

Lecture 14:

Language Models and Transformer



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**Bayesian Data Analysis and
Machine Learning for Physical
Sciences**

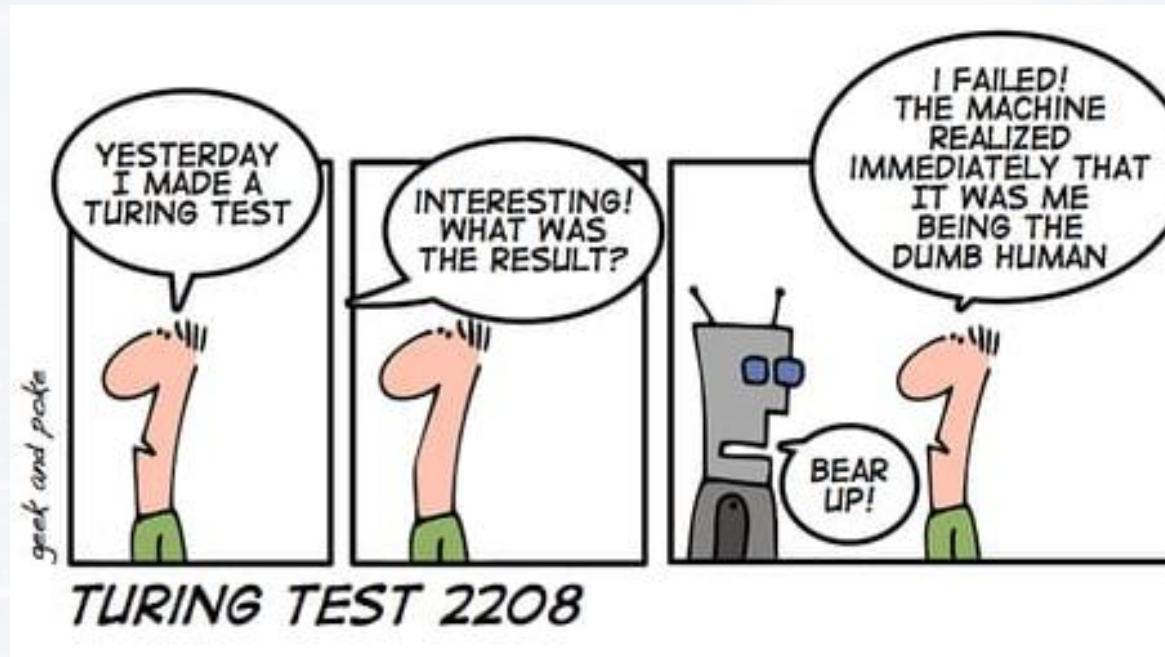


Course Map

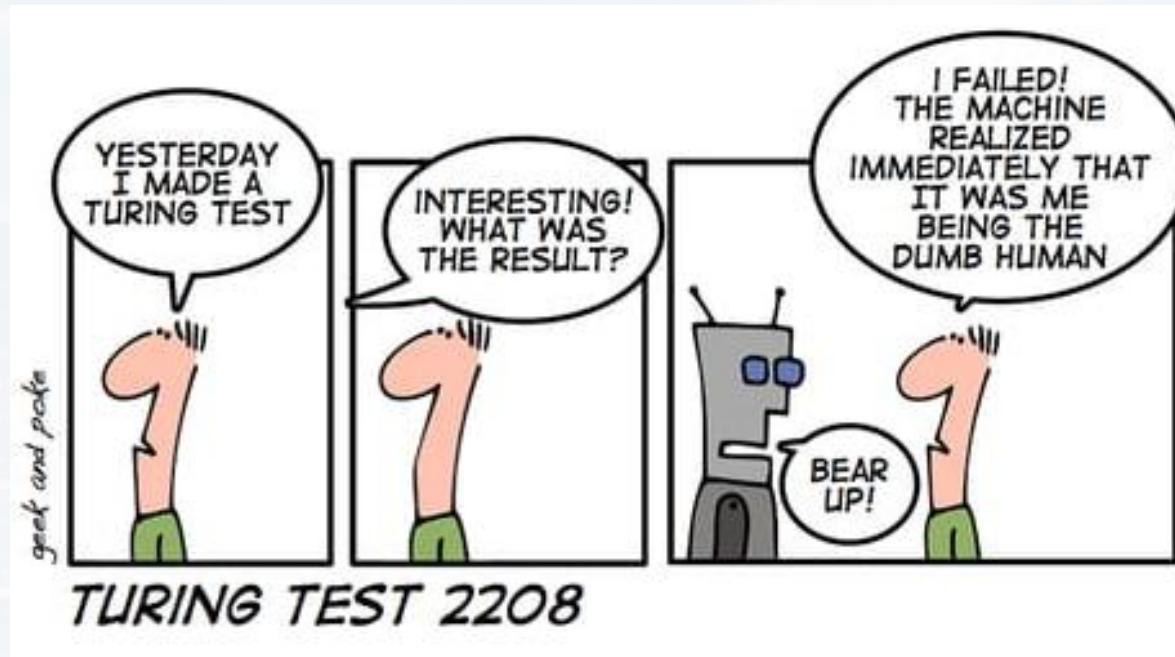
Module 1	Maximum Entropy and Information, Bayes Theorem
Module 2	Naive Bayes, Bayesian Parameter Estimation, MAP
Module 3	MLE, Lin Regression
Module 4	Model selection I: Comparing Distributions
Module 5	Model Selection II: Bayesian Signal Detection
Module 6	Variational Bayes, Expectation Maximization
Module 7	Hidden Markov Models, Stochastic Processes
Module 8	Monte Carlo Methods
Module 9	Machine Learning Overview, Supervised Methods & Unsupervised Methods
Module 10	ANN: Perceptron, Backpropagation, SGD
Module 11	Convolution and Image Classification and Segmentation
Module 12	RNNs and LSTMs
Module 13	RNNs and LSTMs + CNNs
Module 14	Transformer and LLMs
Module 15	Graphs & GNNs



Outline

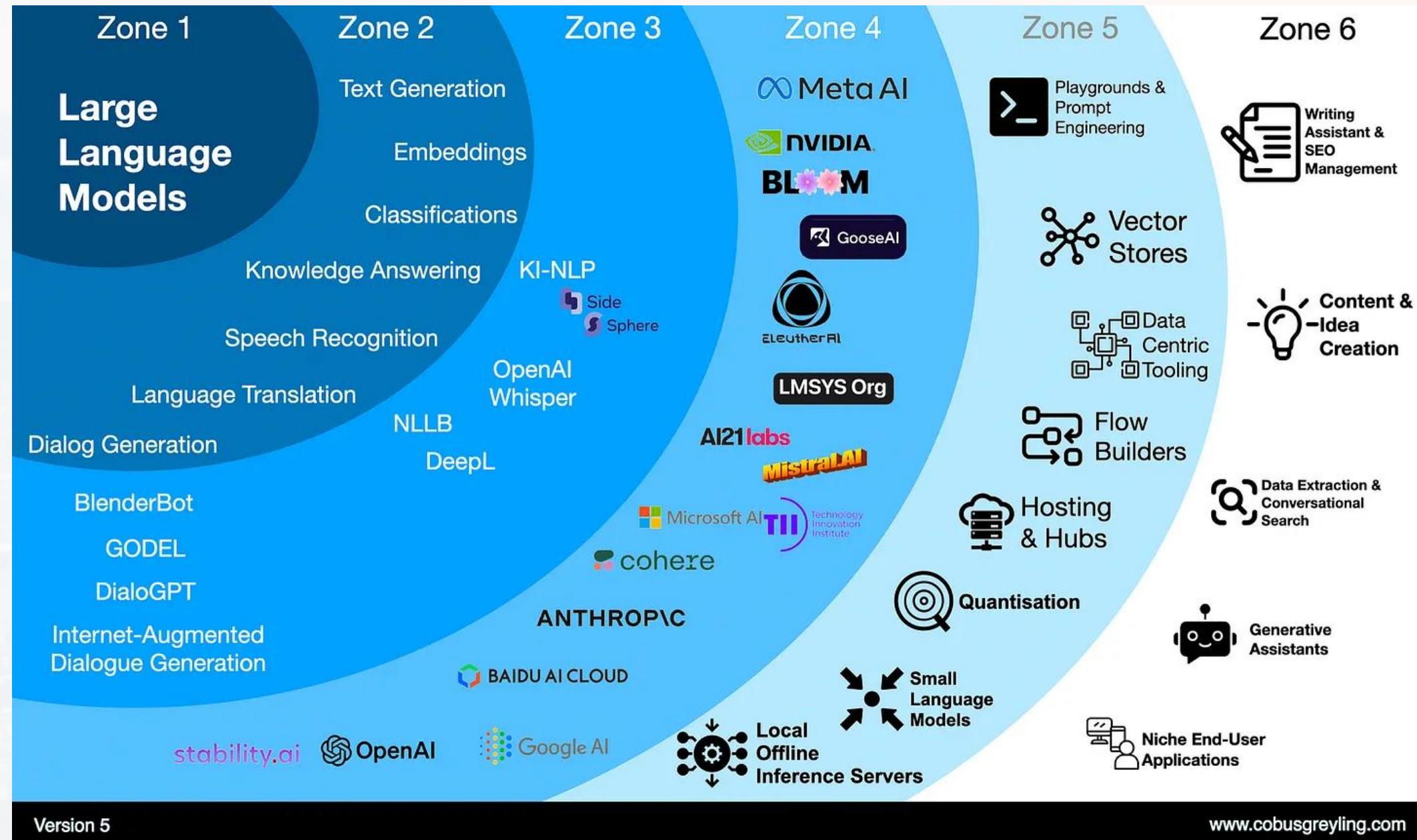


- Introduction
- Bigram and MAP
- Positional Encoding
- Word Embedding
- Attention
- Transformer Architecture



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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

- letters in a word
- words in a sentence

(upper/lower case, cases, gender, tenses, conjugations)

- amino acids in a protein sequence
- nucleotides in a DNA/RNA sequence
- motifs in a DNA/RNA sequence

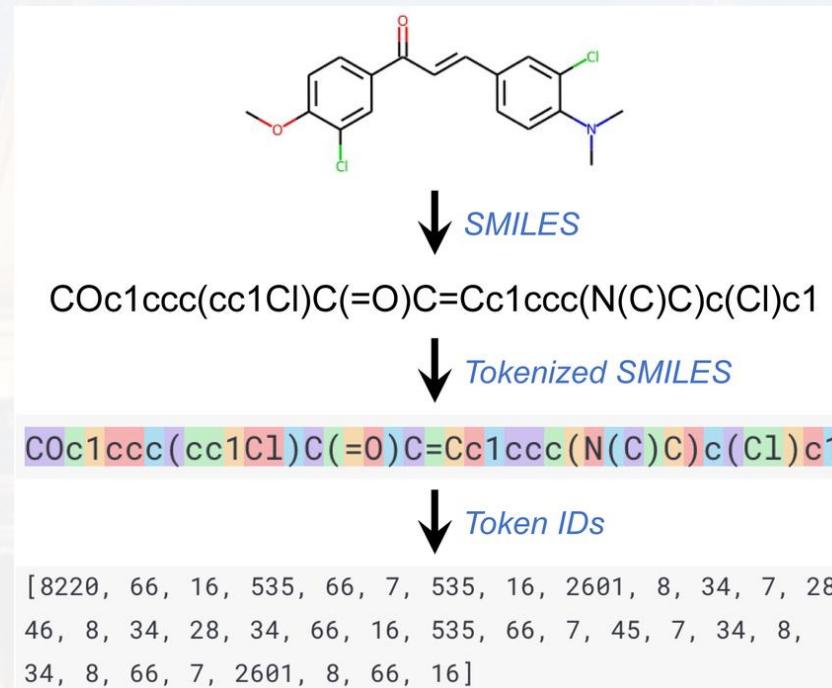
size of alphabet

- 10^2
- $10^4 \dots 10^6$
- 21
- 4
- 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



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

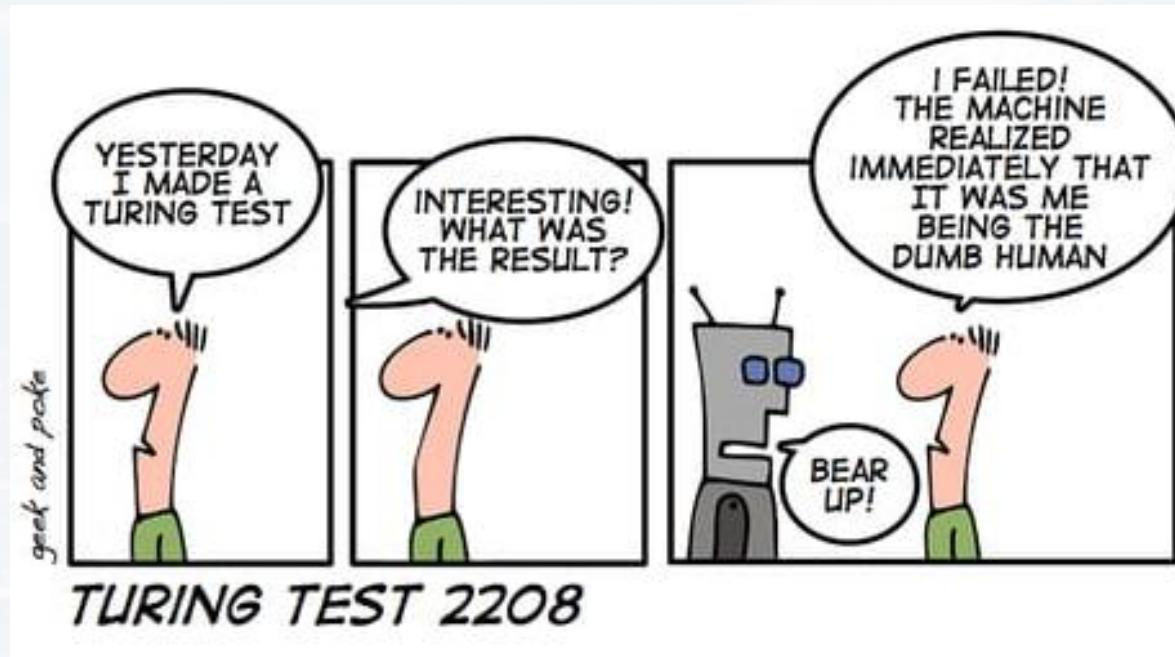
token: individual, independent entity of a language

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):

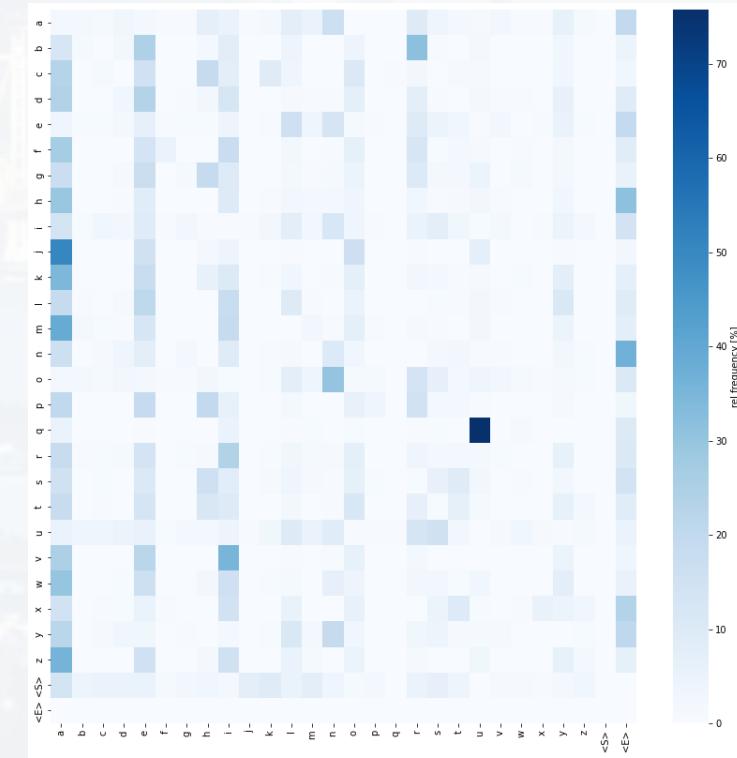
$$P(X_1 X_2 X_3 X_4 X_5 \dots X_n) = P(X_n | X_{n-1}) P(X_{n-1} | X_{n-2}) \dots P(X_1)$$



P(i|j): that token i is generated after token j

→ N x N transition matrix from frequencies

→ “bigram” = “two words”



frequency matrix of letters in common names



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',
'harpers',
'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**

['<S>'] + ['olivia'] + ['<E>']

→ **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

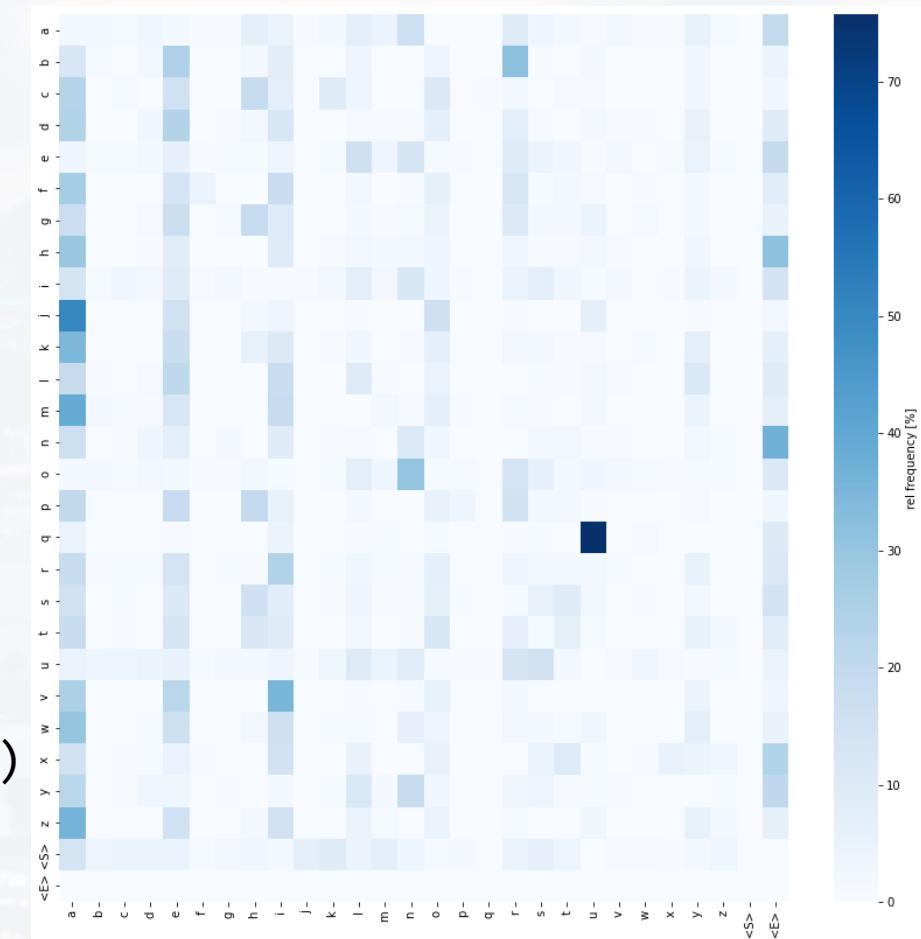
- 1) dictionary first (will help for counting)
- 2) count how often letter i is followed by letter j

→ 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 → 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
drvah
lzaxi
tyunusthun
jorrwro
ja
asoow
s

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

mtkg
yufexhviov
morphqvik
bbbjxebpxwure
jaqlzzuwuan
xmmomhr<S>
uhb
xlmusadjfdzxadaotd
ik<S>vdtydvxev
taselkykcfbamceprtv1
zyr<S>inzoerobz
wuovx
eg<S>pbdvikf<S>
tomcnkfsjay<S>
rikatnaykizszciv
pds<S>zj
kh<S>y<S>ualzug
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bblupnibtqmyl<S>
vyobf
kybs
rznjgpml
tnhoxuckkjzbwmj<S>
vshkycicf<S>
kowskphy
rxodh
jvswmzw
jzpcfnpbg



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
→ essentially **MLE** (problematic if a letter hasn't appeared in the sequence yet
→ $P(X_n)$ 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:

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

binomial process

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

$q - 1$



q



$q = ?$





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

Bayesian
Parameter
Estimation*)

$q - 1$



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

likelihood function (here: binomial)

$$P(q|data\ set) = \frac{P(data\ set|q)P(q)}{P(data\ set)} \text{ prior } (\sim P(X_n|X_{n-1} \dots X_1))$$

evidence (const wrt q)

$q = const$
before 1st data point
(max entropy!)

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

$q = conjugate\ prior$
after nth data point

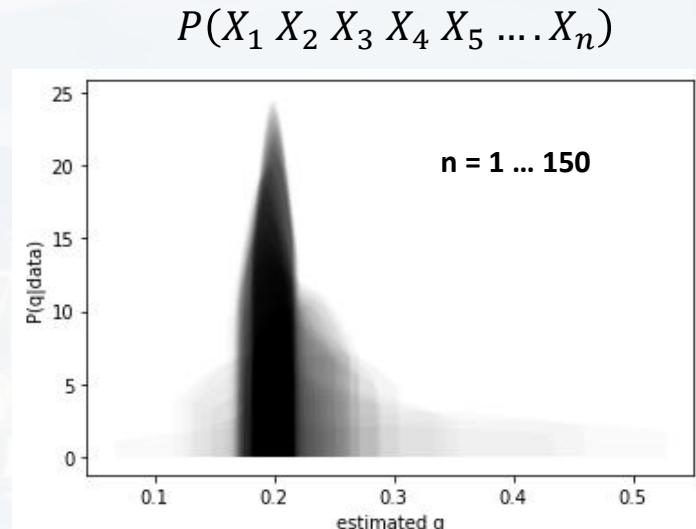
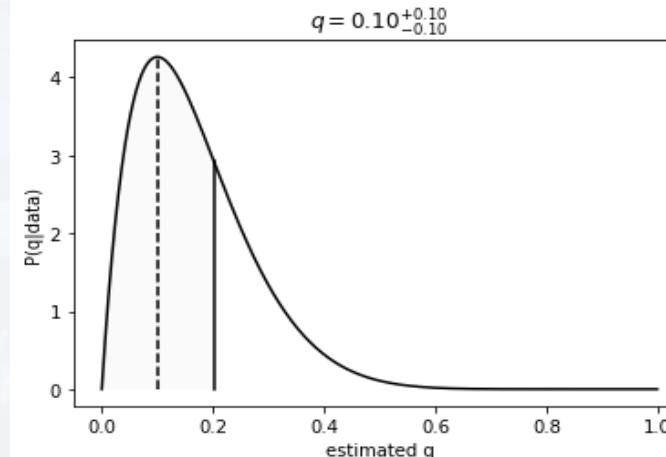
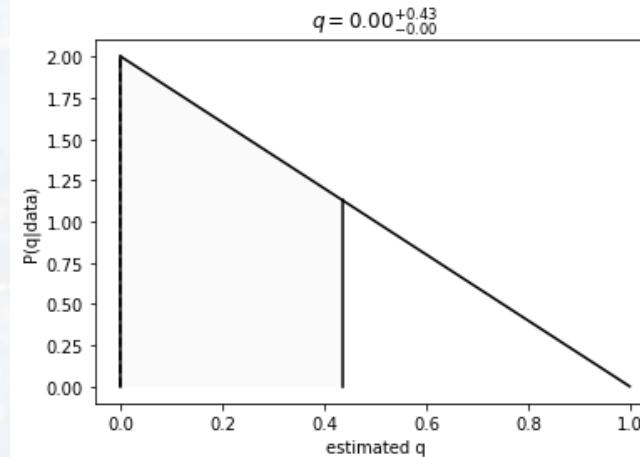
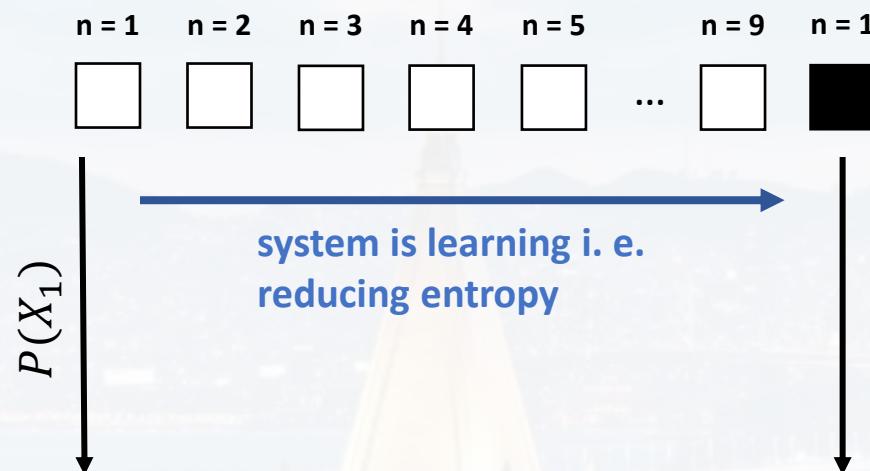
$$= \frac{q^{k+\alpha-1} (1-q)^{n-k+\beta-1}}{\int_0^1 q^{k+\alpha-1} (1-q)^{n-k+\beta-1} dq}$$



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

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

Bayesian
Parameter
Estimation*)



*) see lecture 2



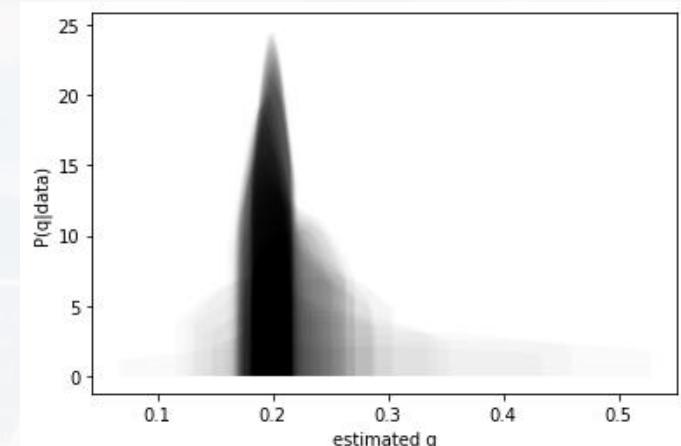
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Bayesian
Parameter
Estimation*)

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

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

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

*) see lecture 2

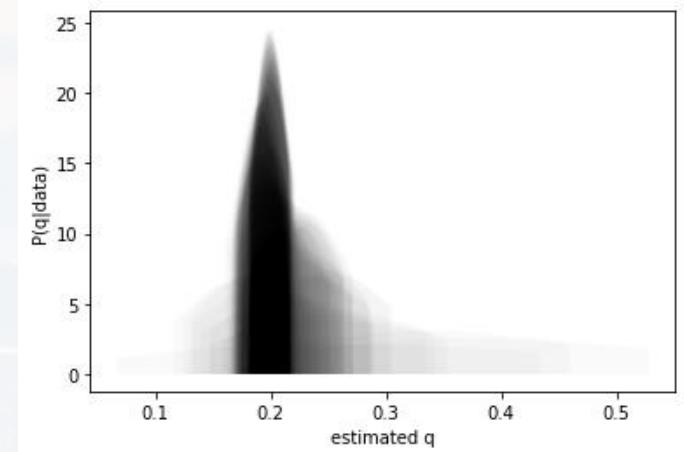


$$P(X_1 X_2 X_3 X_4 X_5 \dots X_n) = P(X_n|X_{n-1} \dots X_1)P(X_{n-1}|X_{n-2} \dots X_1) \dots P(X_1)$$

Dirichlet distribution

$$P(\text{sequence}) \sim \prod_j \prod_a P(a)_j^{\alpha(a)-1}$$

note: $\sum_{\text{over all } a} P(a)_j = 1 \rightarrow N - \text{dim simplex}$



- 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 $P(\text{sequence})$ given the constrain $\sum_{\text{over all } a} P(a)_j = 1$ (**Lagrangian multipliers**)
 - **Maximum a-posteriori (MAP)** approach → see XXmotif (Siebert & Soeding, 2016)

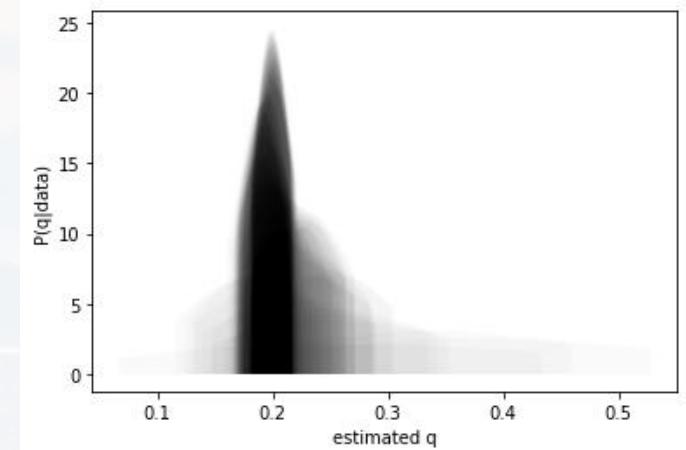


$$P(X_1 X_2 X_3 X_4 X_5 \dots X_n) = P(X_n|X_{n-1} \dots X_1)P(X_{n-1}|X_{n-2} \dots X_1) \dots P(X_1)$$

Dirichlet distribution

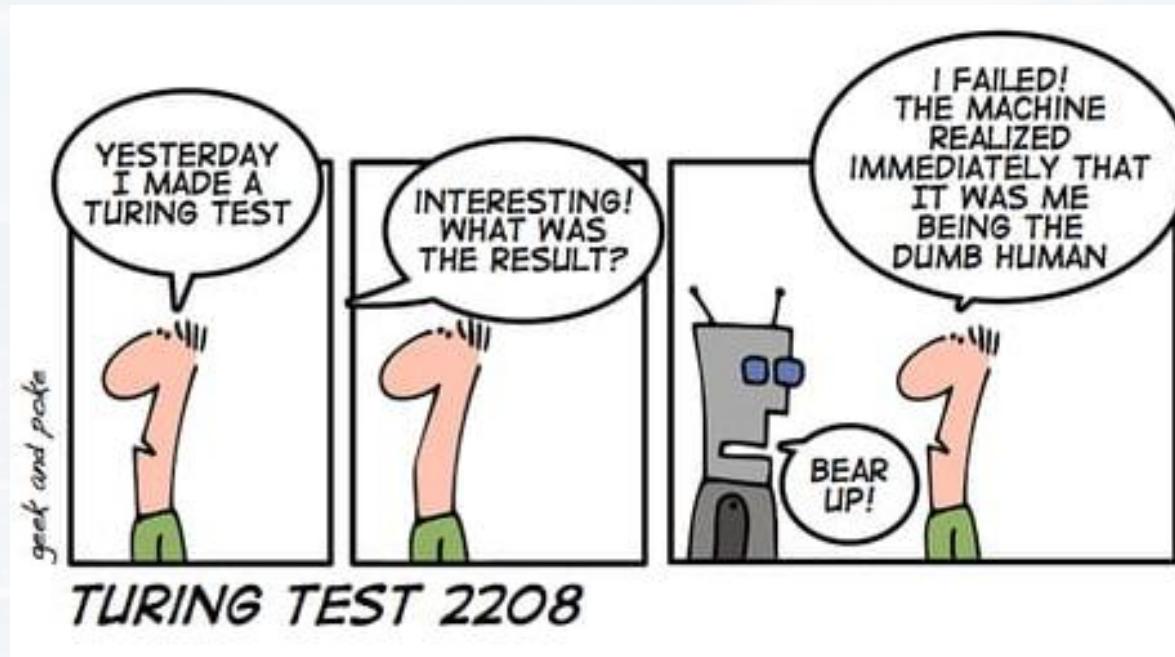
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Maximum a-posteriori (MAP)

- 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:

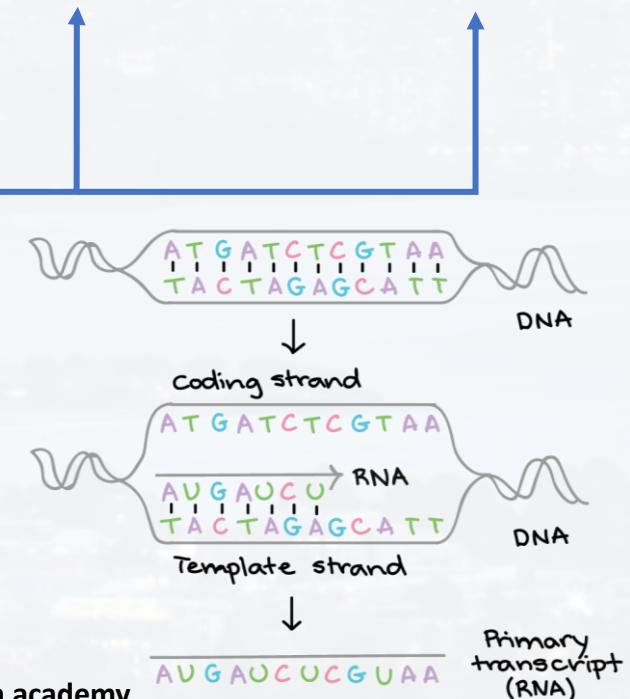
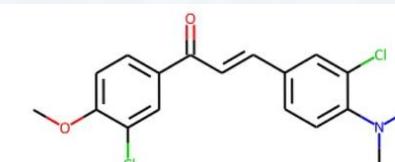
- **positional encoding** (location of token in a sequence)
- **word embedding** (relation between similar/different token)
- **attention** (relation between token within a sequence)

"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

76543210 ← 8bit i.e. eight dimensions

1	00000001
2	00000010
3	00000011
4	00000100
5	00000101
6	00000110
7	00000111
8	00001000
9	00001001
10	00001010
11	00001011
12	00001100
13	00001101
14	00001110
15	00001111
16	00010000

depending on dimensions (bit)

→ different frequencies

bit	frequency
0	1/2
1	1/4
2	1/8
...	

Does that look familiar?
→ like Fourier Series



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

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

p : position in sequence

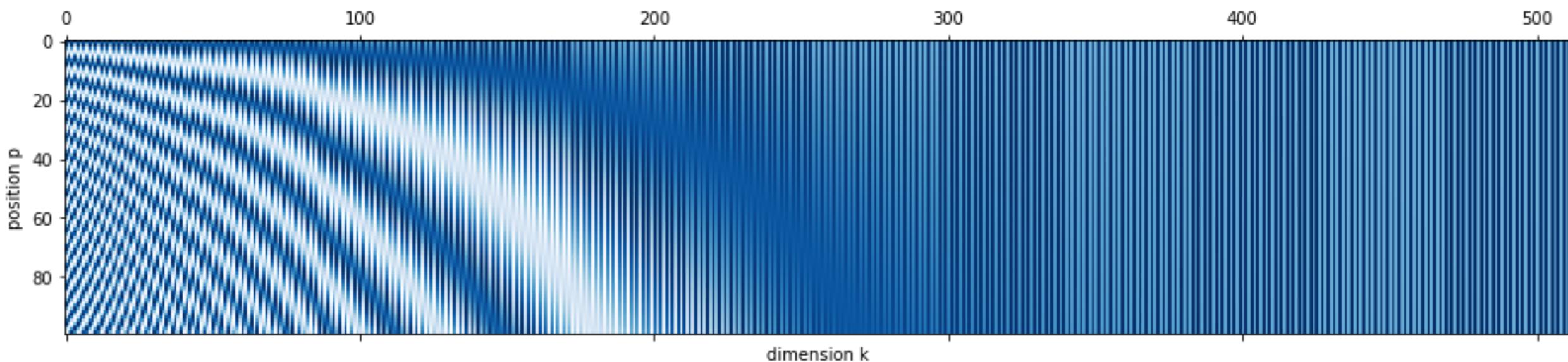
k : dimension index

d : number of dimensions

10,000: an arbitrary number Vaswani et al., 2017

run **PlotPositionEncoding.py**

more info [here](#)





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

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

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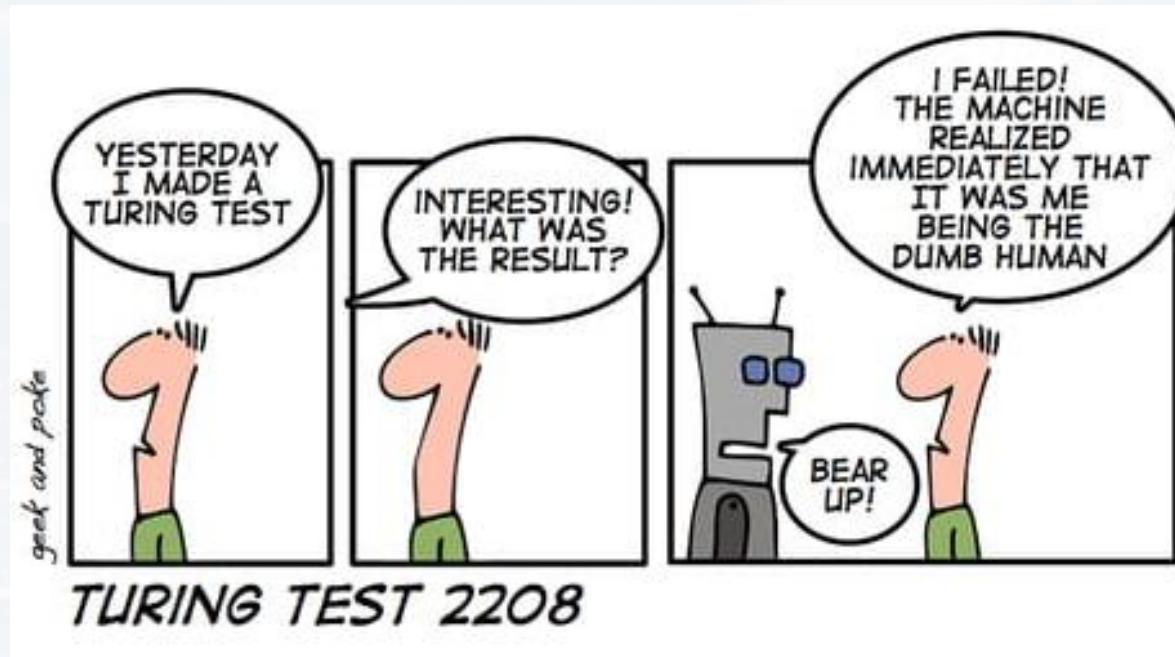
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run **PlotPositionEncoding.py**

note:

- easier to handle numerically vs discrete encoding
- $\cos(x + 2\pi k) = \cos(x)$ and $\sin(x + 2\pi k) = \sin(x)$
→ absolute position not relevant but **relative** position



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three things make context:

- **positional encoding** (location of token in a sequence)
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problem: turning token (words/letters) into numbers

single letters:

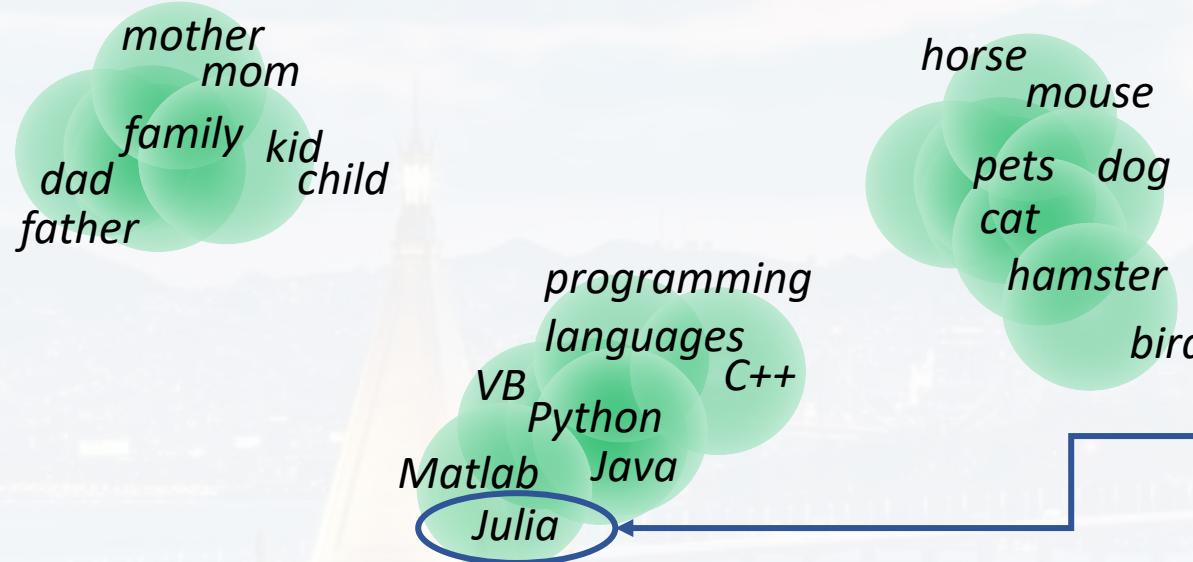
- | | |
|---------|--|
| ACGT | - one – hot works perfectly (four different token) |
| abcd... | - lower/upper case, special characters (50 different token), one – hot is fine too |

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) |
|--------------|--|



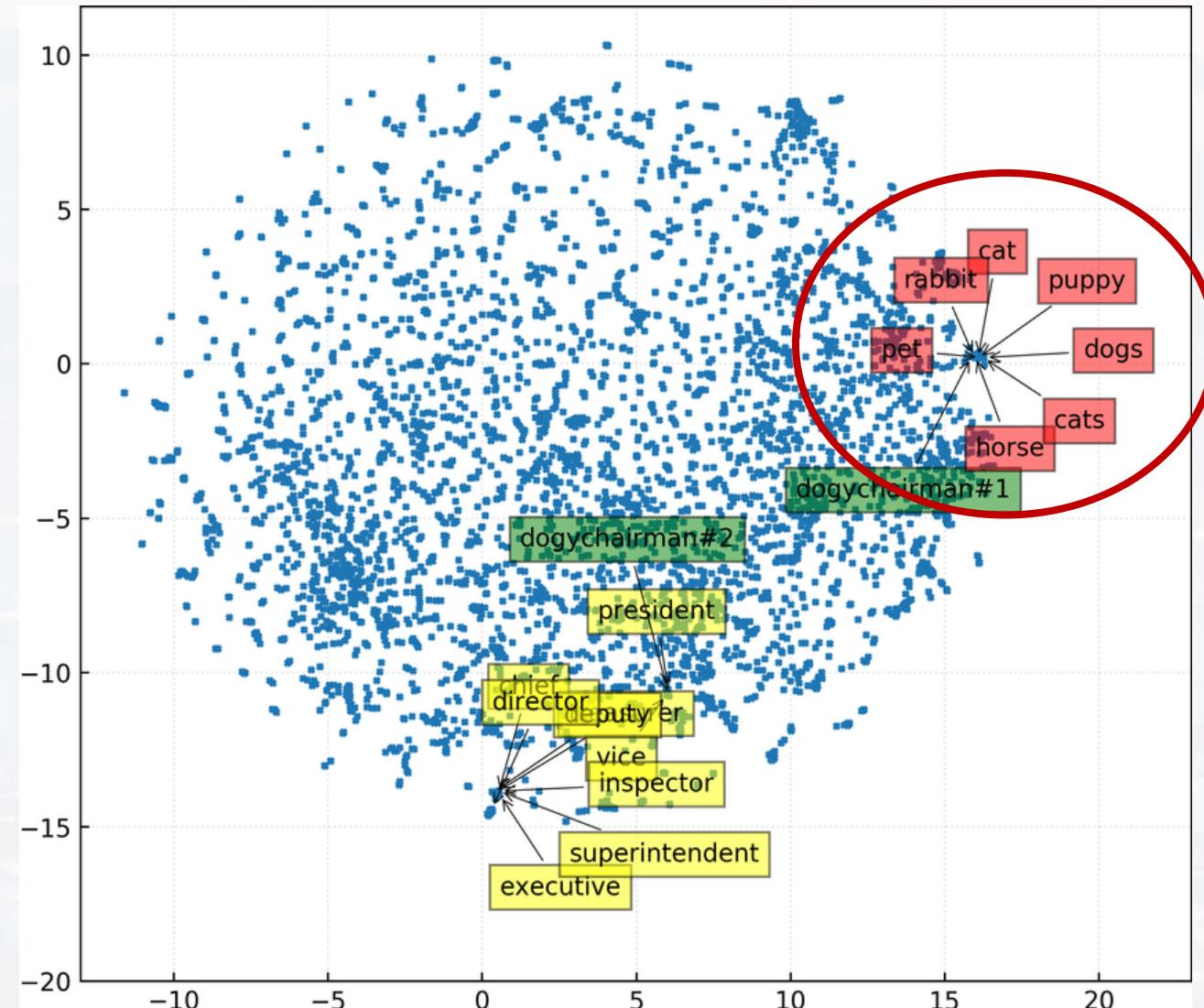
words with a **similar meaning** should form **cluster**



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



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





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 previous 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

The competent services have not included them in the agenda on the grounds that they...

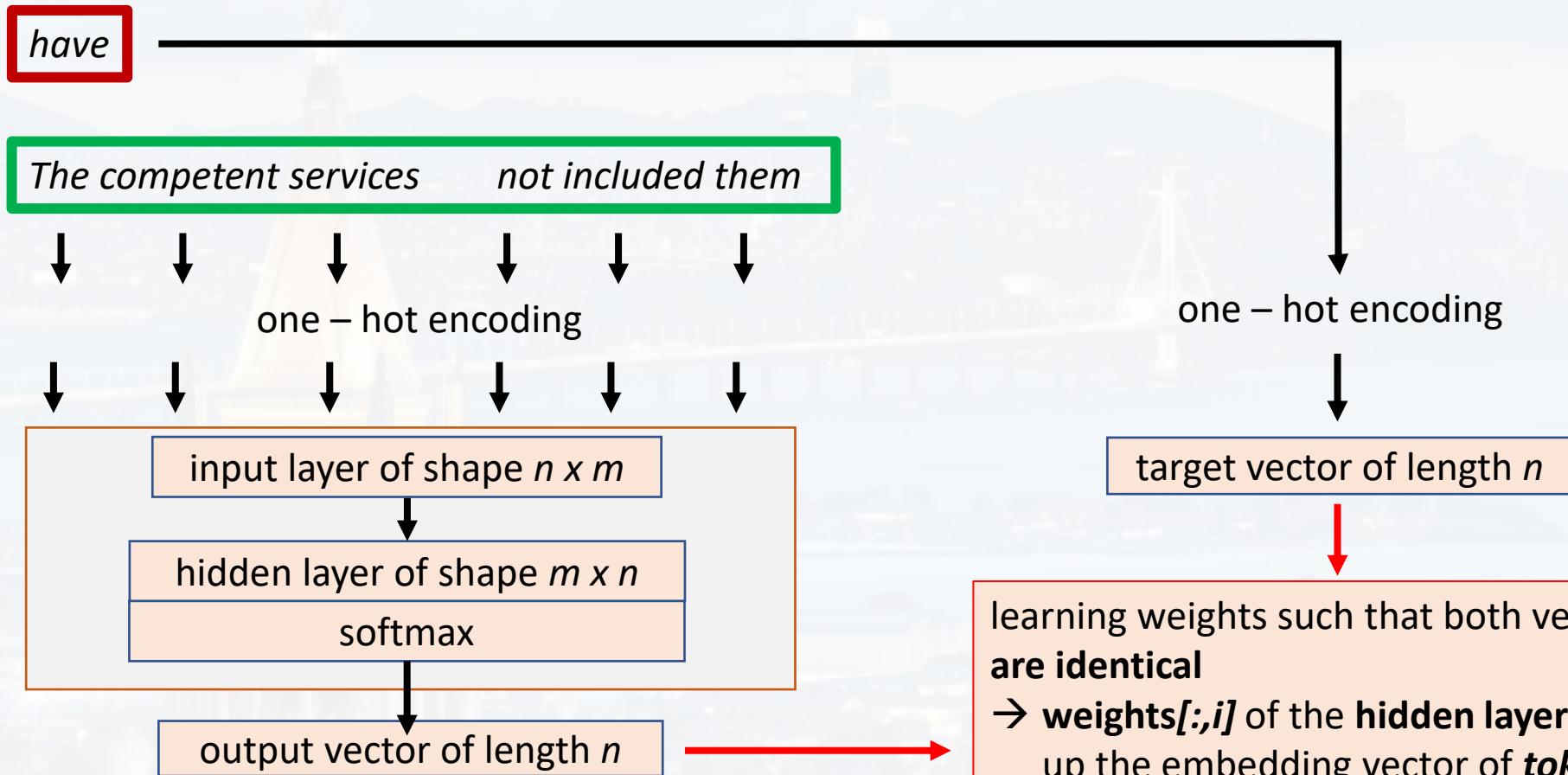
target

have

context window

The competent services not included them

shallow ANN





Continuous Bag Of Words

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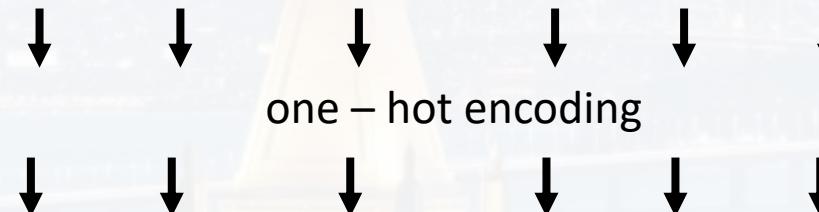
The **competent services have not included them in the agenda on the grounds that they...**

target

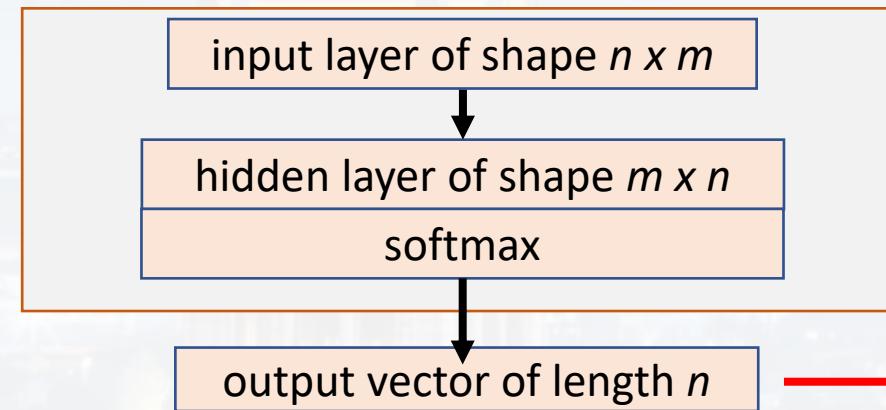
not

context window

competent services have included them in



shallow ANN



one – hot encoding

target vector of length n

learning weights such that both vectors are **identical**
→ **weights $[:,i]$** of the **hidden layer** make up the embedding vector of **token i**



Continuous Bag Of Words

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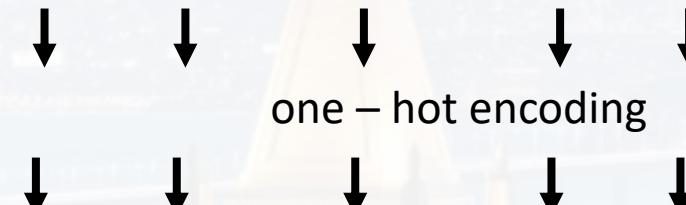
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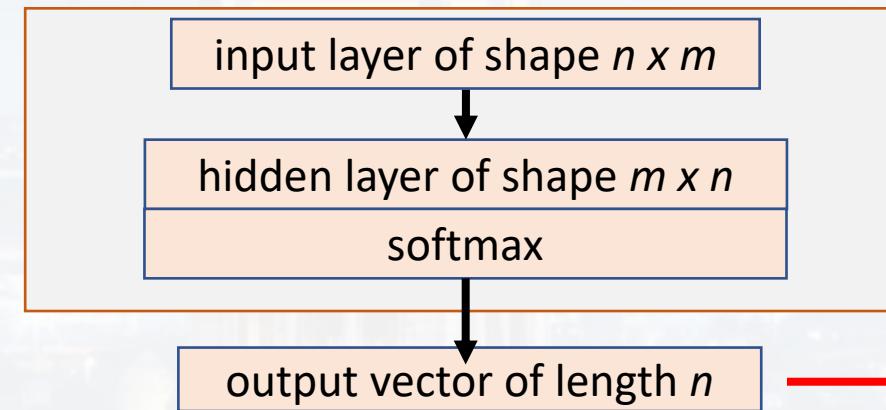
included

context window

services have not them in the



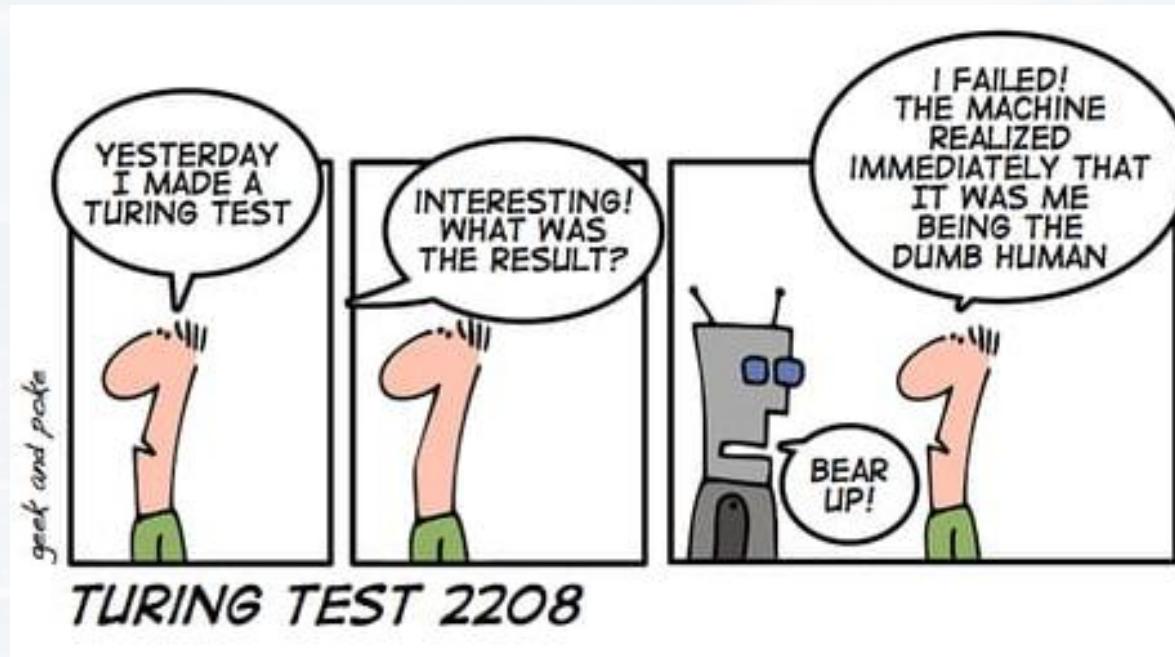
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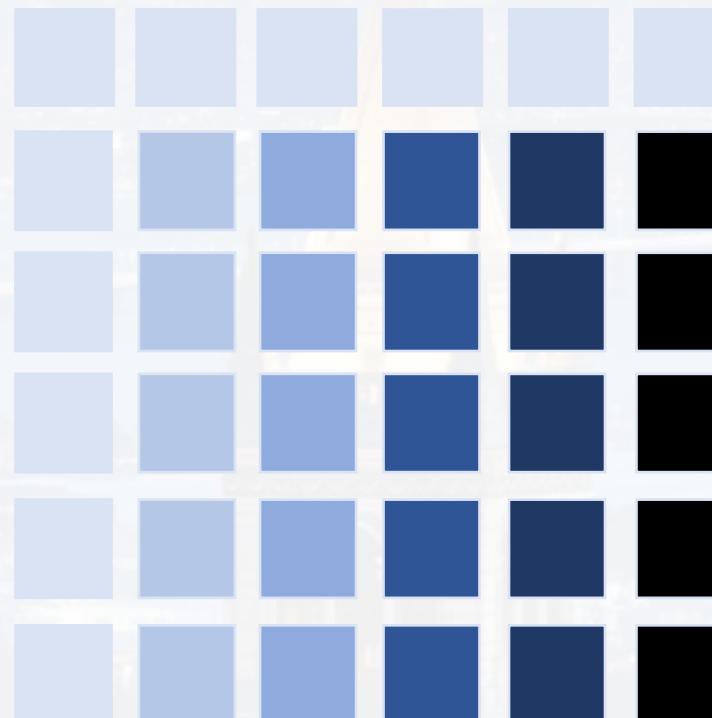
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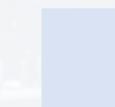
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"The cat jumped on the roof."

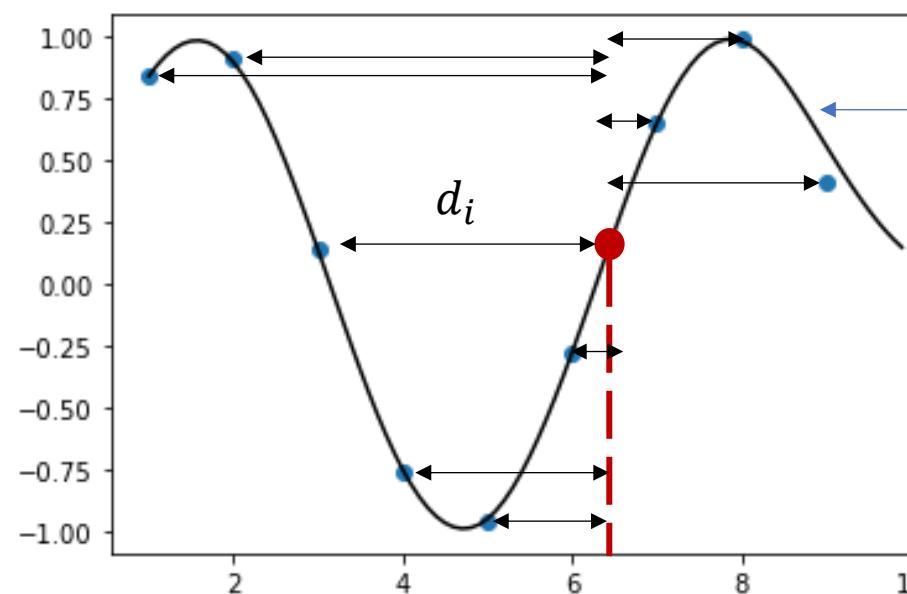


how the first token influences all other token



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!**

- idea:
- 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

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

calculating distance

```
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

Gaussian kernel

```
W      = np.exp(-(D**2)/(sigma))
W      = W/np.sum(W + 1e-16, axis = 0)
yint  = np.dot(W.transpose(), y)
```

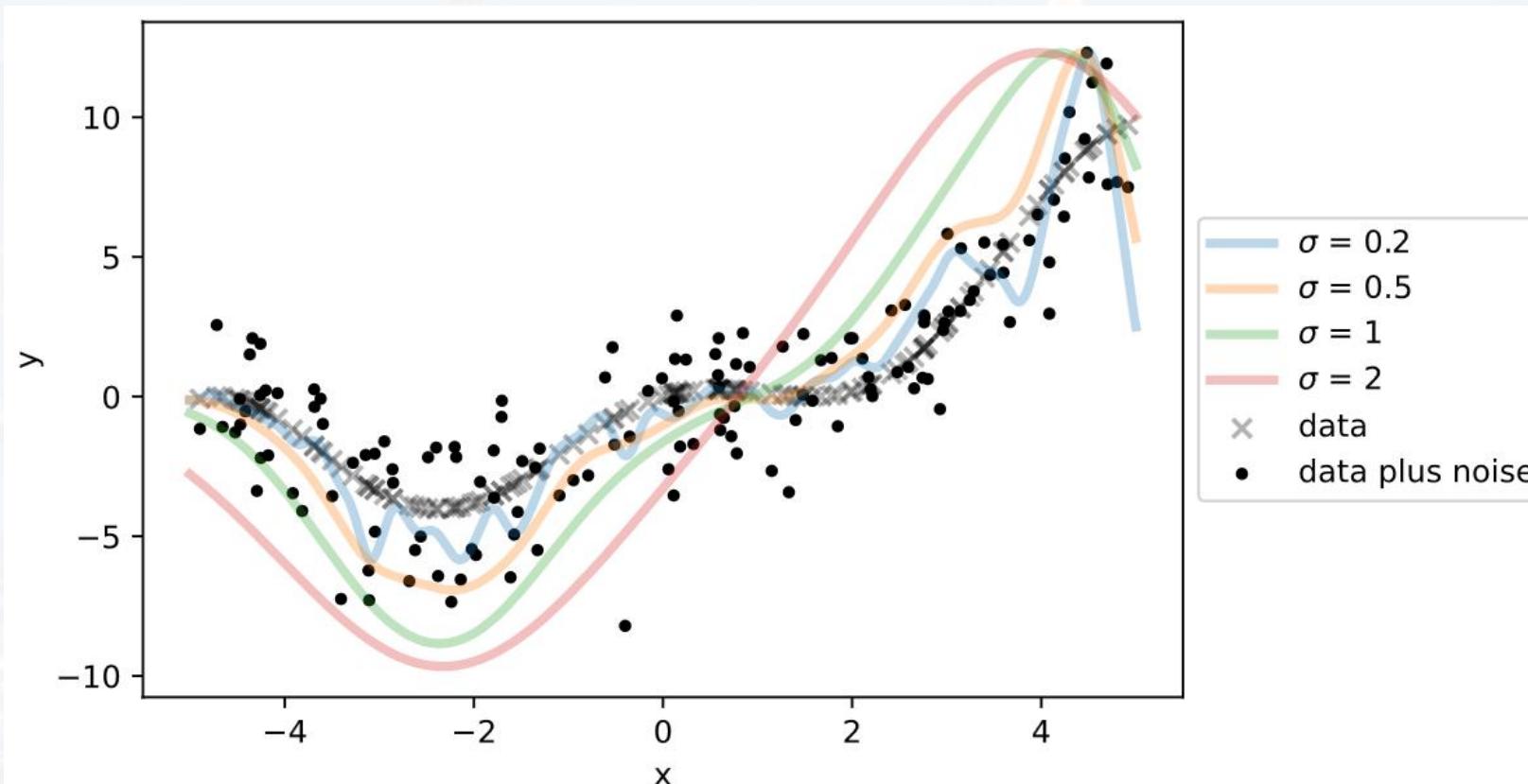
$$y_{int} \sim \sum_{i=1}^I w_i y_i$$



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Gaussian kernel

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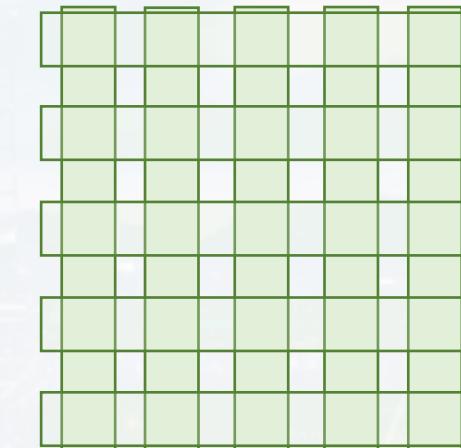
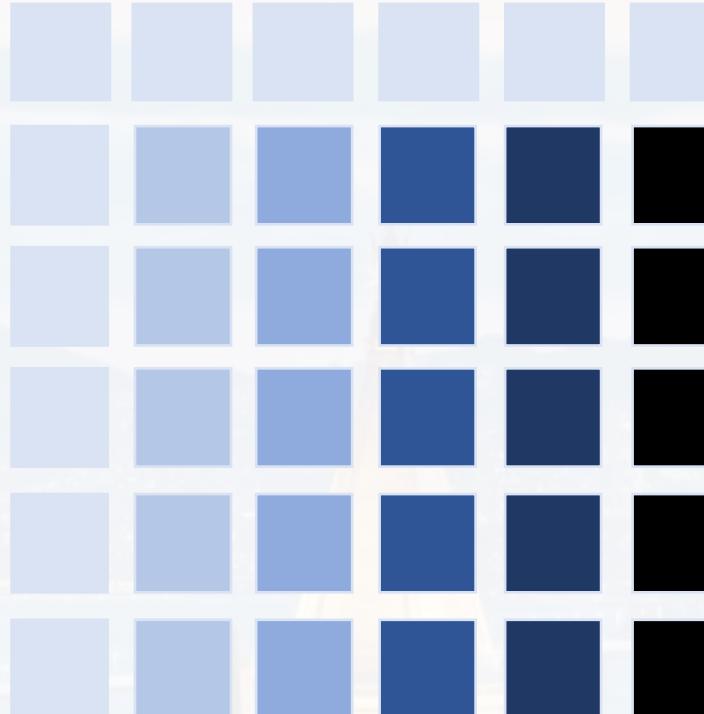


check out:

[SmoothGaussKernel.py](#)
[SmoothExamples.py](#)



"The cat jumped on the roof."



Gaussian kernel	W	$= \text{np.exp}(-(D^2)/(sigma))$
	W	$= W / \text{np.sum}(W + 1e-16, \text{axis} = 0)$
	y_{int}	$= \text{np.dot}(W^\top, y)$

actual attention:
these weights are learnable,
no kernel assumed!



self attention

imagine you want to built & train a movie GenAI **that creates movies based on queries.**

training data

"Thrilling horror science fiction movie, plays in space in a distant future"

$$X = X_1, X_2, \dots, X_N$$

each token is a vector X_n of length E

"Entertaining science fiction movie, plays in space in a distant past"

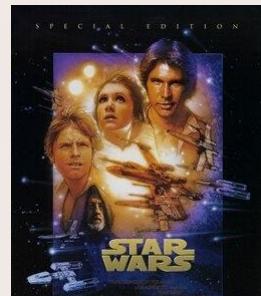
"Boring love story, plays on a ship in the past"

key

Alien



Star Wars



Titanic



value



self attention

imagine you want to built & train a movie GenAI **that creates movies based on queries**.

training data

each token is a vector X_n of length E

$$X = X_1, X_2, \dots, X_N$$

key

Alien



value

"Boring love story, plays in space."

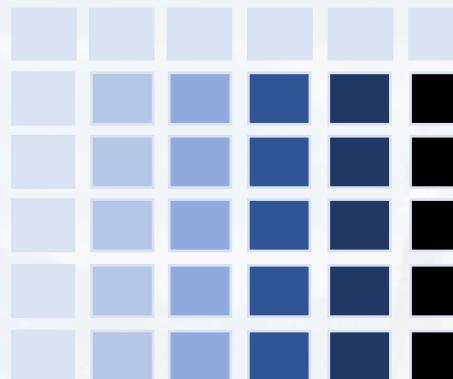
query





self attention

key value query

"Boring love story, plays on a ship in the past"weights w_{nm} each token is a vector X_n of length E $X = X_1, X_2, \dots, X_N$

output:

$$Y_n = \sum_{m=1}^N w_{nm} X_m$$

- weights should be learnable
- weight = 0, X_m has no influence on output
- weights should be positive so that neg weights don't counteract positive weights
- normalization: $\sum_{m=1}^N w_{nm} = 1$

for returning the best suggestion:

comparing key vector X_n to query vector X_m via dot product

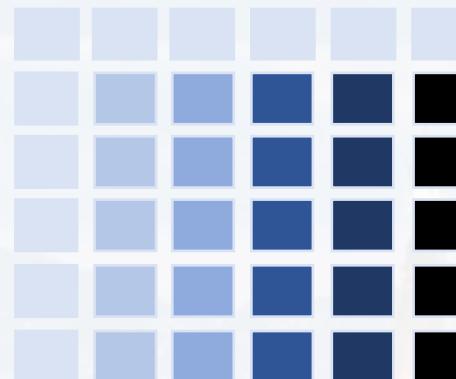
$$w_{nm} = \frac{\exp(X_n \circ X_m)}{\sum_{\mu=1}^N \exp(X_n \circ X_\mu)}$$

softmax



self attention

key value query

"Boring love story, plays on a ship in the past"weights w_{nm} each token is a vector X_n of length E $X = X_1, X_2, \dots, X_N$

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for returning the best suggestion:

comparing key vector X_n to query vector X_m via dot product

$$w_{nm} = \frac{\exp(X_n W(K) \circ X_m W(Q))}{\sum_{\mu=1}^N \exp(X_n W(K) \circ X_\mu W(Q))}$$

softmax



self attention

key value query

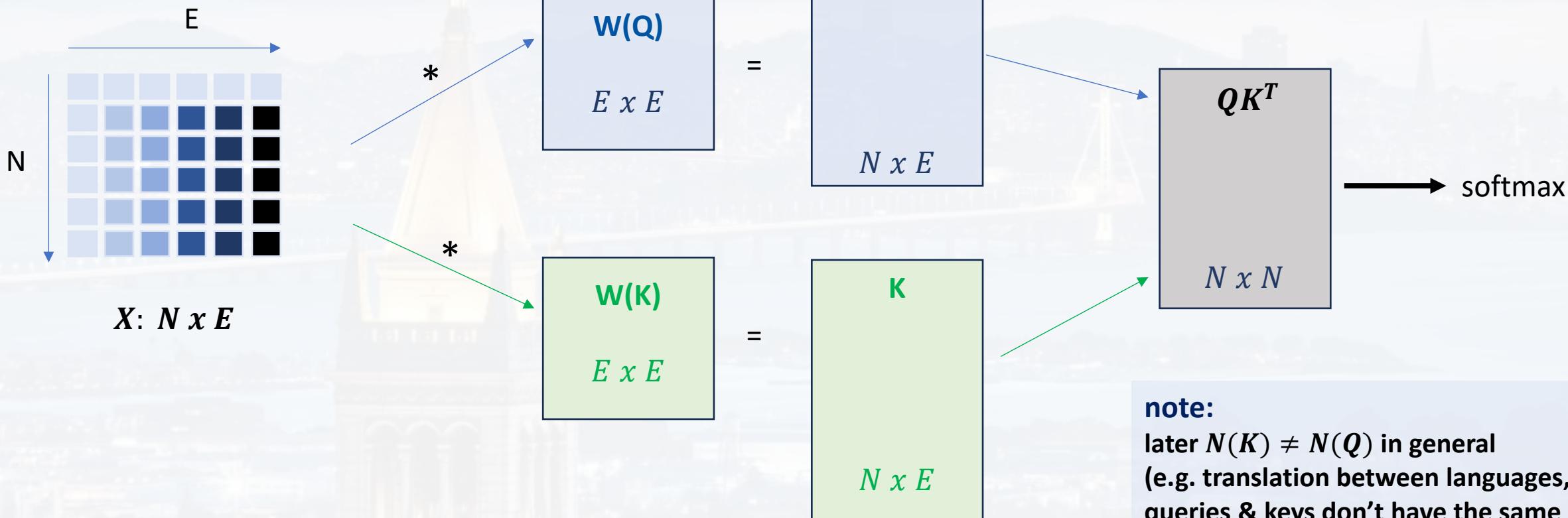
$$w_{nm} = \frac{\exp(X_n W(K) \circ X_m W(Q))}{\sum_{\mu=1}^N \exp(X_n W(K) \circ X_\mu W(Q))}$$

N: number of token

E: number of embedding dimensions

output: $Y_n = \sum_{m=1}^N w_{nm} X_m$

"Boring love story, plays on a ship in the past"



note:

later $N(K) \neq N(Q)$ in general
(e.g. translation between languages,
queries & keys don't have the same
number of tokens in general etc)



self attention

key value query

$$w_{nm} = \frac{\exp(\mathbf{X}_n \mathbf{W}(K) \circ \mathbf{X}_m \mathbf{W}(Q))}{\sum_{\mu=1}^N \exp(\mathbf{X}_n \mathbf{W}(K) \circ \mathbf{X}_{\mu} \mathbf{W}(Q))}$$

N: number of token

E: number of embedding dimensions

output: $Y_n = \sum_{m=1}^N w_{nm} X_m = \sum_{m=1}^N \frac{\exp(\mathbf{X}_n \mathbf{W}(K) \circ \mathbf{X}_m \mathbf{W}(Q))}{\sum_{\mu=1}^N \exp(\mathbf{X}_n \mathbf{W}(K) \circ \mathbf{X}_{\mu} \mathbf{W}(Q))} X_m$

$$= \sum_{m=1}^N \text{softmax}(\mathbf{Q}\mathbf{K}^T) X_m$$

$$\rightarrow \sum_{m=1}^N \text{softmax}(\mathbf{Q}\mathbf{K}^T) X_m \mathbf{W}(V) = \sum_{m=1}^N \text{softmax}(\mathbf{Q}\mathbf{K}^T) \mathbf{V}$$



value

summarizing the characteristics of the movie by using the movie itself

The output would be a movie, generated by weighted contributions of those movies (values), where the keys match well with the query



self attention

key value query

$$w_{nm} = \frac{\exp(\mathbf{X}_n \mathbf{W}(K) \circ \mathbf{X}_m \mathbf{W}(Q))}{\sum_{\mu=1}^N \exp(\mathbf{X}_n \mathbf{W}(K) \circ \mathbf{X}_{\mu} \mathbf{W}(Q))}$$

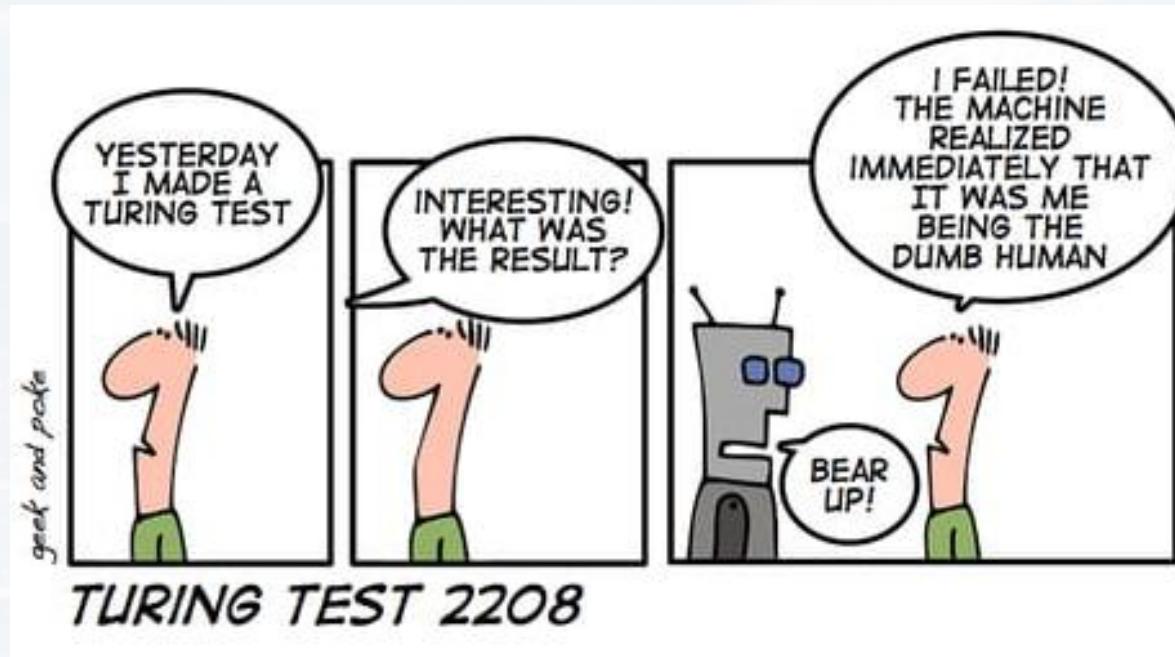
N: number of token

E: number of embedding dimensions

output: $Y_n = \sum_{m=1}^N w_{nm} X_m \rightarrow \sum_{m=1}^N \text{softmax}(\mathbf{Q}\mathbf{K}^T) X_m \mathbf{W}(V) = \sum_{m=1}^N \text{softmax}(\mathbf{Q}\mathbf{K}^T) \mathbf{V}$

note:

- dot product scales with E , therefore normalization: $\text{softmax}\left(\frac{\mathbf{Q}\mathbf{K}^T}{\sqrt{E}}\right)$
- cross attention:
 - eg. key a phrase in language A, query in language B
 - **encoder/decoder** structure, see next slides
- we want to recognize many underlying pattern → **multiple attention** layers in parallel → transformer



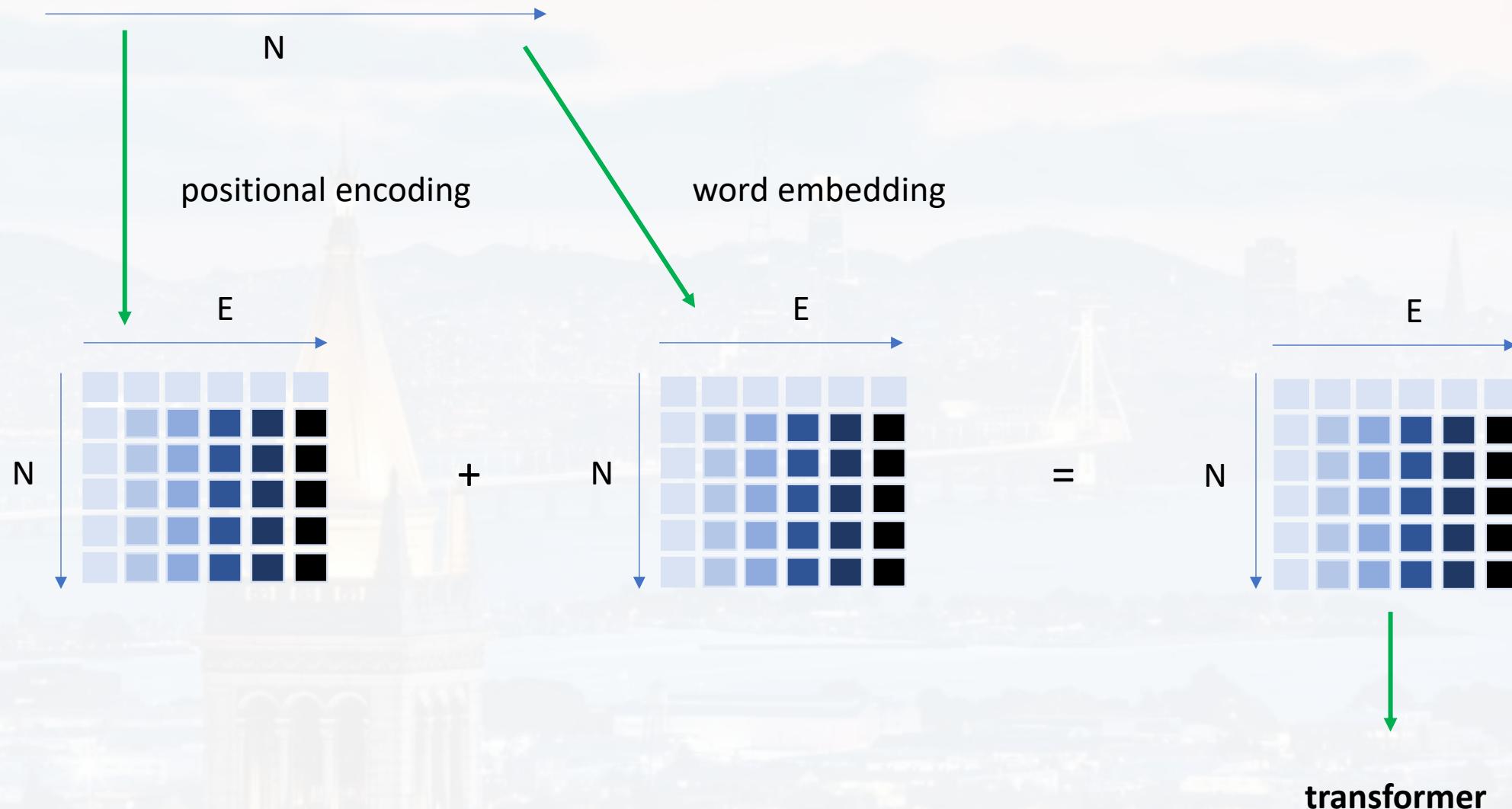
Outline

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



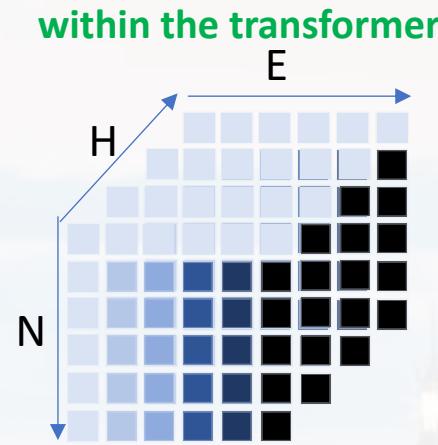
"The cat jumped on the roof."

N: number of token
E: number of embedding dimensions





attention:



$$* \quad \begin{matrix} \text{W(Q)} \\ \text{E} \\ \text{W(K)} \end{matrix}$$

$$= \quad \begin{matrix} \text{Q} \\ \text{N} \\ \text{H} \\ \text{K} \end{matrix}$$

query

$$* \quad \begin{matrix} \text{W(V)} \\ \text{E} \\ \text{H} \end{matrix}$$

$$= \quad \begin{matrix} \text{M} \\ \text{N} \\ \text{H} \\ \text{V} \end{matrix}$$

key

$$* \quad \begin{matrix} \text{M} \\ \text{E} \\ \text{H} \end{matrix}$$

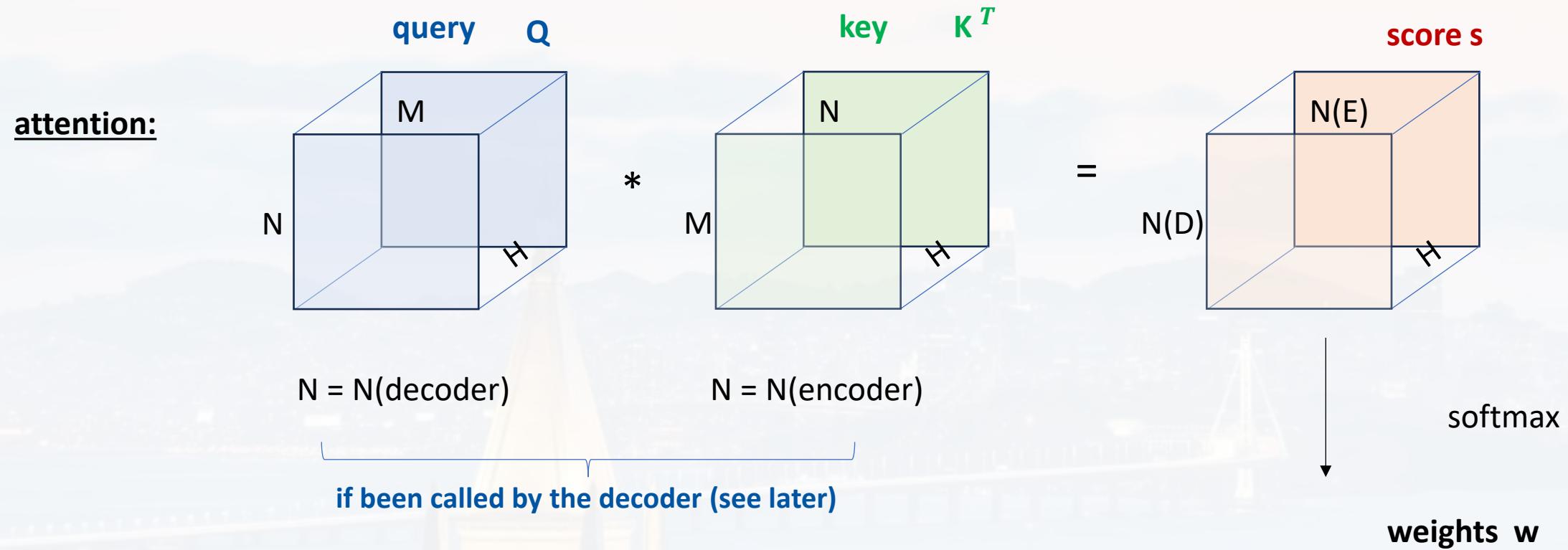
$$= \quad \begin{matrix} \text{M} \\ \text{N} \\ \text{H} \\ \text{value} \end{matrix}$$

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)

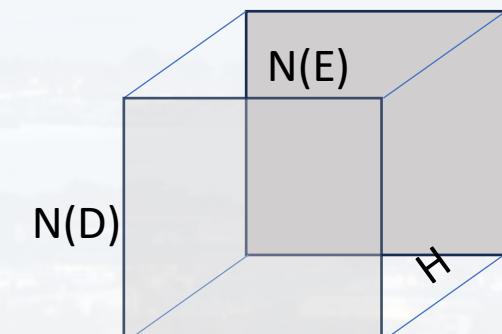


within the transformer:



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

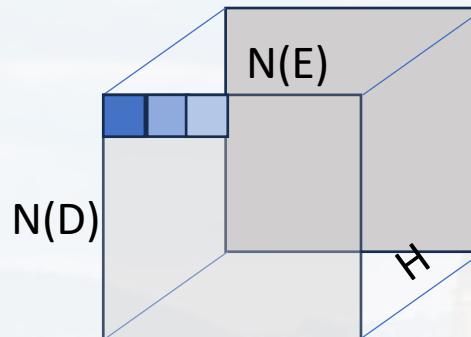
- N: number of token
- E: number of embedding dimensions
- H: number of heads (= 8)
- M: head size (= 64)





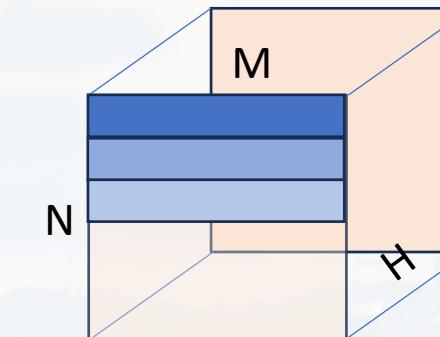
within the transformer:

weights w



attention:

value v



N:

number of token

E:

number of embedding dimensions

H:

number of heads (= 8)

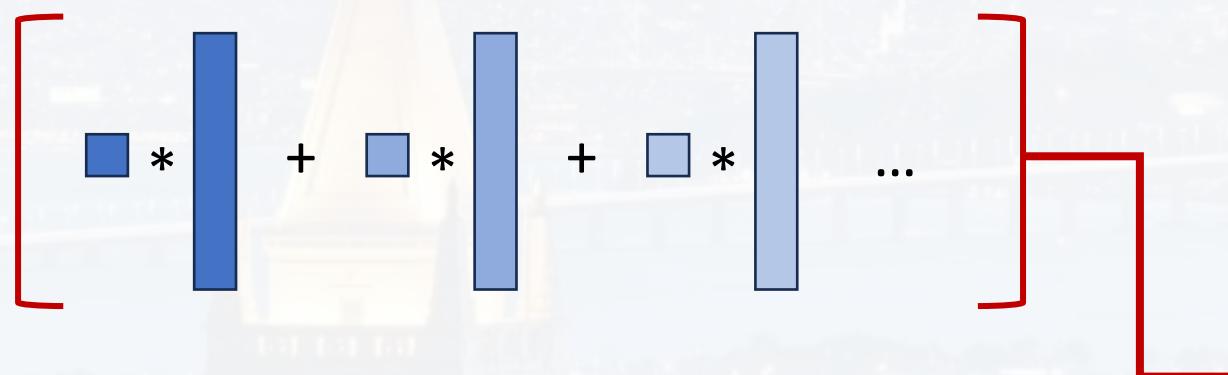
M:

head size (= 64)

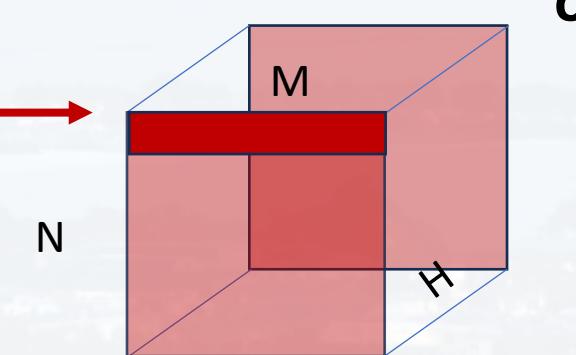
N(E)
N(D)

= N(encoder)

= N(decoder) , [see later](#)



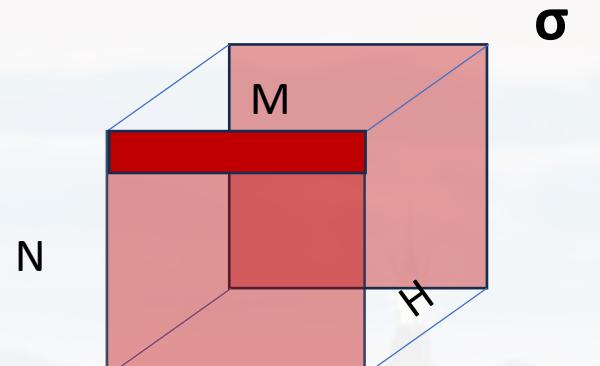
$$\sigma[i,:,k] = \sum_j w[i,j,k] * v[j,:,k]$$



σ



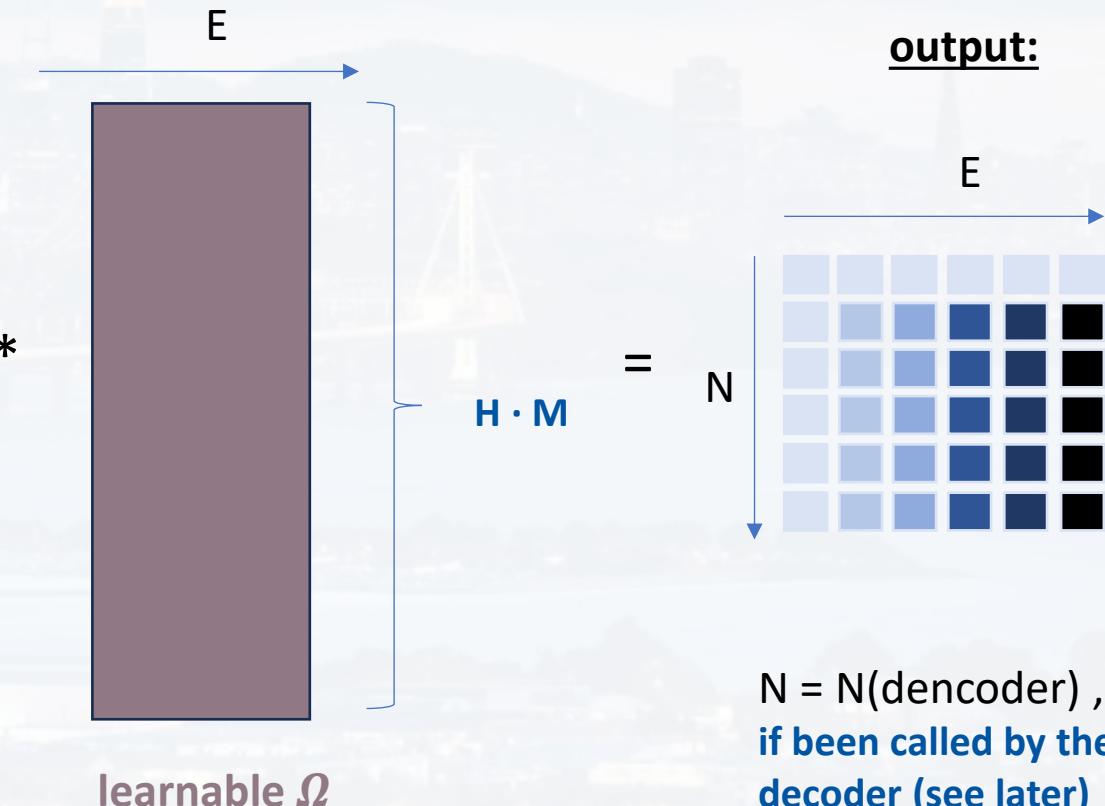
within the transformer:



concatenating σ

$$\sigma_{con} = [\sigma[:, :, 0] | \sigma[:, :, 1] | \dots | \sigma[:, :, H]]$$

The output is a sequence of $H \cdot M$ columns, indicated by a bracket under the concatenated rows.



$N = N(\text{decoder})$,
if been called by the
decoder (see later)

N:	number of token
E:	number of embedding dimensions
H:	number of heads (= 8)
M:	head size (= 64)

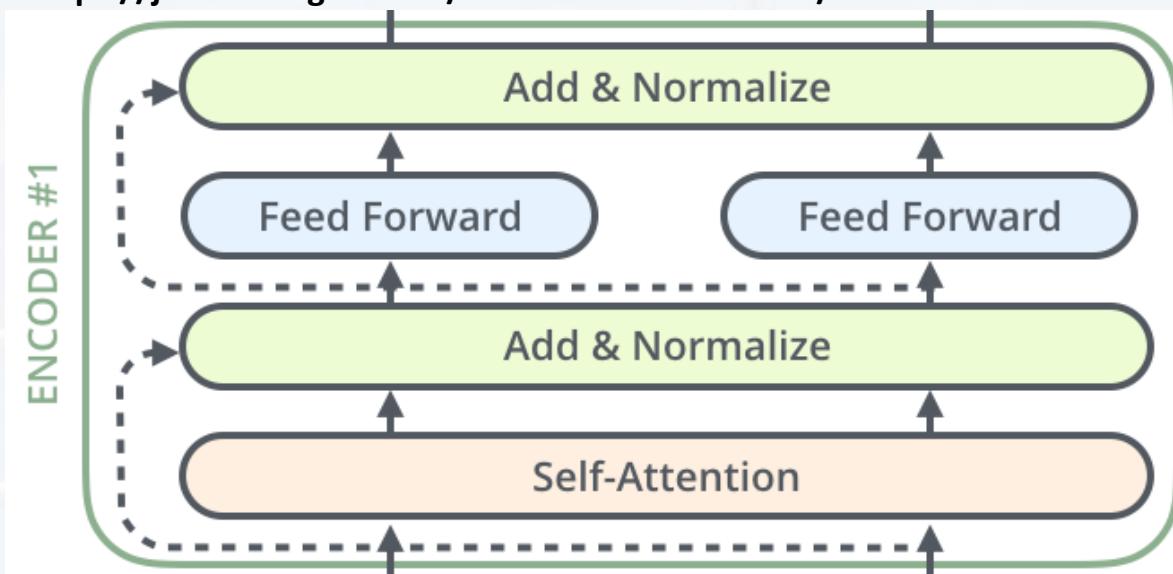


Berkeley LLM & Transformer:

Transformer Architecture

that was attention → now: encoder

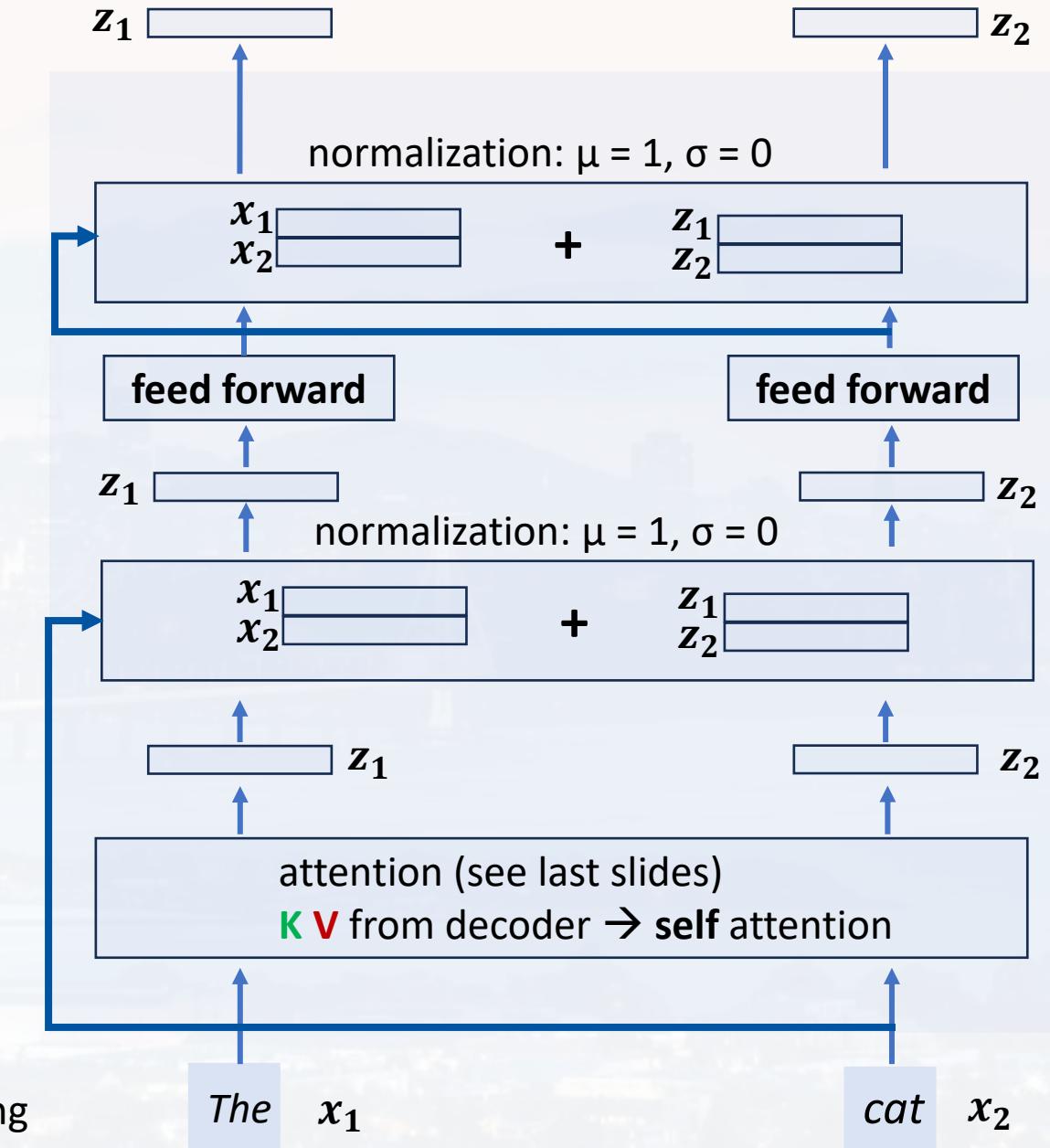
<https://jalammar.github.io/illustrated-transformer/>



positional encoding

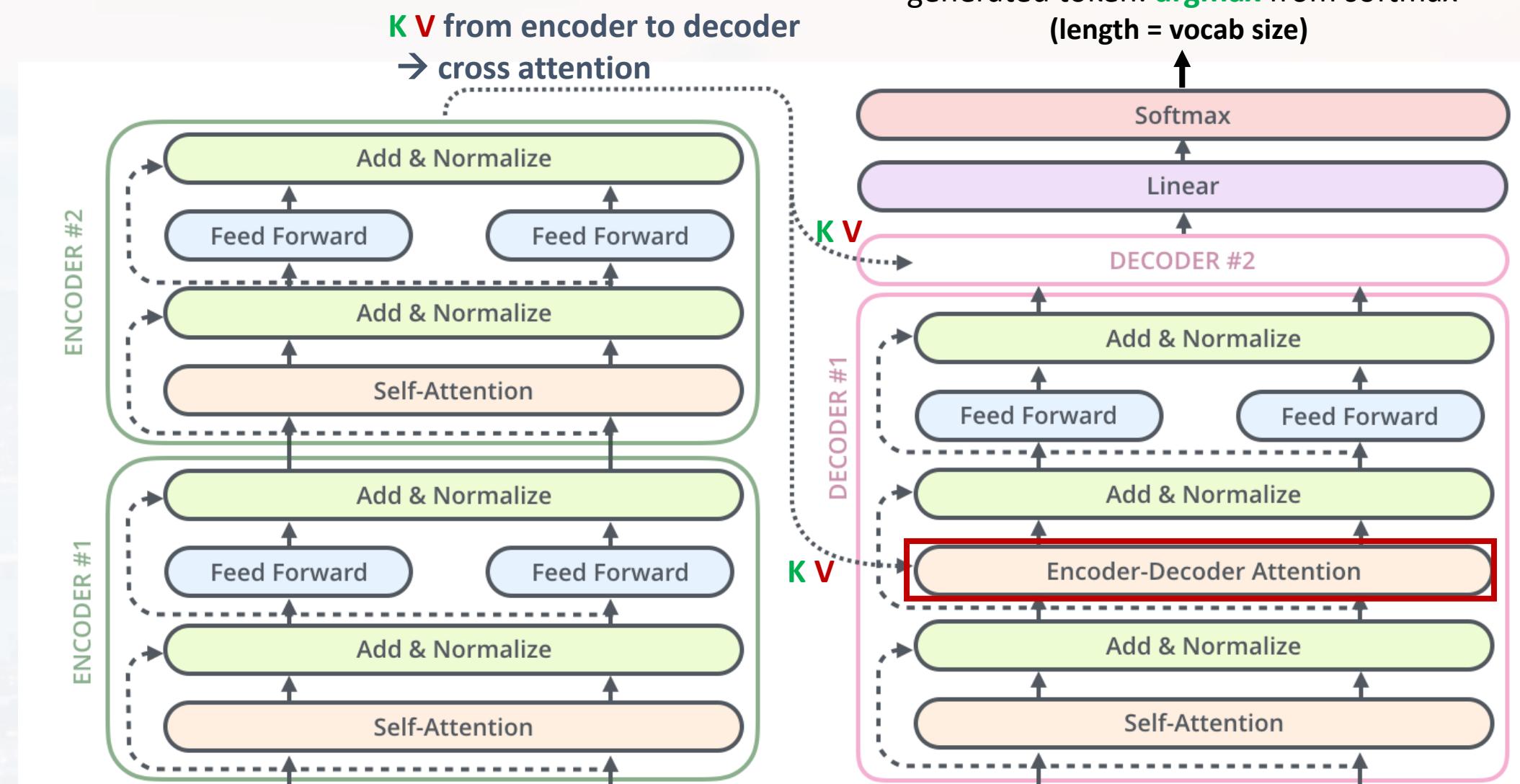
+

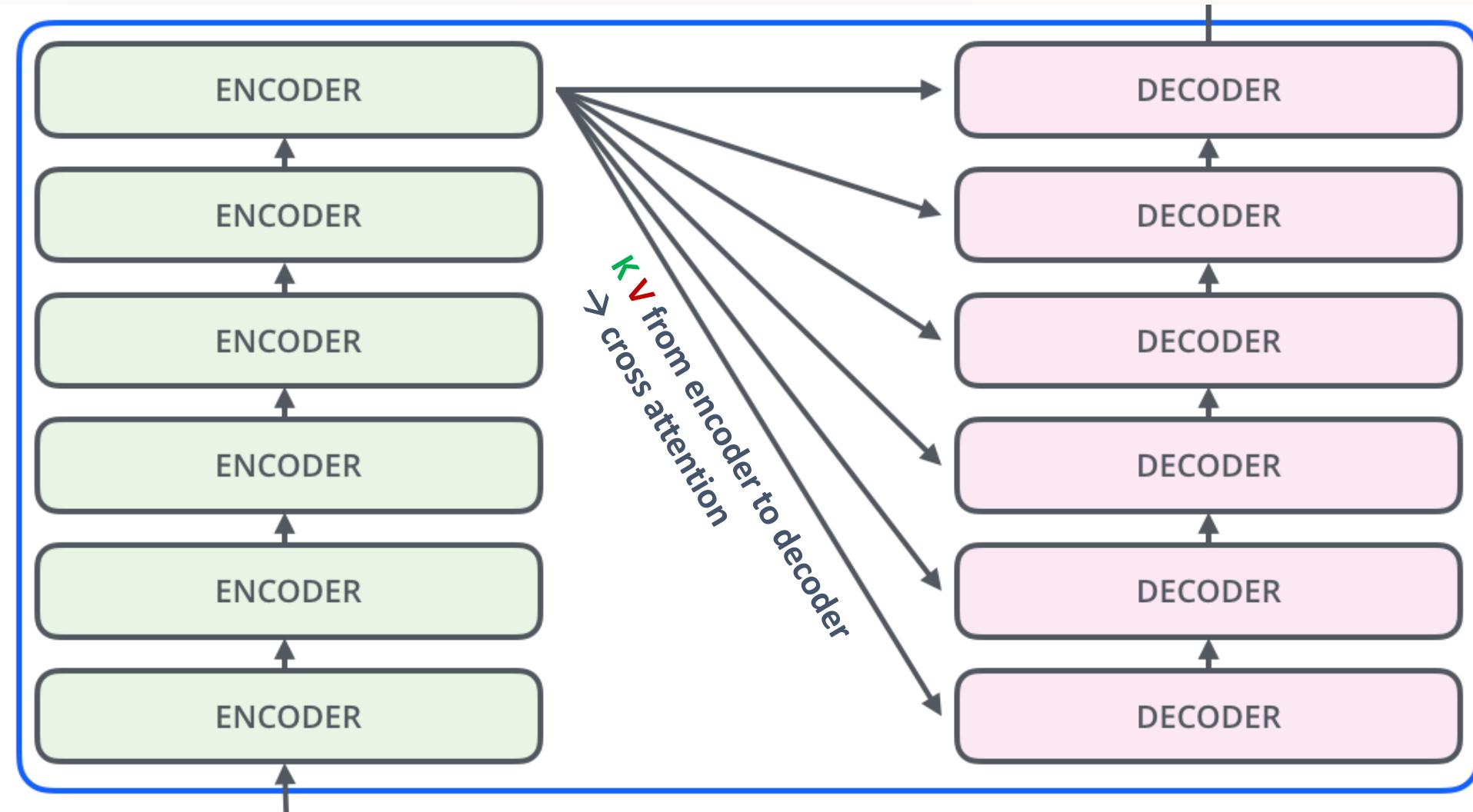
word embedding



The x_1

cat x_2

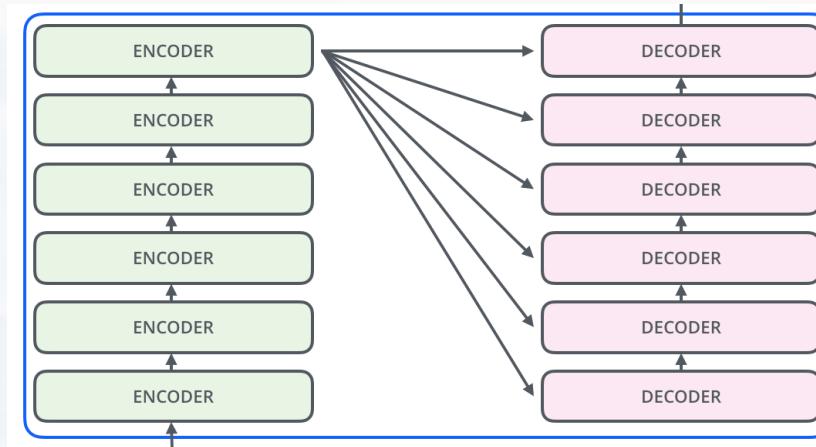






K V from encoder to decoder

→ cross attention



general: $N(E) \neq N(D)$

English: Let there be light.

$$N(E) = 4$$

German: Es werde Licht.

$$N(D) = 3$$

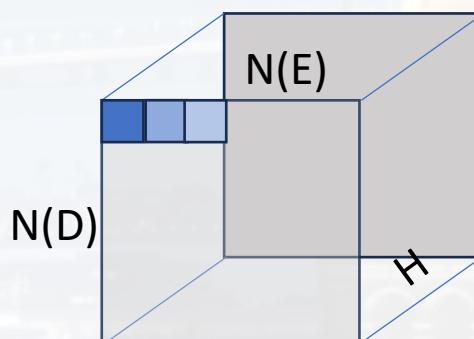
Latin: Fiat lux.

$$N(D) = 2$$

Hebrew: yehi, or

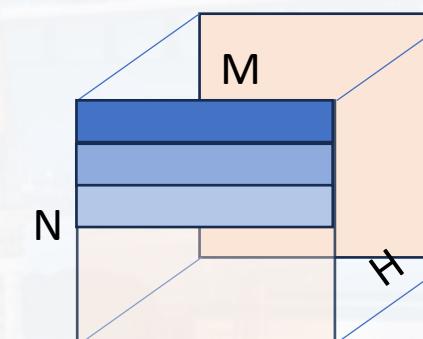
$$N(D) = 2$$

weights w

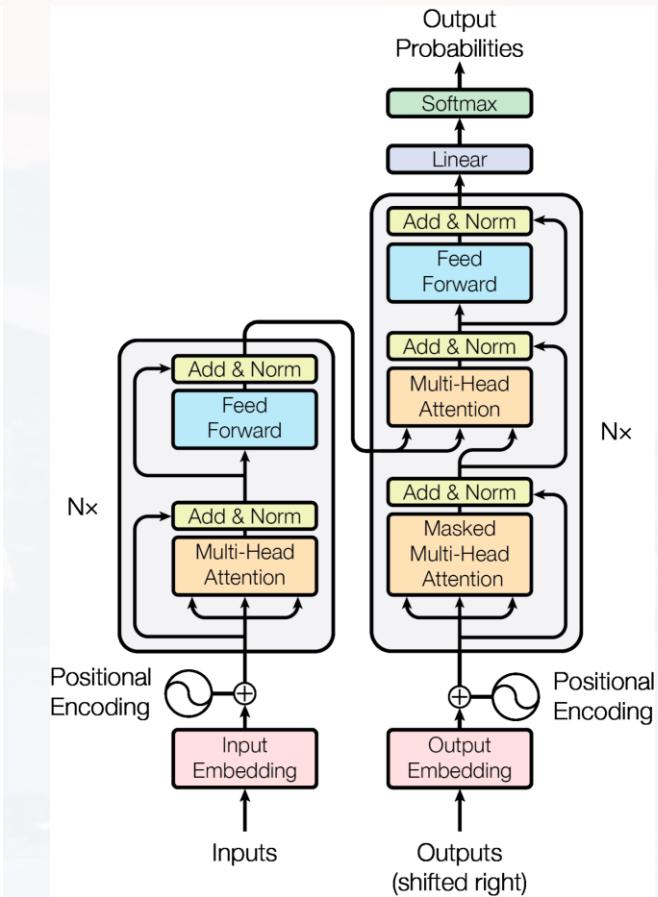
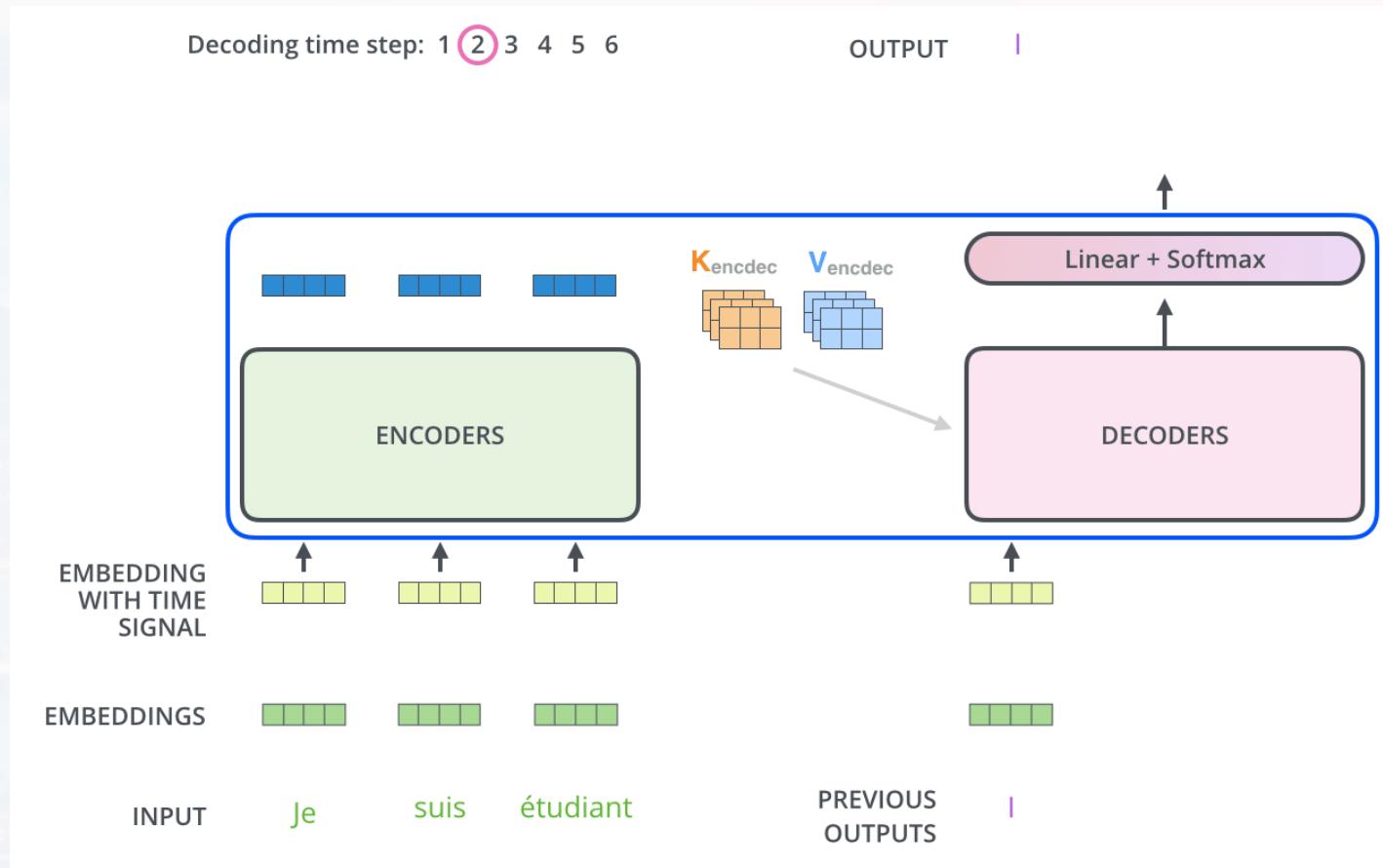


attention:

value V



$N = N(\text{encoder})$, if been called by the decoder





more about transformers:

[Jay Alammar](#)

[Interactive Visualization](#)

[transformers intro](#)



Misra Turp

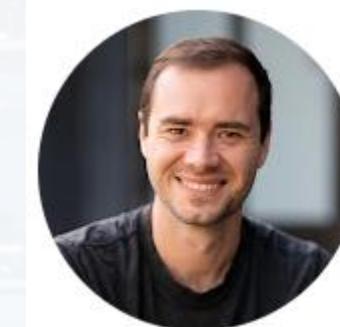
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Thank you very much for your

