Title: Transformers

Speakers: Mohamed Hibat Allah

Collection: Navigating Quantum and AI Career Trajectories: A Beginnerâ€™s Mini-Course on Computational Methods and their Applications

Date: May 24, 2024 - 9:30 AM

URL: https://pirsa.org/24050087

Lecture 3: Transformers

Energy-based model (Intractable)

Last time:

"Generative modeling"

Restricted Boltzmann Machines (RBM)

Recurrent Neural Networks (RNN) } Auto… (Trac…

Transformers

Other architectures (Not covered in this mini-cour…

Outline:

1. Attention mechanism
2. Transformer architecture
3. Transformer Wave function

① Attention mechanism:

Most famous paper:

"Attention is All you need"

Vaswani et. al (2017)

* Why it's interesting?

→ Enabled state of the art results in Natural Language processing (NLP)

→ Transformer is the basic building block of ChatGPT, GPT4, GPT4o

GPT = Generative Pre-trained Transformer.

based on the "attention" mechanism

→ Other architectures (Not covered in this ...)

$$\vec{X} = (x_1, x_2, \ldots, x_N)$$

$x_i \in 0, 1$

Query: $[d_k]$ $\vec{q}_i \equiv \vec{x}_i \, W^{(Q)}$

Key: $\vec{K}_i \equiv \vec{x}_i \, W^{(K)}$ $\rightarrow [d_e \times d_k]$

Value: $\vec{V}_i \equiv \vec{x}_i \, W^{(V)}$

Embedding of x_i: $\vec{x}_i = \begin{pmatrix} \vdots \end{pmatrix} \Big\} d_e$

"↓" $\rightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

"↑" $\rightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

Example of Youtube

↳ Query: Text on search bar.

↳ Key: Videos, titles & descriptions

↳ Value: Best video matches.

→ We can use $\vec{q}_i, \vec{K}_i, \vec{v}_i$ to compute self-attention.

$$\vec{A}_i = \sum_{j=1}^{N} \underbrace{\alpha\left(\vec{q}_i , \vec{K}_j^{\dagger}\right)}_{\text{“Correlation between site “}i\text{” and “}j\text{””}} \cdot \vec{v}_j$$

Solves the vanishing gradient problem in RNNs

Attention that has information about the most relevant « x_j »$_{j=1}^{N}$ on “x_i”

“Attention of x_i on x_j”

d_e

attention mechanism

« I live in France, hence I speak French »

i

$$\alpha(\vec{q}_i, K_j^T) = \mathrm{Softmax}\left(\frac{\vec{q}_i \cdot \vec{K}^T}{\sqrt{d_k}}\right)_j$$

$$\begin{pmatrix} \vec{K}_1 \\ \vec{K}_2 \\ \vdots \\ \vec{K}_N \end{pmatrix}$$

For normalization purposes

$$\sum_{j=1}^{N} \alpha(\vec{q}_i, \vec{K}_j^T) = 1$$

$$\vec{q}_i \cdot \vec{K}_j \in \mathbb{R}$$

$$\vec{q}_i \cdot K = \begin{pmatrix} \vdots \\ \vdots \end{pmatrix} \updownarrow N$$

mechanism

“I live in France, hence I speak French”

i

$$\sum_{j=1}^{N} \alpha(\vec{q}_i, \vec{K}_j^{\dagger}) = 1$$

$$\begin{pmatrix} \vec{K}_1 \\ \vec{K}_2 \\ \vdots \\ \vec{K}_N \end{pmatrix}$$

$$\vec{q}_i \cdot \vec{K}_j \in \mathbb{R}$$

$$\alpha(\vec{q}_i, K_j^{\dagger}) = \mathrm{Softmax}\left(\frac{\vec{q}_i \cdot \vec{K}^{\dagger}}{\sqrt{d_K}}\right)_j$$

$$\vec{q}_i \cdot \vec{K} = \begin{pmatrix} \vdots \\ \vdots \end{pmatrix} \Big\updownarrow N$$

For normalization purposes.

For normalization purposes

$$\vec{A}_i = \sum_{j=1}^{N} \mathrm{Softmax}\left(\frac{\vec{q}_i \cdot K^T}{\sqrt{d_k}}\right)_j \vec{v}_j$$

$[d_k]$

$$A = \underbrace{\mathrm{Softmax}\left(\frac{Q \cdot K^T}{\sqrt{d_k}}\right)}_{N \times N} \cdot V$$

$[N \times d_k]$

Takes advantage of GPU parallelization power

↳ Value : Best video matches.

* Positional encoding

$$\vec{X} = \overset{x_1}{\text{I}}\text{'}\overset{x_2}{\text{m}}\ \overset{x_3}{\text{not}}\ \overset{x_4}{\text{sad}},\ \overset{x_5}{\text{I}}\text{'m}\ \overset{x_6}{\text{happy}}.$$

$$\vec{X} = \text{I'm not happy, I'm sad}$$

Idea $\quad \vec{x}_i + \underbrace{\vec{PE}(i)}_{[d_e]} \longrightarrow \vec{x}_i'$

on "x_i"

$$\vec{PE}(i)_{2j} = \sin\left(\frac{i}{10000^{2j/d_e}}\right)$$

$$\vec{PE}(i)_{2j+1} = \cos\left(\frac{i}{\underbrace{10000}_{\text{Max sequence length}}{}^{2j/d_e}}\right)$$

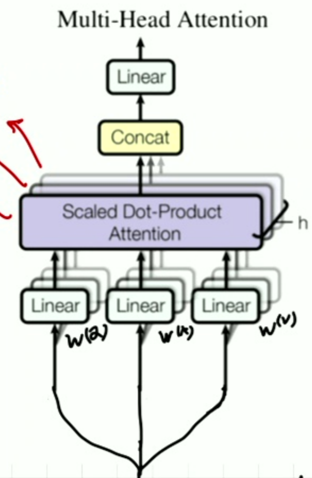
↳ Nearby positions have similar PE at particular component "k"

↳ Each component of the PE has a different wavelength → Short - long range dependencies.

* **Multi-head Attention:** allows to learn attention about different features

A^μ
Q^μ
K^μ
V^μ
← New index $\mu = 1 \to h$

A^1 A^2 A^3



different self-attentions

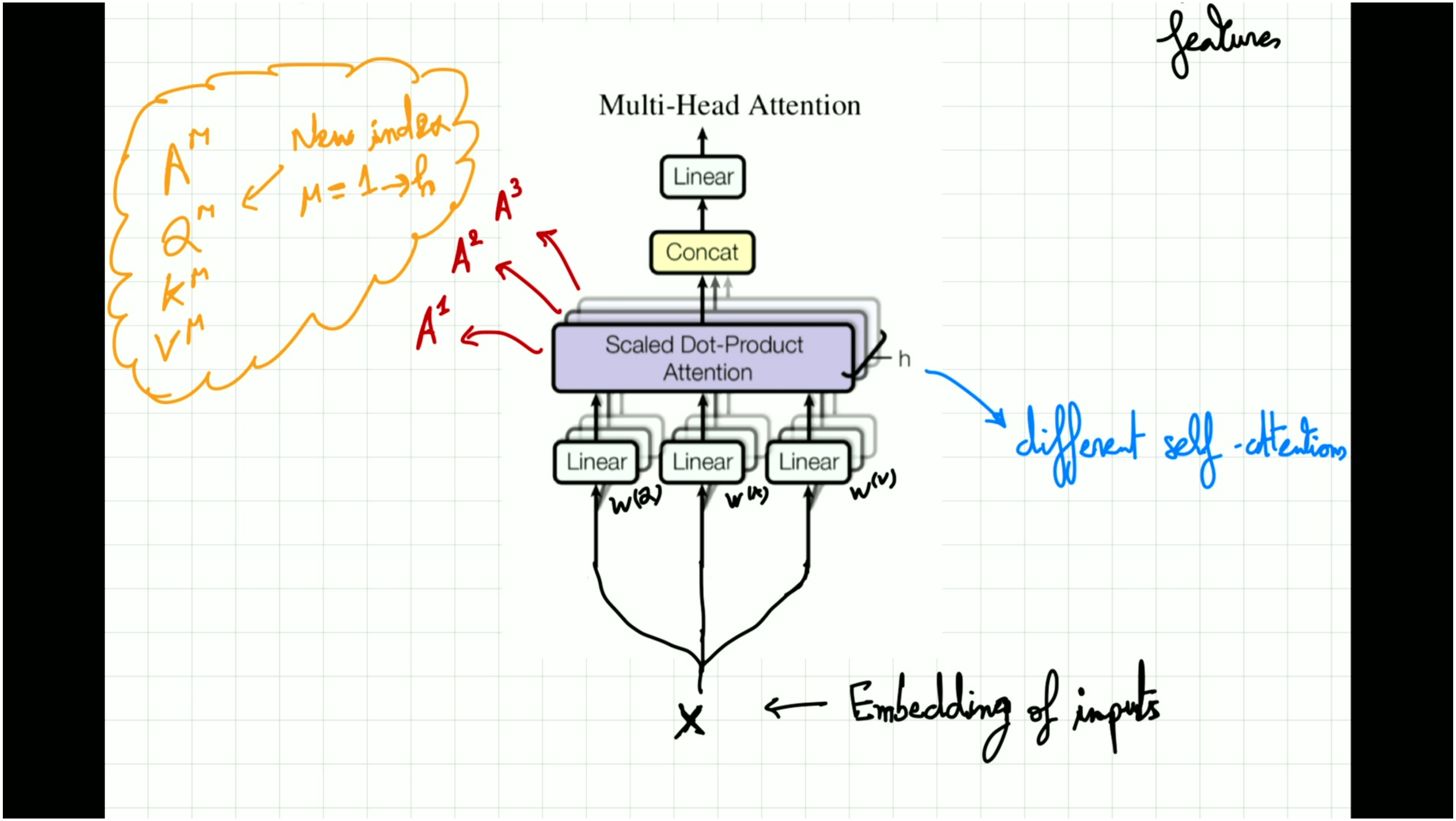
X ← Embedding of inputs

Example: Group of people ⟶ Character, Job, Age, Gender...

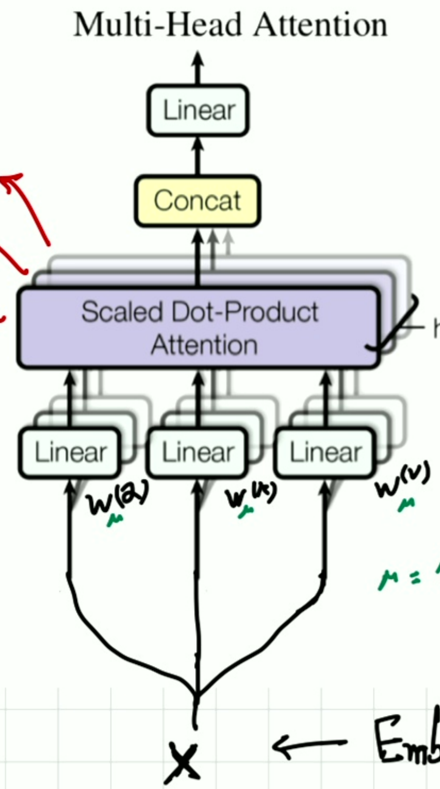
Spins ⟶ Correlation, magnetization, ...

In equation:

$$\text{Multi head Attention} = \text{Concat}(A^1, A^2, \dots, A^h)\, W^{(O)},$$


features
Multi-Head Attention
Linear
Concat
Scaled Dot-Product Attention
h
Linear
Linear
Linear
$W^{(Q)}$
$W^{(K)}$
$W^{(V)}$
A^1
A^2
A^3
A^μ
Q^μ
K^μ
V^μ
New index
$\mu = 1 \to h$
different self-attentions
X
Embedding of inputs

A^μ, Q^μ, K^μ, V^μ ← New index $\mu = 1 \to h$



A^1, A^2, A^3

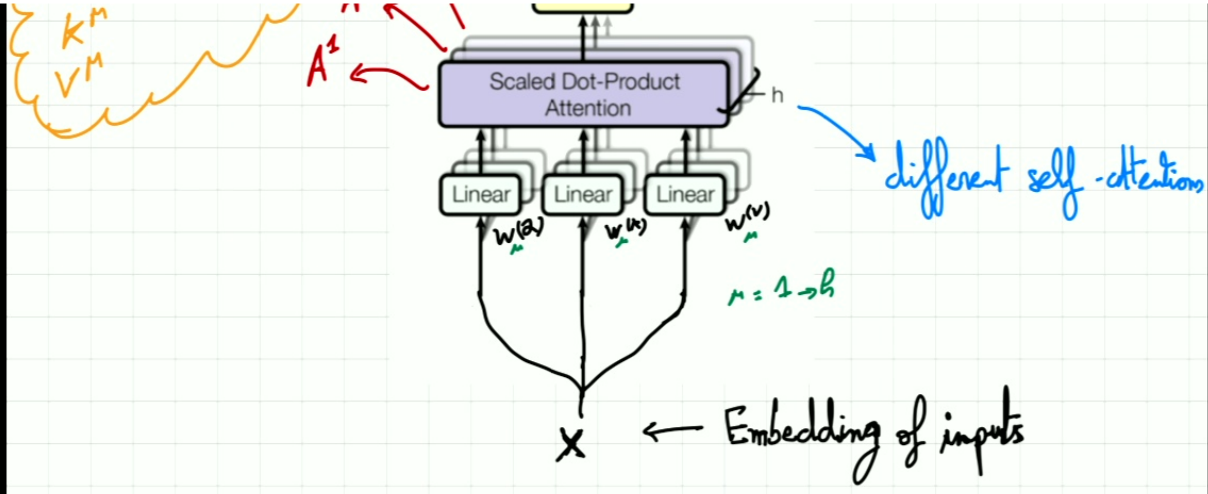
different self-attentions

$W^{(Q)}_\mu$ $W^{(K)}_\mu$ $W^{(V)}_\mu$

$\mu = 1 \to h$

X ← Embedding of inputs

Example: Group of people ⟶ Character, Job, Age, Gender...



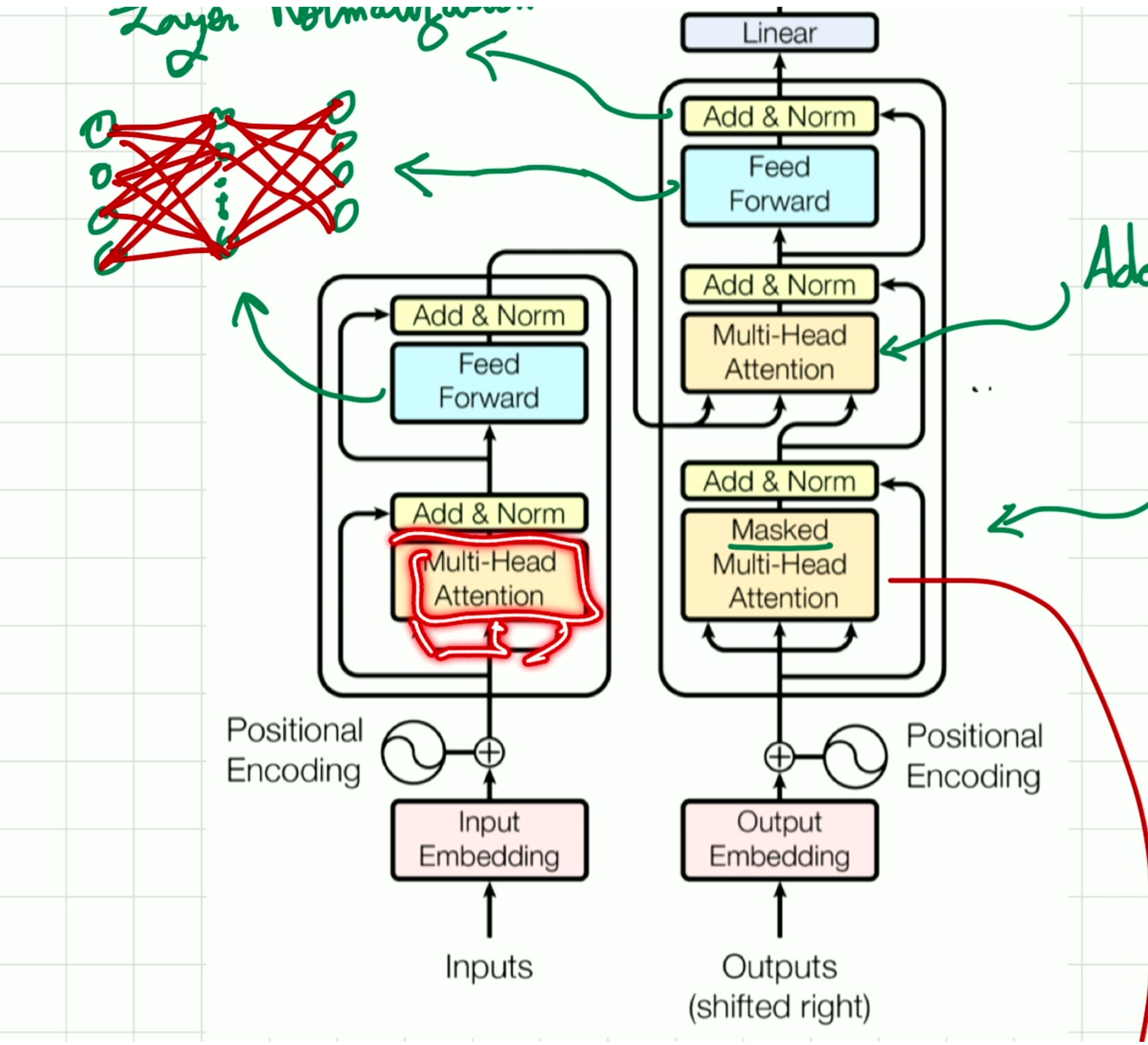
Example: Group of people ⟶ Character, Job, Age, Gender...

Spins ⟶ Correlation, magnetization, ...

In equation:

$$\text{Multi head Attention} = \text{Concat}\left(A^1, A^2, \ldots, A^h\right) W^{(0)}$$

Learnable weights



probability

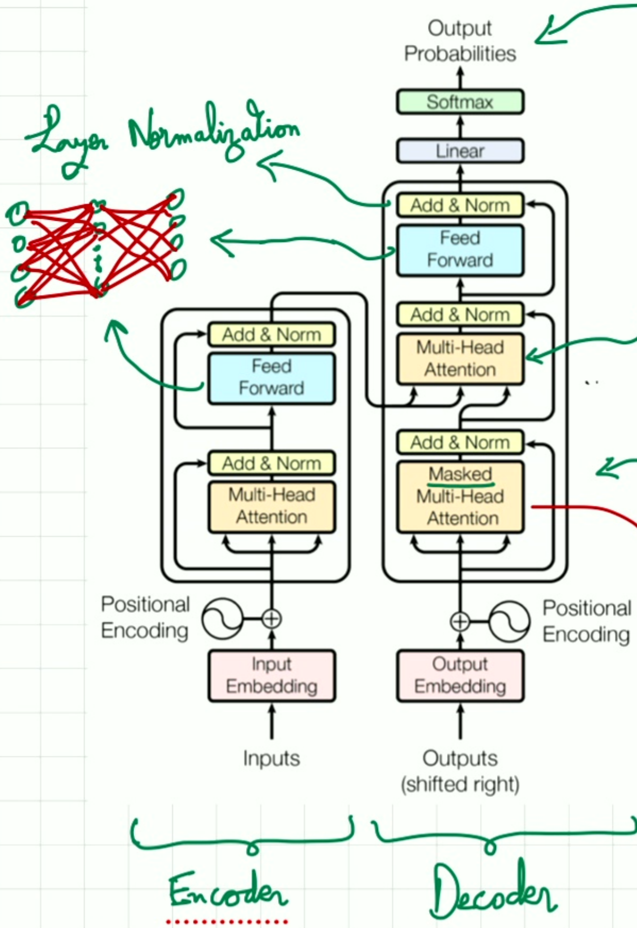
Adding Attention on inputs Y

At step i

Masking

$x_1, x_2, \ldots, x_i, \cancel{x_{i+1}}, \ldots, \cancel{x_N}$

$$\vec{A}_i = \sum_{j<i} \alpha\left(\vec{q}_i, \vec{k}_j^{\,t}\right) \cdot \vec{v}_j$$



Conditional probability

Input

Adding Attention on inputs Y

At step i

Masking

$$x_1, x_2, \dots, x_i, \cancel{x_{i+1}}, \dots, \cancel{x_N}$$

$$\vec{A}_i = \sum_{j<i} \alpha\left(\vec{q}_i, \vec{k}_j^{\,t}\right) \cdot \vec{v}_j$$

|GPT-3|

175 B parameters

$W^{(Q)}, W^{(K)}, W^{(V)}$

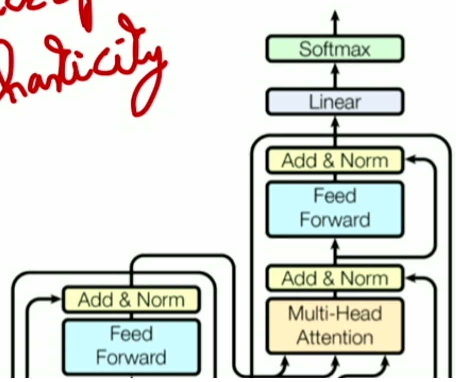
$W^{(O)}, \ldots$

96 Transformer layers

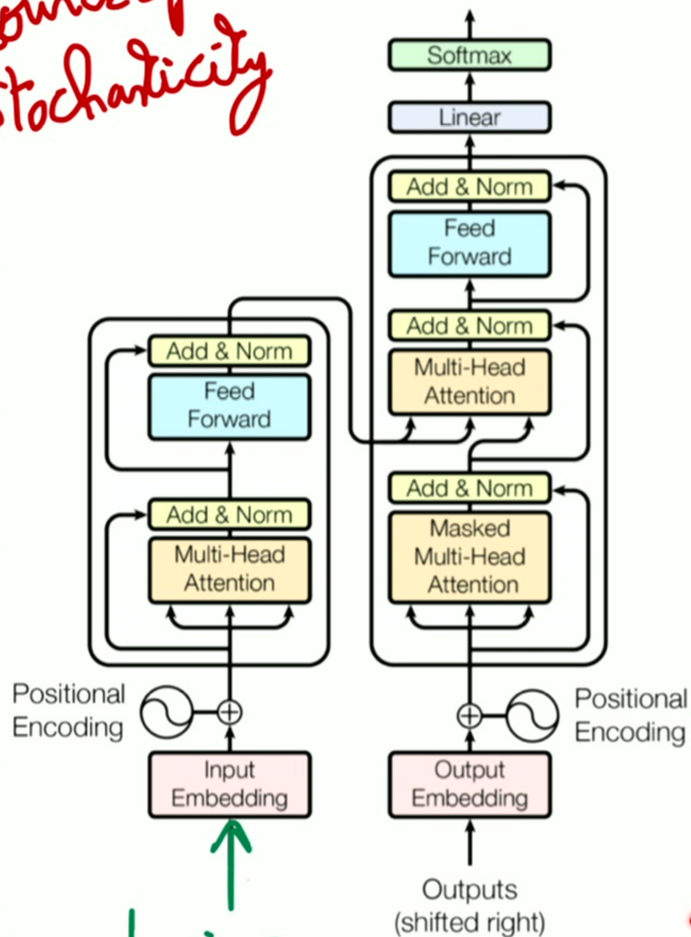
Training using massive Dataset D ~ 300 B words

Human feedback (Reward) to fine tune the parameters

Source of Stochasticity ← P(Next word | X)



Source of Stochasticity



Sentence beginning

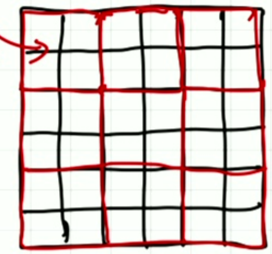
Human feedback (Reward) to fine tune the parameters

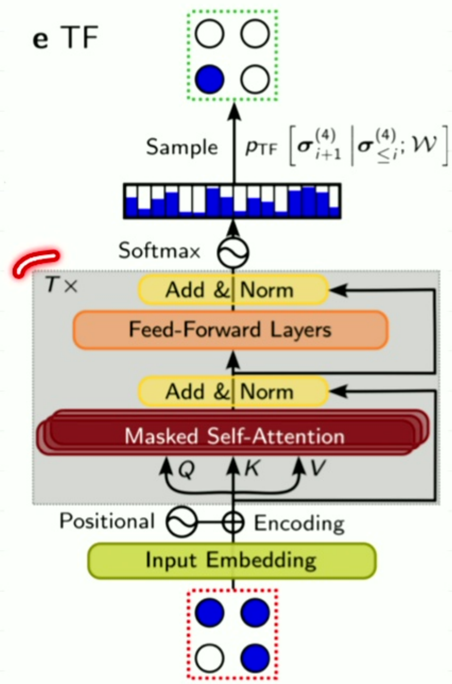
⚠ Training cost: ~ 4.6 million $ to train.

550 tons of CO_2 → Climate Change

(3) Transformer Wavefunctions

Patch
eg: 4 spins





$$\Psi_{TF}(\sigma_1, \sigma_2, \dots, \sigma_N)$$

$$= \sqrt{P_{TF}(\sigma_1, \sigma_2, \dots, \sigma_N)}$$

↳ For Stoquastic Hamiltonians

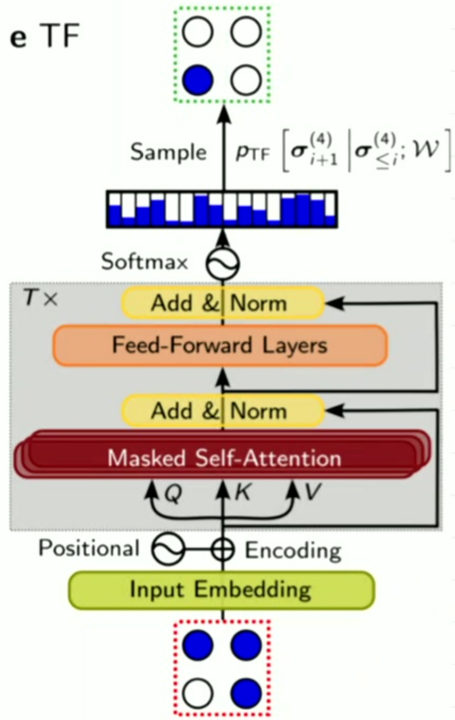
Cost function:

$$E = \langle \Psi_{TF} | \hat{H} | \Psi_{TF} \rangle$$

K. Sprague & S. Czischek, Comms Phys 2024

(3) Transformer Wavefunctions

Patch
eg: 4 spins



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$$= \sqrt{P_{TF}(\sigma_1, \sigma_2, \dots, \sigma_N)}$$

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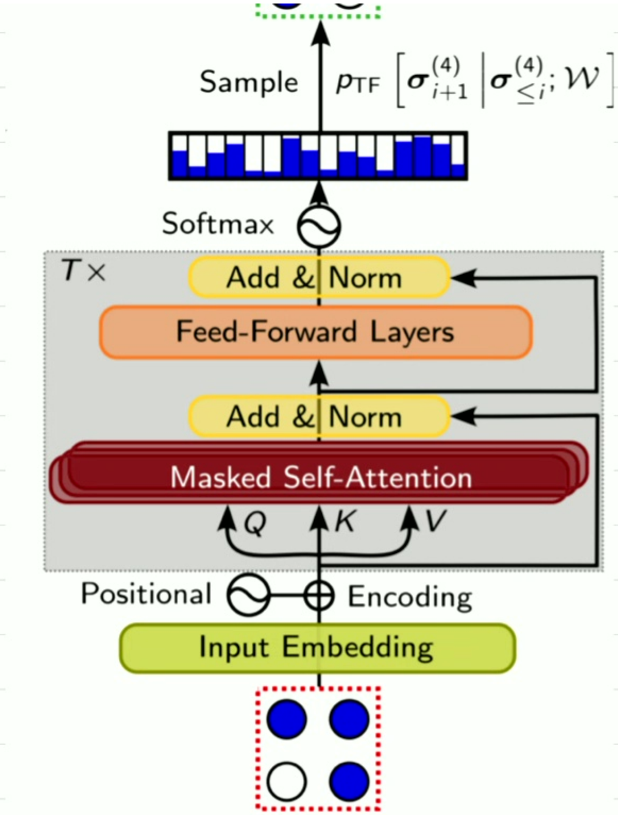


$$\Psi_{TF}(\sigma_1, \sigma_2, \dots, \sigma_N) = \sqrt{P_{TF}(\sigma_1, \sigma_2, \dots, \sigma_N)}$$

For Stoquastic Hamiltonians

Cost function:

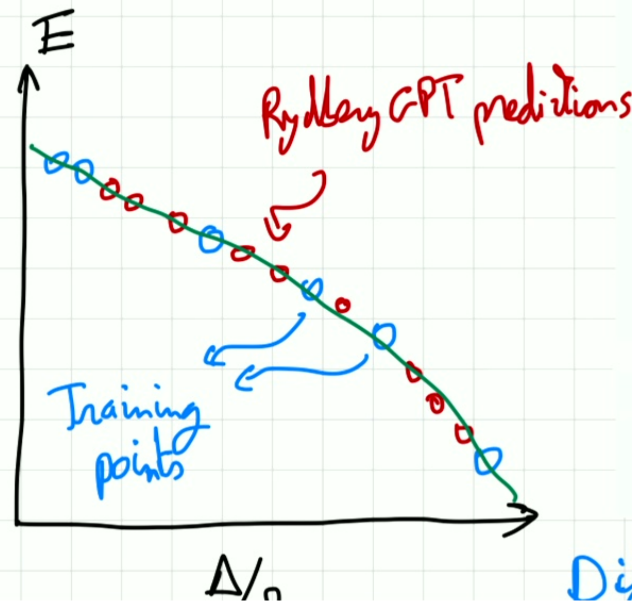
$$E = \langle \Psi_{TF} | \hat{H} | \Psi_{TF} \rangle$$

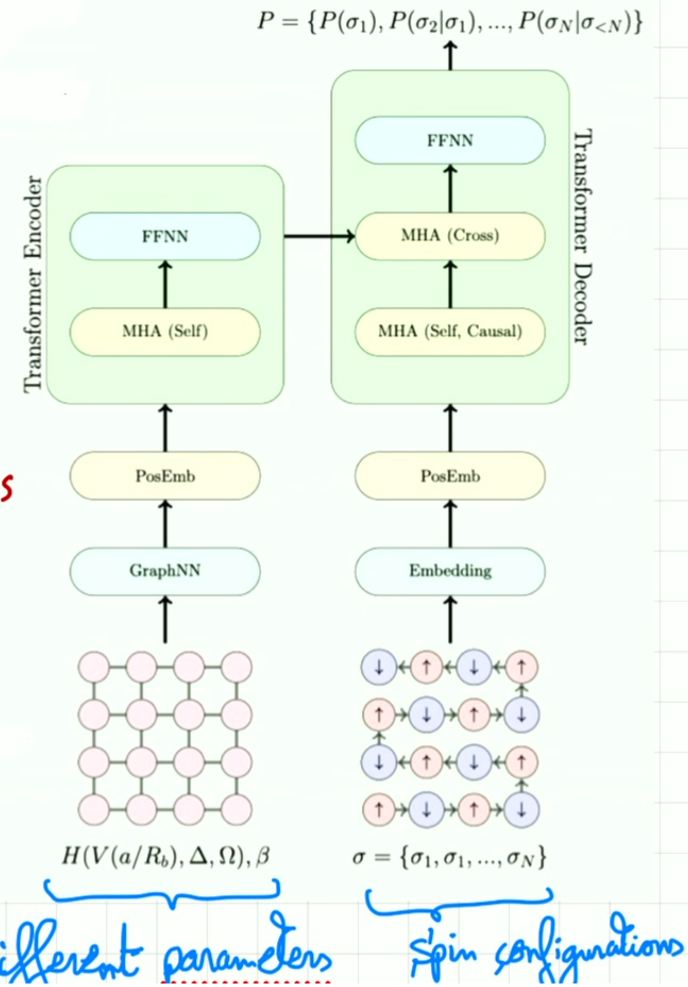
K. Sprague & S. Czischek, Comms Phys 2024

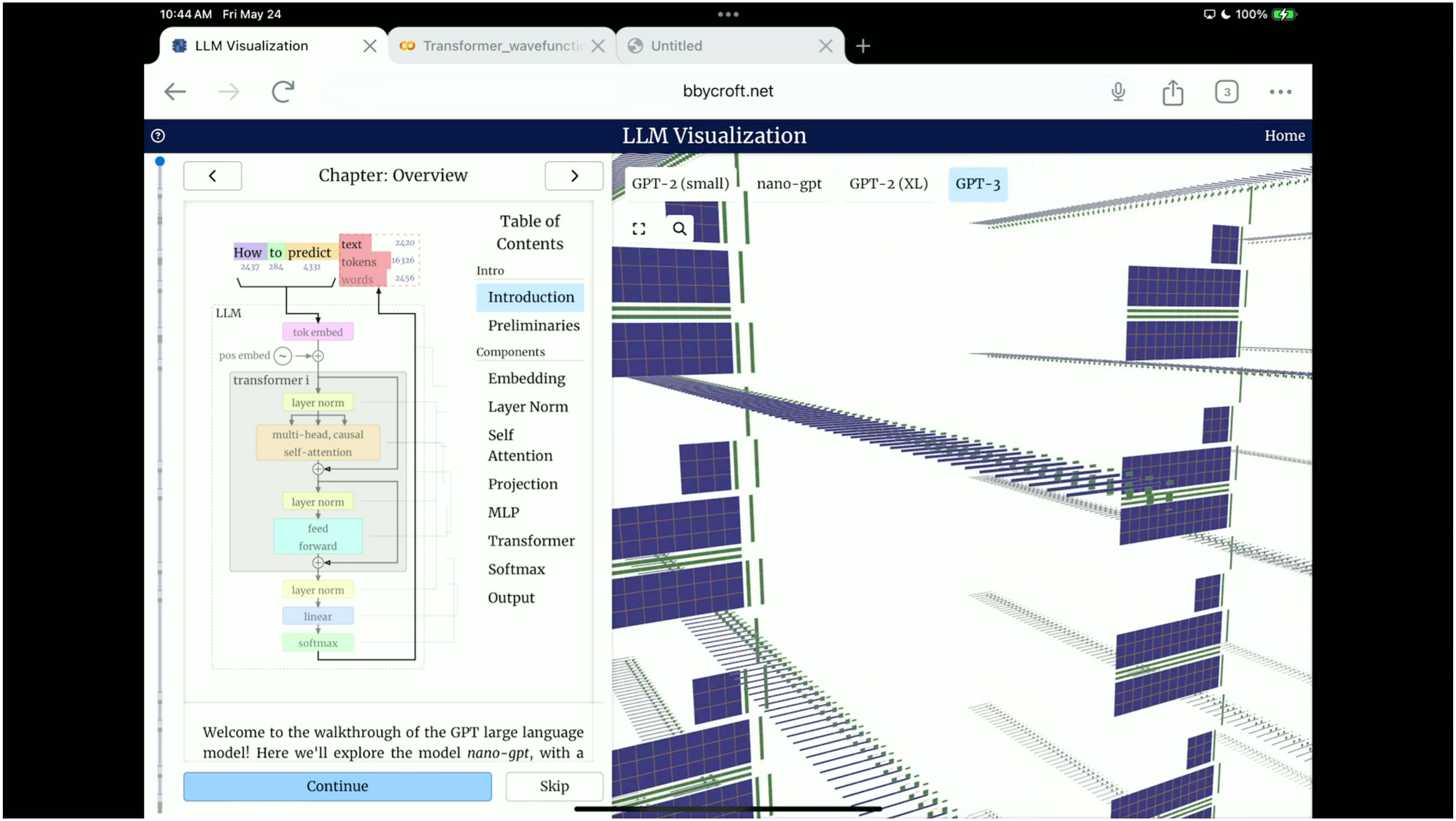
Another paper: "ArXiv: 2310.05715"

*Rydberg atoms Hamiltonian:

$$H = \Omega \sum_i \sigma_i^x - \Delta \sum_i n_i + \sum_{i<j} V_{ij} n_i n_j$$







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LLM Visualization
Transformer_wavefunctic
Untitled
bbycroft.net
LLM Visualization
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2437 284 4331
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tok embed
pos embed
transformer i
layer norm
multi-head, causal self-attention
layer norm
feed forward
layer norm
linear
softmax
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Welcome to the walkthrough of the GPT large language model! Here we'll explore the model *nano-gpt*, with a
Continue
Skip
GPT-2 (small)
nano-gpt
GPT-2 (XL)
GPT-3

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LLM Visualization | Transformer_wavefuncti | GitHub - APRIQuOt/VMC

colab.research.google.com

Transformer_wavefunctions_on_Rydberg_Hamiltonian_on_square_lattice.ipynb

Transformer wave functions

This notebook is based on code implemented on this repository: https://github.com/APRIQuOt/VMC_with_LPTFs based on this paper: https://www.nature.com/articles/s42005-024-01584-y

Cloning github repository:

```
!git clone https://github.com/mhibatallah/VMC_with_TF.git
```

```
Cloning into 'VMC_with_TF'...
remote: Enumerating objects: 96, done.
remote: Counting objects: 100% (96/96), done.
remote: Compressing objects: 100% (94/94), done.
remote: Total 96 (delta 45), reused 0 (delta 0), pack-reused 0
Receiving objects: 100% (96/96), 47.67 KiB | 185.00 KiB/s, done.
Resolving deltas: 100% (45/45), done.
```

Training Arguments:

```
L         (int)     -- Total lattice size (8x8 would be L=64).

    Q         (int)     -- Number of minibatches per batch.

    K         (int)     -- size of each minibatch.

    B         (int)     -- Total batch size (should be Q*K).

    NLOOPS    (int)     -- Number of loops within the off_diag_labels function. Higher values save ram and
                           generally makes the code run faster (up to 2x). Note, you can only set this
```

10:46 AM Fri May 24

LLM Visualization | Transformer_wavefuncti | GitHub - APRIQuOt/VMC

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roximate the gradients, more efficient but approximate.

he end of the output directory (inside a subfolder).

```
n L=16 steps=1000 --ptf patch=2x2 Nh=32 nhead=1 --rydberg V=7 delta=

tf', 'patch=2x2', 'Nh=32', 'nhead=1', '--rydberg', 'V=7', 'delta=1',
s/torch/nn/modules/transformer.py:306: UserWarning: enable_nested_te
 is True, but self.use_nested_tensor is False because {why_not_spars
          {'L': 16, 'Q': 1, 'K': 256, 'B': 256, 'NLOOPS': 1, 'steps'
          {'L': 16, 'patch': '2x2', 'Nh': 32, 'dropout': 0.0, 'num_l
          {'Lx': 4, 'Ly': 4, 'V': 7, 'Omega': 1, 'delta': 1, 'L': 16

077 , Transformer energy variance= 471.61472
```

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LLM Visualization | Transformer_wavefuncti | GitHub - APRIQuOt/VMC

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Transformer_wavefunctions_on_Rydberg_Hamiltonian_on_square_lattice.ipynb

```
1 !python VMC_with_TF/train.py --train L=16 steps=1000 --ptf patch=2x2 Nh=32 nhead=8 --rydberg V=7 delta=
```

```
['--train', 'L=16', 'steps=1000', '--ptf', 'patch=2x2', 'Nh=32', 'nhead=8', '--rydberg', 'V=7', 'delta=1', 'Omega=1']
/usr/local/lib/python3.10/dist-packages/torch/nn/modules/transformer.py:306: UserWarning: enable_nested_tensor is True, but self.use_
  warnings.warn(f"enable_nested_tensor is True, but self.use_nested_tensor is False because {why_not_sparsity_fast_path}")
train                                          {'L': 16, 'Q': 1, 'K': 256, 'B': 256, 'NLOOPS': 1, 'steps': 1000, 'dir': 'PTF', 'lr':
model                                          {'L': 16, 'patch': '2x2', 'Nh': 32, 'dropout': 0.0, 'num_layers': 2, 'nhead': 8, 'rep
hamiltonian                                    {'Lx': 4, 'Ly': 4, 'V': 7, 'Omega': 1, 'delta': 1, 'L': 16, 'name': 'RYDBERG'}

Output folder path established
Step : 0 , Transformer energy = 31.8925 , Transformer energy variance= 543.7189

Step : 50 , Transformer energy = 7.497976 , Transformer energy variance= 179.69516

Step : 100 , Transformer energy = -2.9836862 , Transformer energy variance= 35.55628

Step : 150 , Transformer energy = -5.044218 , Transformer energy variance= 19.876806

Step : 200 , Transformer energy = -6.4999714 , Transformer energy variance= 2.637269

Step : 250 , Transformer energy = -6.633377 , Transformer energy variance= 3.255067

Step : 300 , Transformer energy = -6.476509 , Transformer energy variance= 8.979716

Step : 350 , Transformer energy = -6.746655 , Transformer energy variance= 1.1118166

Step : 400 , Transformer energy = -6.842925 , Transformer energy variance= 1.4557284
```

```
[ ] 1 !python VMC_with_TF/train.py --train L=16 steps=1000 --ptf patch=2x2 Nh=128 nhead=8 --rydberg V=7 delta=1 Omega=1
```

Final Remarks:

* Complexity:

Computationally more expensive

* Regular Transformer: $\mathcal{O}(N^3)$ sampling, $\mathcal{O}(N^2)$ inference

* RNN: $\mathcal{O}(N)$ for sampling and inference

Linear transformers: $\mathcal{O}(N)$

One example: « Transformers are RNNs »

* The intersection of $\langle \text{NLP} \,|\, \text{Many body physics} \rangle$ is very promising.

Modern applications of machine learning in quantum sciences

Anna Dawid[1,2,3⋆], Julian Arnold[4†], Borja Requena[2†], Alexander Gresch[5,6†], Marcin Płodzień[2], Kaelan Donatella[7], Kim A. Nicoli[8,9], Paolo Stornati[2], Rouven Koch[10], Miriam Büttner[11], Robert Okuła[12,13], Gorka Muñoz–Gil[14], Rodrigo A. Vargas–Hernández[15,16,17], Alba Cervera-Lierta[18], Juan Carrasquilla[16], Vedran Dunjko[19], Marylou Gabrié[20], Patrick Huembeli[21,22], Evert van Nieuwenburg[19,23], Filippo Vicentini[21,24], Lei Wang[25,26], Sebastian J. Wetzel[27], Giuseppe Carleo[21], Eliška Greplová[28], Roman Krems[29], Florian Marquardt[30,31], Michał Tomza[1], Maciej Lewenstein[2,32] and Alexandre Dauphin[2,33⋆]