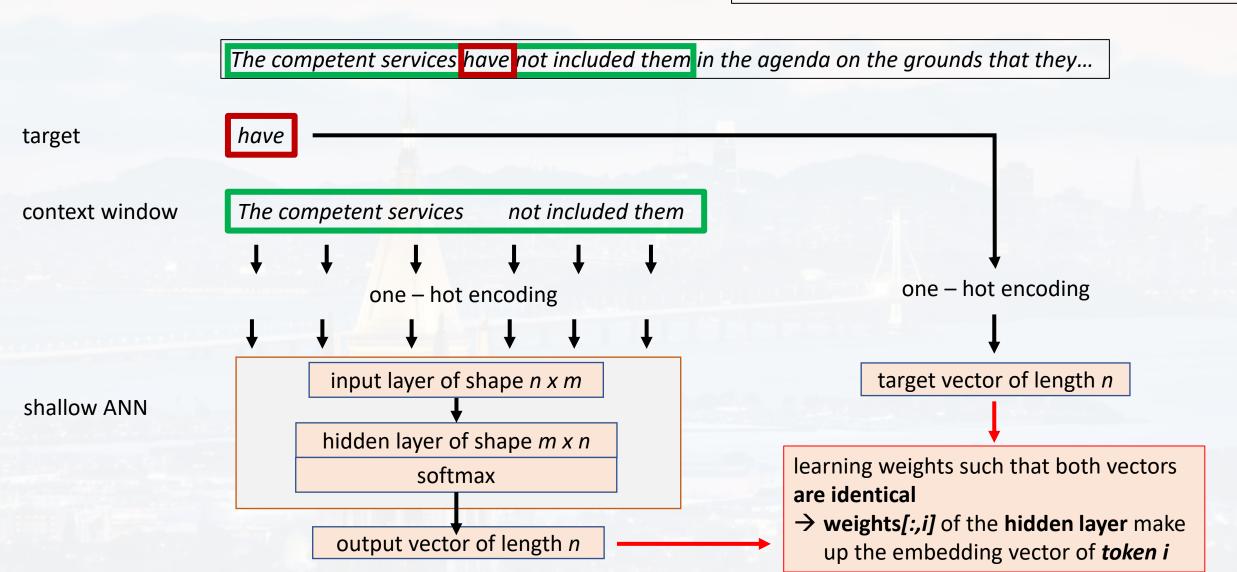
Two common algorithms are Continuous Bag Of Words and skip gram



Continuous Bag Of Words

n: number of unique token from corpus

m: desired number of dimensions for embedding





Continuous Bag Of Words

n: number of unique token from corpus

m: desired number of dimensions for embedding

The competent services have not included them in the agenda on the grounds that they... target competent services have included them in context window one – hot encoding one – hot encoding input layer of shape *n x m* target vector of length *n* shallow ANN hidden layer of shape m x n learning weights such that both vectors softmax are identical → weights[:,i] of the hidden layer make output vector of length *n* up the embedding vector of token i



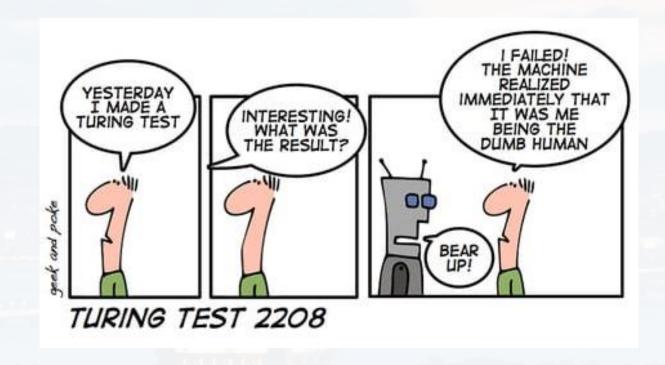
Continuous Bag Of Words

n: number of unique token from corpus

m: desired number of dimensions for embedding

The competent services have not included them in the agenda on the grounds that they... included target ... and so on... services have not them in the context window one – hot encoding one – hot encoding input layer of shape *n x m* target vector of length *n* shallow ANN hidden layer of shape m x n learning weights such that both vectors softmax are identical → weights[:,i] of the hidden layer make output vector of length *n* up the embedding vector of token i

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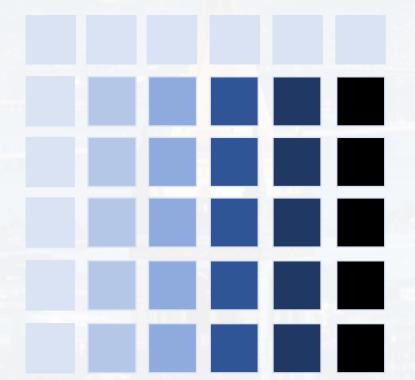


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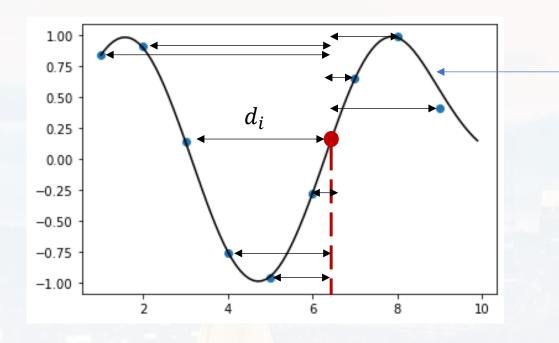
"The cat jumped on the roof."



how the first token influences all other token

how the second token influences all other token

.... and so on



We want to interpolate between the blue dots

- → generating the black line
- → no curve fitting!

<u>idea:</u>

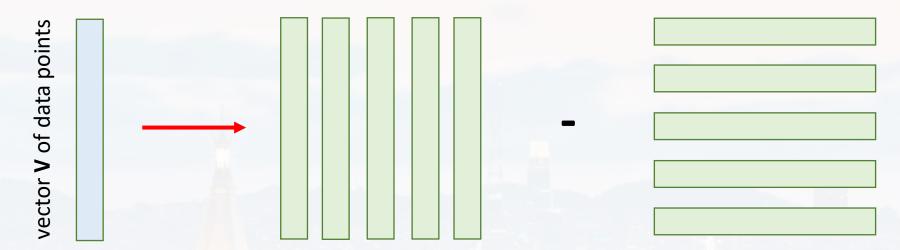
- select a point for which we want the interpolation for
- calculate distance d_i to every other point
- each data point should influence the value of the interpolated point
- the closer, the stronger the influence → weighted mean

$$y_{int} \sim \sum_{i=1}^{I} w_i y_i$$

$$w_i \gamma \frac{1}{d_i}$$



<u>calculating distance</u>

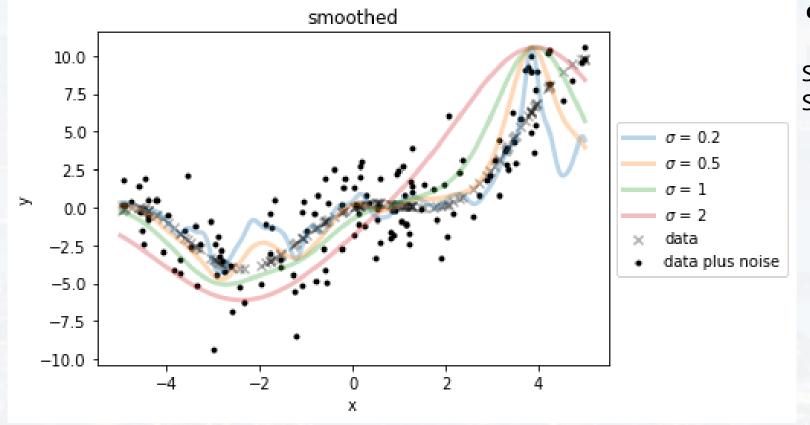


$$D = np.tile(V, (1, len(V))) - np.tile(L.transpose(), (len(V), 1))$$

- each data point should influence the value of the interpolated point
- the closer, the stronger the influence → weighted mean

$$y_{int} \sim \sum_{i=1}^{I} w_i \ y_i$$

```
D = np.tile(V, (1, len(V))) - np.tile(L.transpose(), (len(V), 1))
W = np.exp(-(D**2)/(sigma))
W = W/np.sum(W)
yint = np.dot(W.transpose(), y)
```

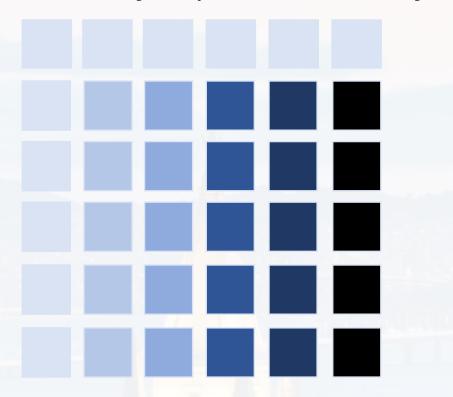


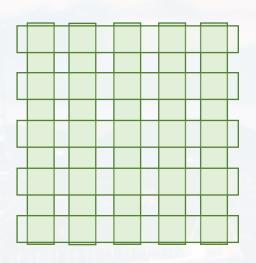
check out:

SmoothGaussKernel.py
SmoothExamples.py



"The cat jumped on the roof."



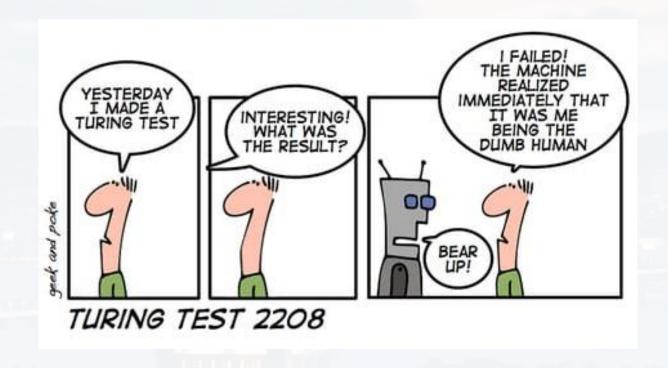


Gaussian kernel	W W	<pre>= np.exp(-(D**2)/(sigma)) = W/np.sum(W)</pre>
	yint	<pre>= np.dot(W.transpose(), y)</pre>

actual attention:

these weights are learnable, no kernel assumed!

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Transformer Architecture

number of token N: "The cat jumped on the roof." number of embedding dimensions E: Ν positional encoding word embedding Ε Ε Ν + Ν N transformer

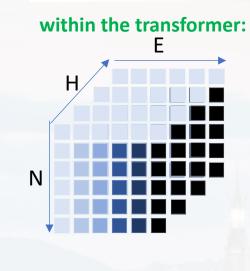
query

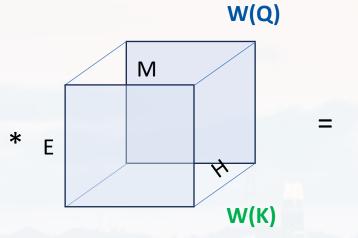
Q

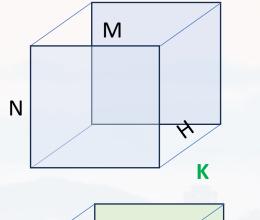


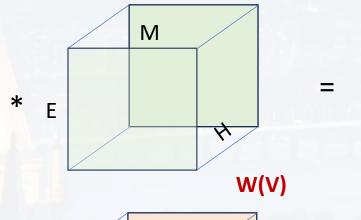
attention:

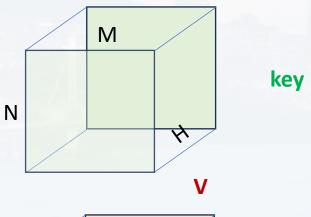
Berkeley LLM & Transformer:











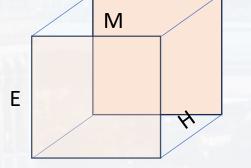
W(Q), W(K), W(V): learnable

N: number of token

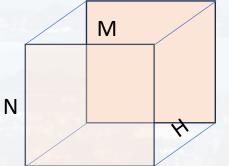
E: number of embedding dimensions

H: number of heads (= 8)

M: head size (= 64)



*



value

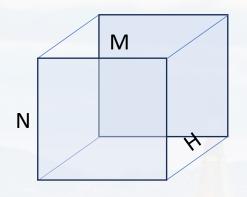


within the transformer:

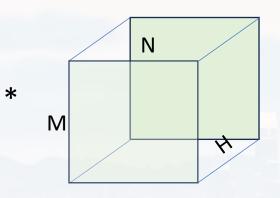


query

attention:



N = N(decoder)

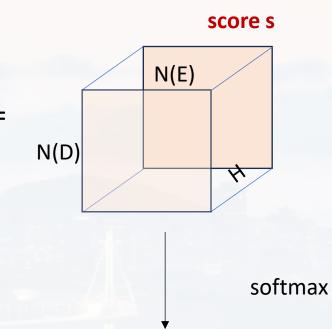


key

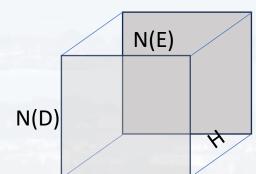
 K^{T}

N = N(encoder)

if been called by the decoder (see later)



weights w



W(Q), W(K), W(V): learnable

number of token N:

number of embedding dimensions E:

number of heads (= 8)

head size (= 64) M:

within the transformer:

weights w

value V

N: number of token

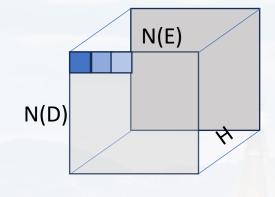
E: number of embedding dimensions

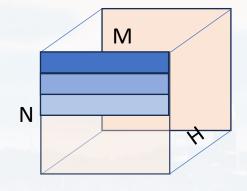
H: number of heads (= 8)

M: head size (= 64)

M

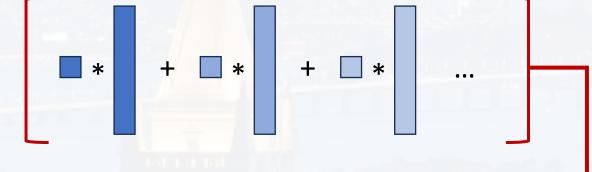
attention:





N = N(encoder), if been called by the decoder (see later)

σ

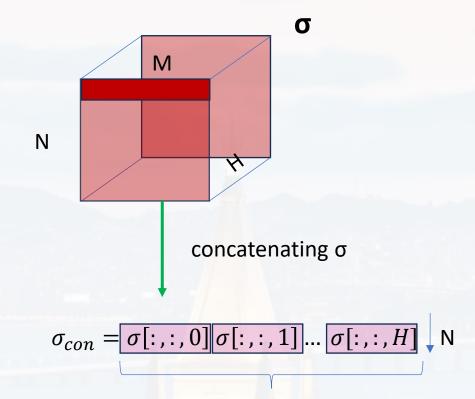


$$\sigma[i,:,k] = \sum_{j} w[i,j,k] * v[j,:,k]$$



Transformer Architecture





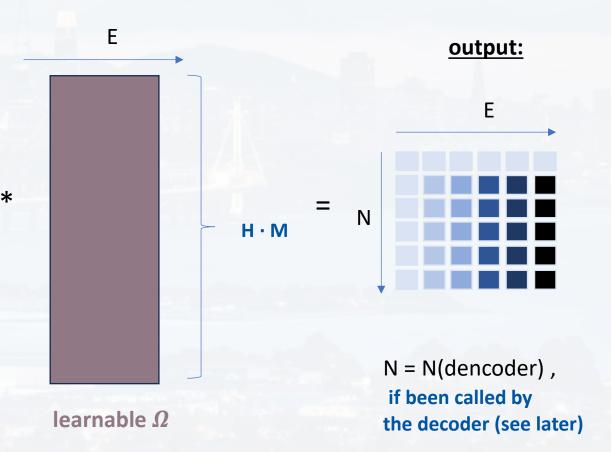
 $H \cdot M$

N: number of token

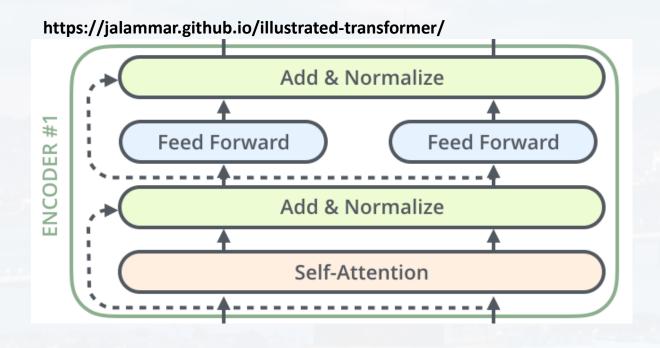
E: number of embedding dimensions

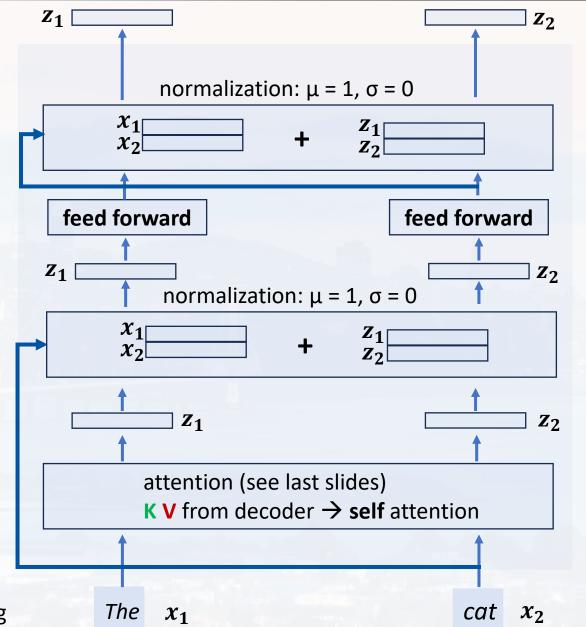
H: number of heads (= 8)

M: head size (= 64)

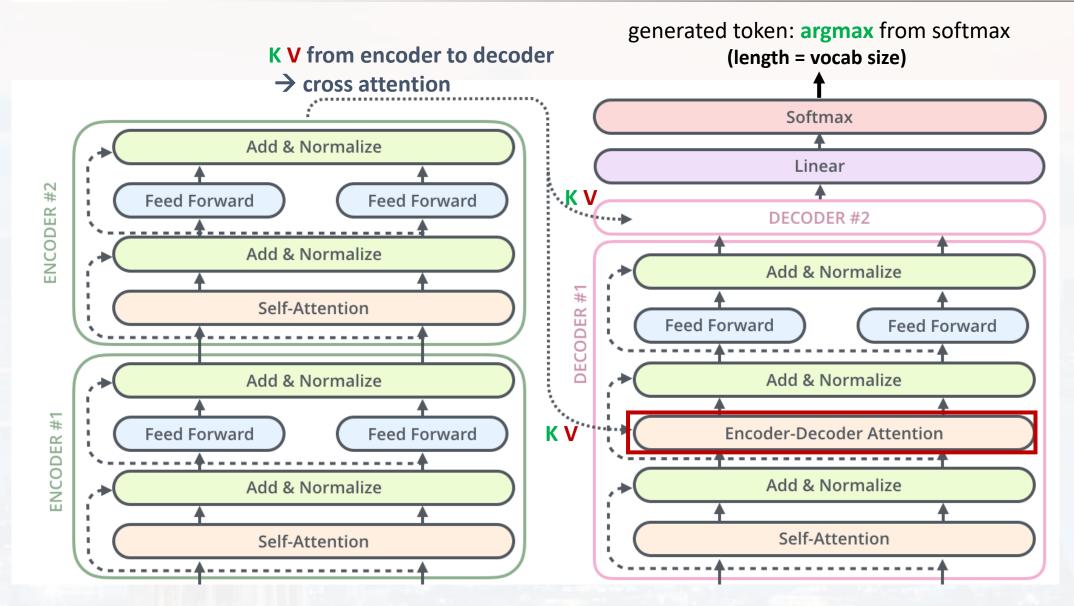


that was attention → now: encoder

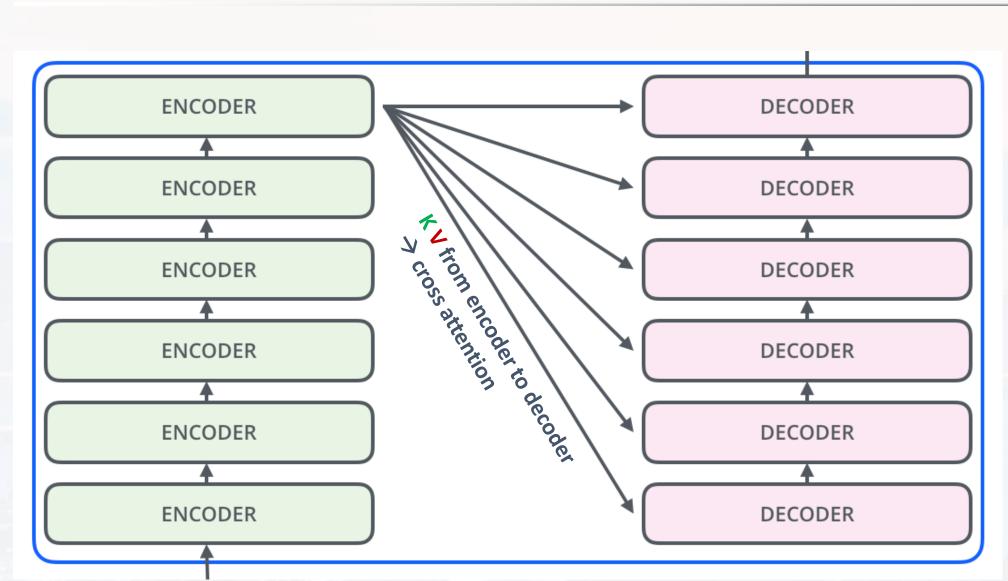




Transformer Architecture



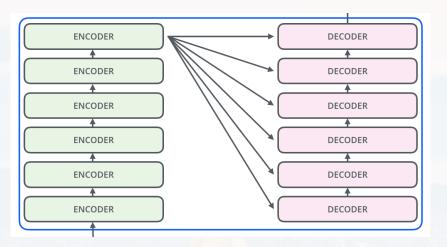






K V from encoder to decoder

→ cross attention



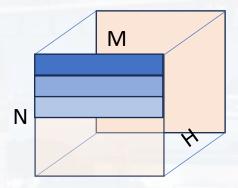
general:	N	(E)	≠	Ν	D)
Belleran	, ,	- /	,	, ,	<i>''</i>	,

English: Let there be light. N(E) = 4German: Es werde Licht. N(D) = 3Latin: Fiat lux. N(D) = 2Hebrew: yehi,or N(D) = 2

weights w

attention: N(E)

value V



N = N(encoder), if been called by the decoder

Transformer Architecture

Output

Softmax

Linear

Feed

Forward

Attention

Masked

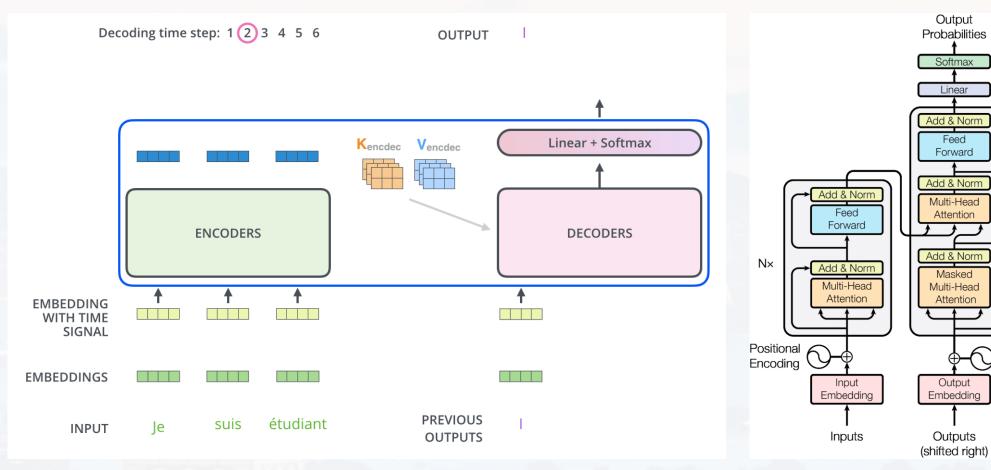
Multi-Head

Output

Outputs

N×

Positional Encoding



https://jalammar.github.io/illustrated-transformer/

Attention Is All You Need (Vaswani et al, 2017)

more about transformers:

Jay Alammar

Interactive Visualization

transformers intro



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