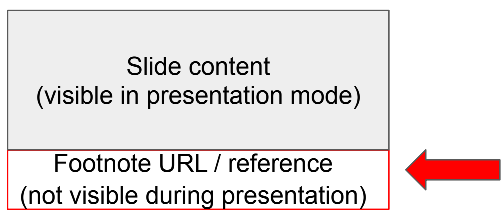
Transformers Workshop
Internals and Insights

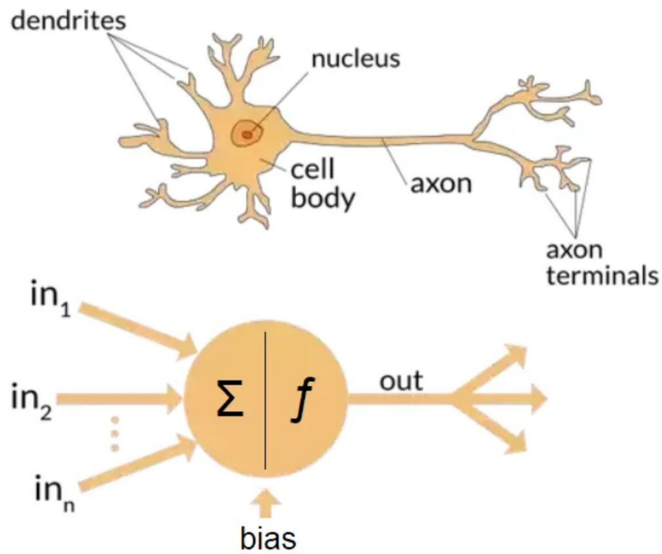
Caus Danu

Background

- This resource is intended to **explain Transformers** to a scientific audience.
- Transformers will be presented in the broader context of AI, so touching **different other relevant topics**.
- **I will act** therefore **as a synthesizer** of many resources created by the broader AI community.
- Hence, **Many Thanks!** to all the creators of the helper material. All credits and references are visible on the last slides.
- Same references are also given in the **footnotes section** of each individual slide, which is **not visible in presentation mode**, but will be useful for referencing at home for extra study if need be.

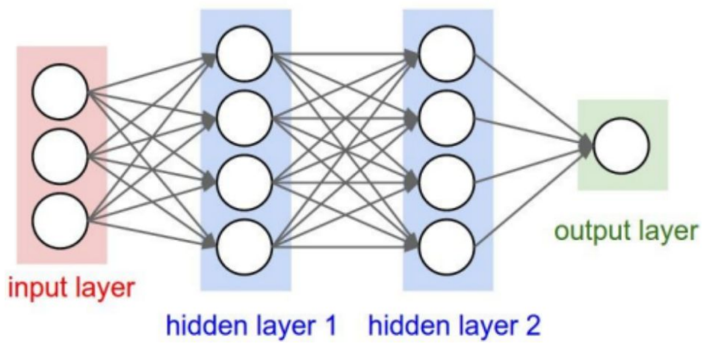


Artificial Neural Nets and Brain Parallels



https://towardsdatascience.com/the-differences-between-artificial-and-biological-neural-networks-a8b46db828b7

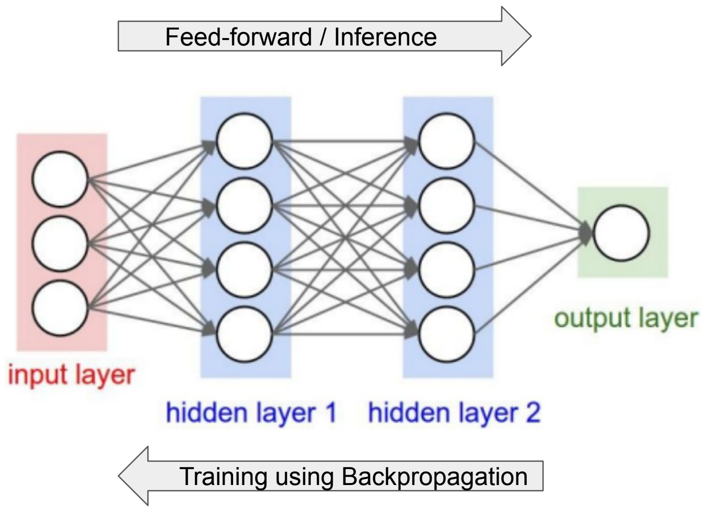
Artificial Neural Networks (ANNs)



CS231n course from Stanford University

http://cs231n.stanford.edu/slides/2019/cs231n_2019_lecture04.pdf

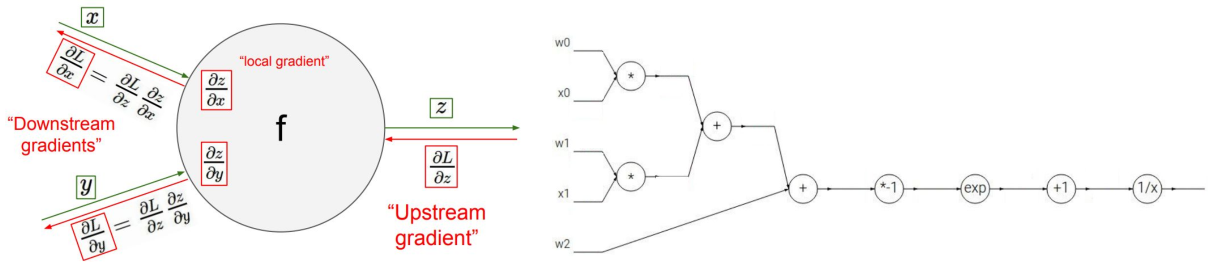
Backpropagation



CS231n course from Stanford University

http://cs231n.stanford.edu/slides/2019/cs231n_2019_lecture04.pdf

Backpropagation using Local Gradients and Chain Rule



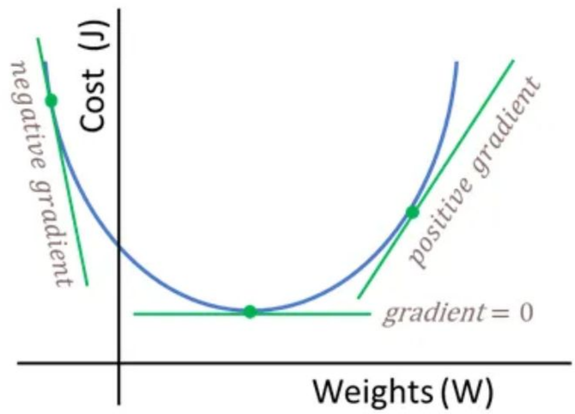
➢ The Chain Rule is implemented with the help of **local gradients**.

➢ We **recursively multiply** the local derivatives.

➢ Backpropagation is a **recursive** application of the chain rule backwards through the **computation graph**.

http://cs231n.stanford.edu/slides/2019/cs231n_2019_lecture04.pdf

Cost function



https://towardsdatascience.com/neural-networks-backpropagation-by-dr-lihi-gur-arie-27be67d8fdce

Weights update

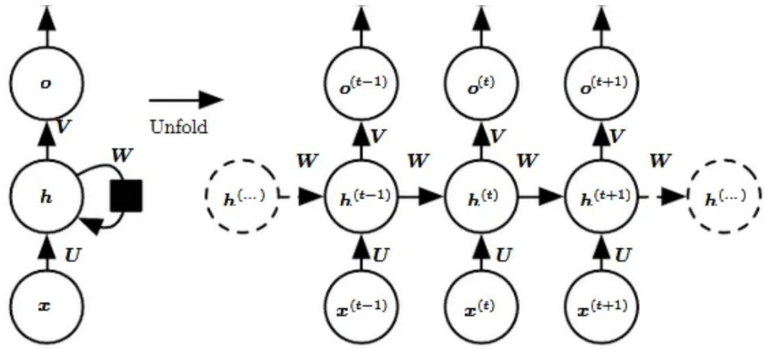
$$\underbrace{W_{new} = W_{old} - \alpha \frac{dJ}{dW}}$$

$$W_{new} = W_{old} - \alpha \underbrace{\frac{dJ}{dW}}_{\text{gradient}}$$

- ➢ **J** and **L** are usual notations for the **Loss** / **Error** / **Cost** function, i.e. the difference between what the model **predicts** and what it should predict according to the **ground truth**.
- ➢ The **weights are updated** in the direction of the **negative** gradient, so that the **cost function is minimized** as much as possible.

https://towardsdatascience.com/neural-networks-backpropagation-by-dr-lihi-gur-arie-27be67d8fdce

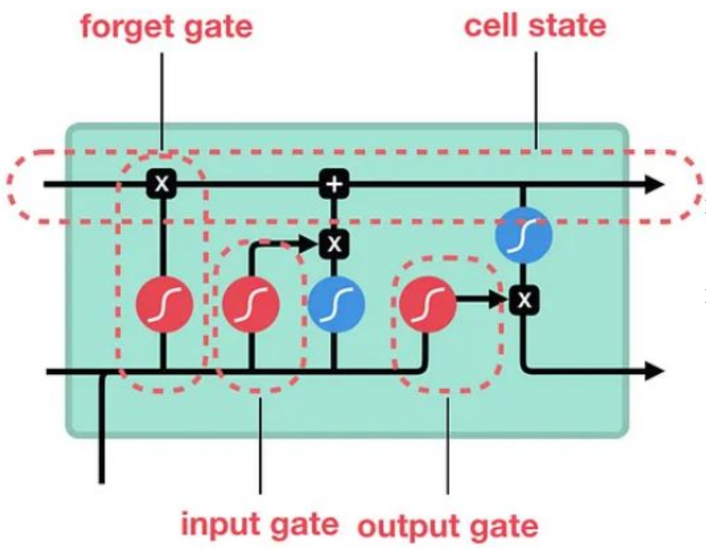
Sequential nature of Recurrent Neural Networks (RNNs)



- By **unfolding** the feedback loop in time, we become aware of the complexity of these networks. It is as if we train a **very deep network** and that is why they are harder to train.
- With **RNNs** things are done **sequentially** => **deep** graph structure.
- With **Transformers** things happen **parallely** => **broad** graph structure.
- **Transformers** might simply be **easier to train stably**, and maybe that is why they have better results.

https://towardsdatascience.com/recurrent-neural-networks-rnns-3f06d7653a85

Long short-term memory (LSTMs)

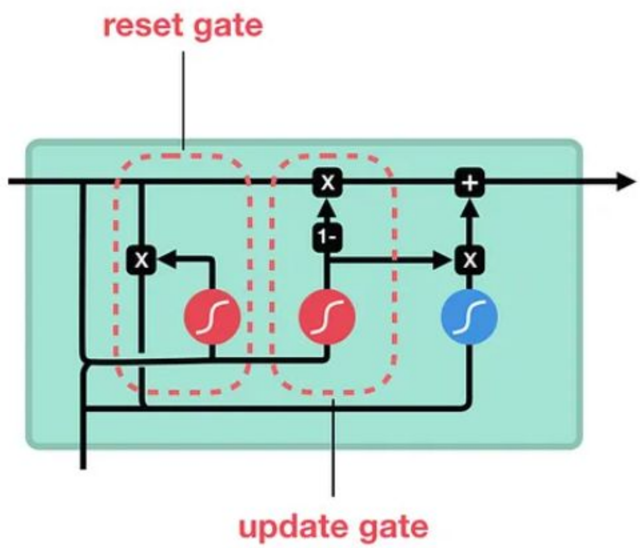


➢ Contains special **gates** that address the problem of **vanishing gradients**.

➢ Addresses the problem of **exploding gradients**.

https://medium.com/towards-data-science/illustrated-guide-to-lstms-and-gru-s-a-step-by-step-explanation-44e9eb85bf21

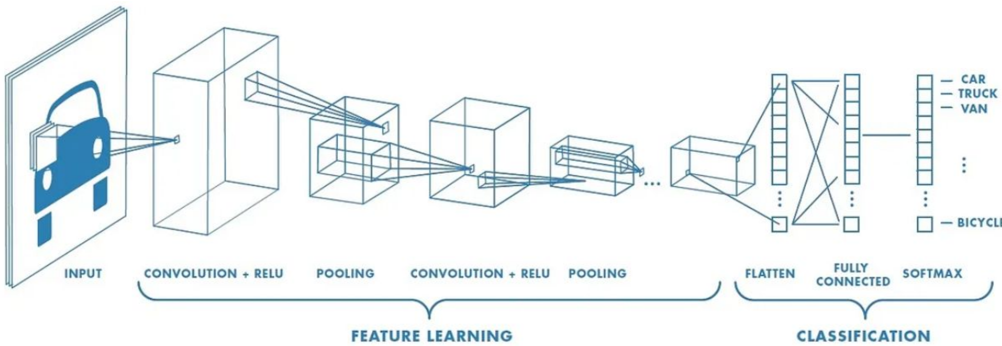
Gated Recurrent Units (GRUs)



- ➢ Generally considered **faster** than LSTMs.
- ➢ In practice => **similar outcomes to** what **LSTM** provides.

https://medium.com/towards-data-science/illustrated-guide-to-lstms-and-gru-s-a-step-by-step-explanation-44e9eb85bf21

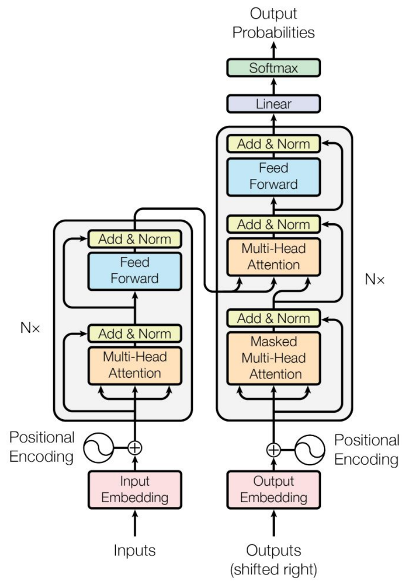
Convolutional Neural Networks (CNNs)



- Generally applied in **computer vision** tasks, i.e. **2D image focused, not time sequence data**.
- We can use **3D CNNs to handle sequences of data**, where 3rd dimension is time. Here we talk about a cube kernel, instead of a plane 2D kernel.
- CNNs are very amenable to **parallelism**.

https://medium.com/@RaghavPrabhu/understanding-of-convolutional-neural-network-cnn-deep-learning-99760835f148

Transformers



“Attention is all you need” paper from 2017 by Vaswani et al.

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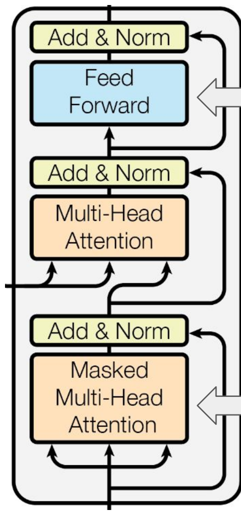
Figure 1 taken from paper “Attention is all you need” by Vaswani et al. -> https://arxiv.org/pdf/1706.03762.pdf

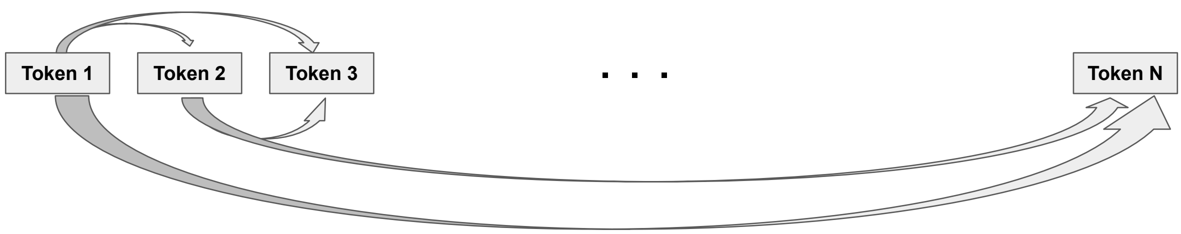
Transformer Block



2. Secondly, a **Multilayer Perceptron (MLP)** crunches the data that was communicated amongst tokens in the previous self-attention phase.

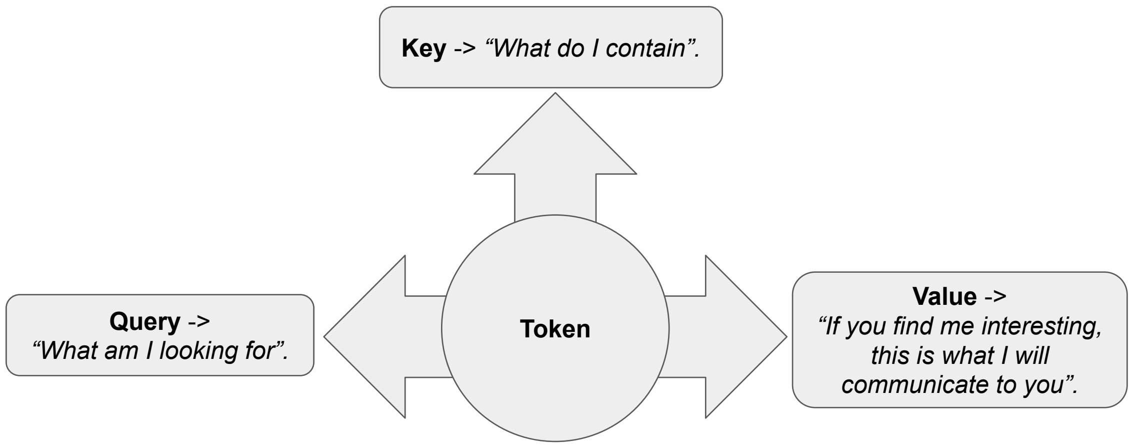
1. First the tokens **communicate** between themselves / they attend to each other (**self-attention**).

Self-Attention



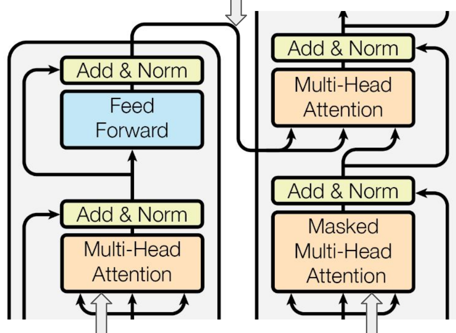
- ➢ **All tokens communicate with one another**.
- ➢ This is computationally expensive because **each token has to look at every other token** to compute an **attention score / attention weight**.

Key, Query and Value Embeddings



Self-Attention vs Cross-Attention

Cross-Attention -> the *queries* come from the **decoder**, whereas the *keys* and *values* are from the **encoder** side.



Self-attention -> the *key*, *query* and *value* vectors are related to the **same entity**, either the encoder, or the decoder.

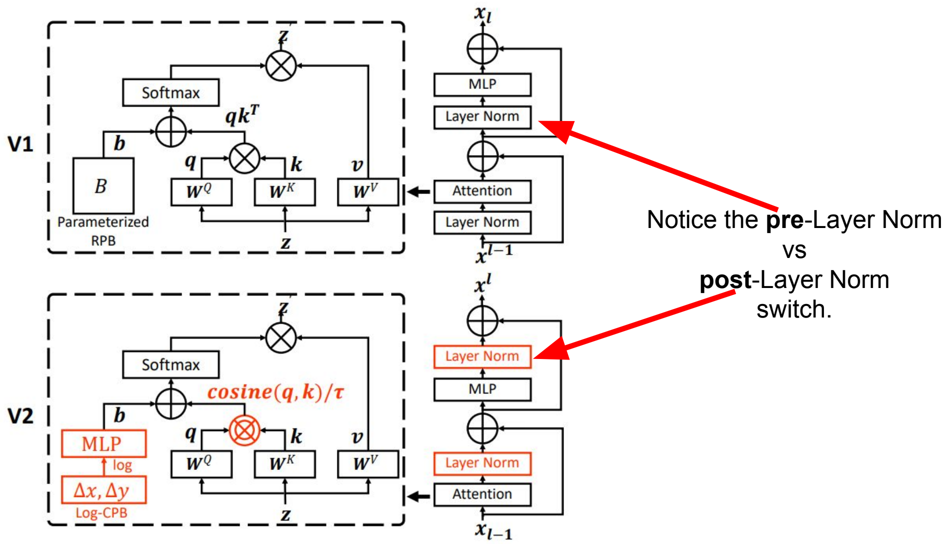
Mathematically Expressing Self-Attention

- The dot product **Query ・ Key** is the attention score.

- Dot product measures **similarity between vectors** => **Attention** can be interpreted as the **alignment** between the **Key** and the **Query** vectors (i.e. two tokens find each other interesting).

- Instead of the dot product, other measures can be used, like the **cosine similarity** for example (**Swin Transformer Version 2** paper).

Cosine similarity

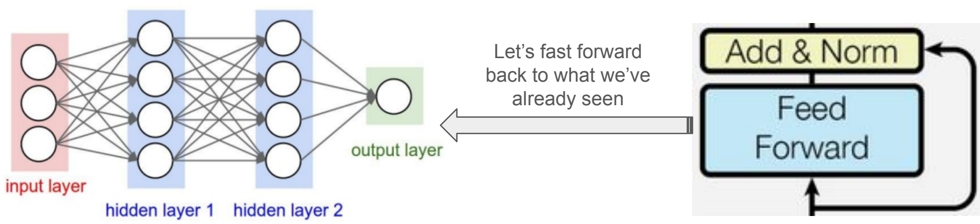


"Swin Transformer V2: Scaling Up Capacity and Resolution" by Liu et al.

Figure 1 from "Swin Transformer V2: Scaling Up Capacity and Resolution" paper by Liu et al. -> https://arxiv.org/abs/2111.09883

Computation Phase / Feed-Forward MLP

- ➢ After the communication between tokens is finished, an MLP has to **“think”** on what was **“said”** during the self-attention phase.
- ➢ This basically means that new features are computed / derived as a result of the communication.



Positional encoding

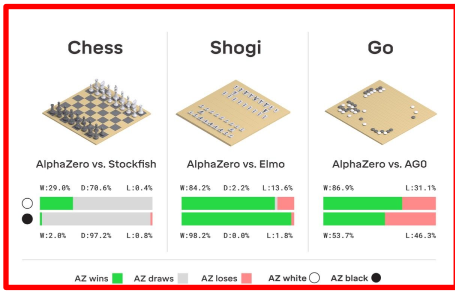
- ➢ The transformer treats the tokens as a **Bag of Words (BOG)**.
- ➢ We need to give each token a label that specifies its position in the form of a **counter ID** for instance.
- ➢ It is interesting that the positional encoding information is simply **added literally** by a **“+”**/ **plus** operation.

*There are various encoding schemes such as for example **absolute encoding**, **relative encoding**, that have a significant impact on how the transformer ends up performing. Check out the Swin Transformer paper for empirical proof.*

ChatGPT Pipeline

1) Pretraining the **base model**.
2) Supervised Fine-Tuning (**SFT**).
3) **Reward** Modeling / **RM**.
4) Reinforcement Learning / **RL** (Very much research territory at the moment).

Personal opinion: ChatGPT works so well, because it borrowed many insights from the AlphaZero games playing engine from back in 2016.



DeepMind subsequently created **AlphaStar** and **AlphaFold** using similar principles.

https://arstechnica.com/science/2018/12/move-over-alphago-alphazero-taught-itself-to-play-three-different-games/

Pretraining the Foundational Model

- Use **raw data** to train a **Base Model**.
- The dataset is **huge** => potentially low quality, but **very large quantity**.
- We obtain a **document completer** in the end.
- Thousands of GPUs work in parallel (ex: 1000-2000 A100 GPUs)

Supervised Fine Tuning (SFT stage)

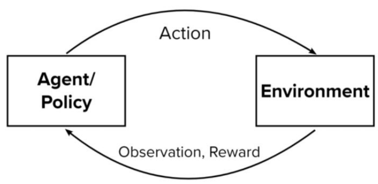
- **Low quantity, high quality data**: ~ 100K (prompt, response) tuples.
- Domain Specialists / Contractors have to scrutinize the dataset so that close to ideal **(prompt, response) tuples** are assembled.
- Less GPUs are required (ex: 1-100).
- The outcome is the so-called **SFT model**.

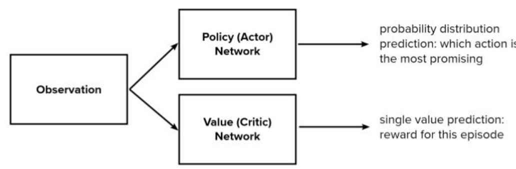
Reward Modeling

- ➢ Ask the SFT model to produce **multiple answers** per prompt.
- ➢ Ask contractors to carefully **rank these answers**.
- ➢ Train a reward model on these rankings.
- ➢ Order of 1 to 100 GPUs for training.
- ➢ The outcome is the so-called **Reward Model / RM** => **Evaluates token trajectories.**

Reinforcement Learning

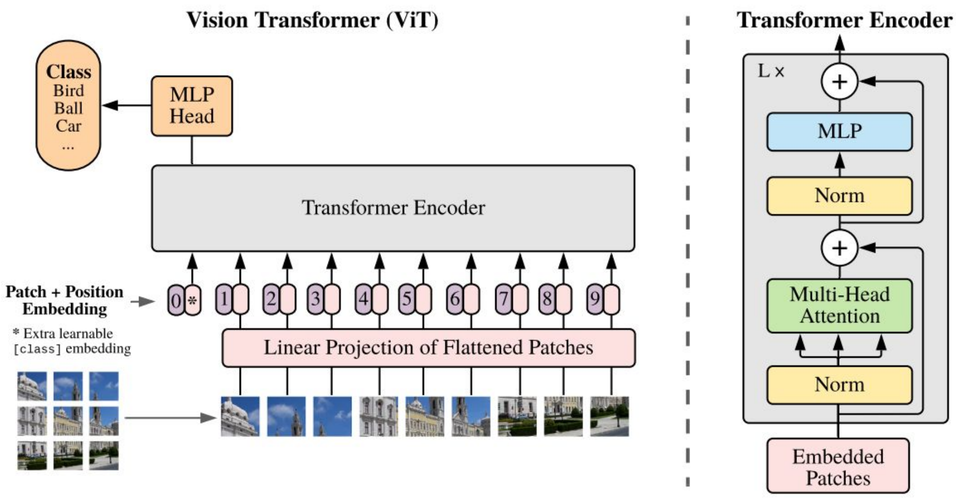
- ➢ Train a **PPO** algorithm (**Proximal Policy Optimization**).
- ➢ Use the previously trained reward model to **evaluate the reward**.
- ➢ PPO will have the job of generating **token "trajectories"** that will have a **very good overall score**.
- ➢ Order of 1 to 100 GPUs for training.
- ➢ The outcome is the so called **RL model / RLHF** (reinforcement learning with **human feedback**).





https://odsc.com/blog/reinforcement-learning-with-ppo/

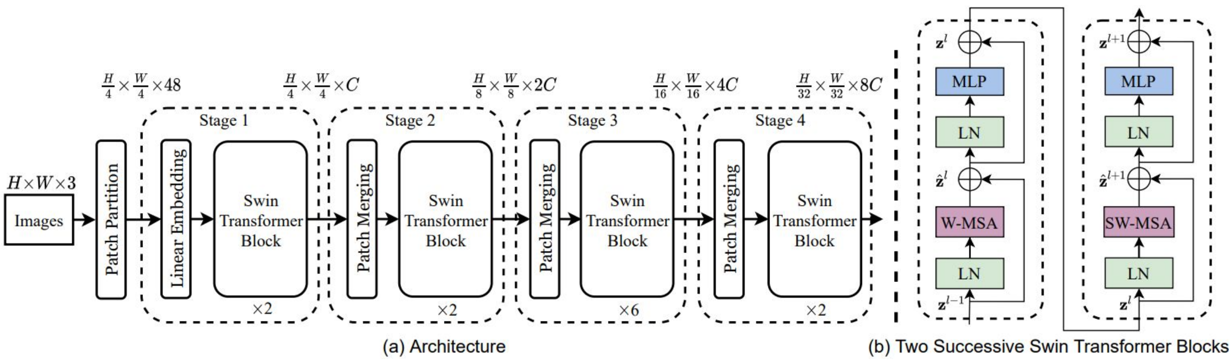
Vision Transformer / ViT



“An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale” by A. Dosovitskiy et al. (2021)

Figure 1 from the paper “An image is worth 16x16 words: Transformers for image recognition at scale” by A. Dosovitskiy et al. -> https://arxiv.org/pdf/2010.11929v2.pdf

Swin Transformer

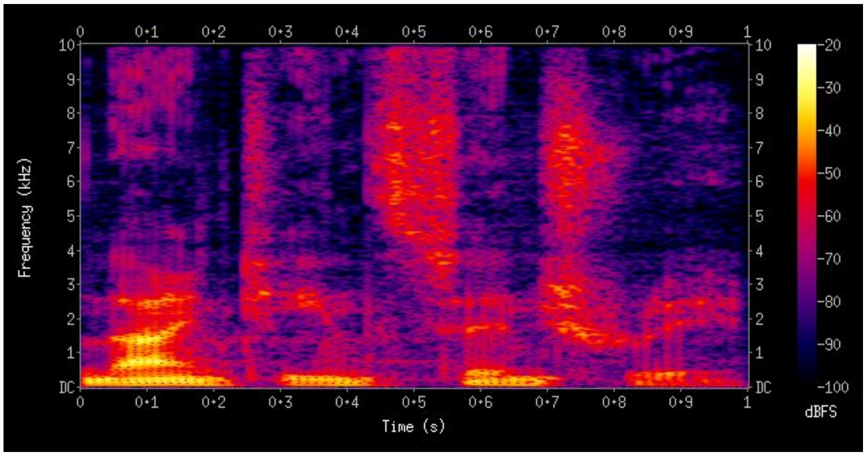


“Swin Transformer: Hierarchical Vision Transformer using Shifted Windows” by Liu et al. (2021)

Figure 3 from the paper “Swin Transformer: Hierarchical Vision Transformer using Shifted Windows” by Liu et al. -> https://arxiv.org/pdf/2103.14030.pdf

Audio Transformer

Raw sound waves can be mapped to a different space using **STFT** (Short-time Fourier Transform).



Here time series become images => **problem is adapted** to be addressed by the ViT / Swin Transformer.

https://en.wikipedia.org/wiki/Short-time_Fourier_transform#/media/File:Spectrogram-19thC.png

Time Series Transformer (TST)

Continuous data is **sampled** and **quantized** into **discrete tokens**.

Implementations available at: https://huggingface.co/docs/transformers/model_doc/time_series_transformer

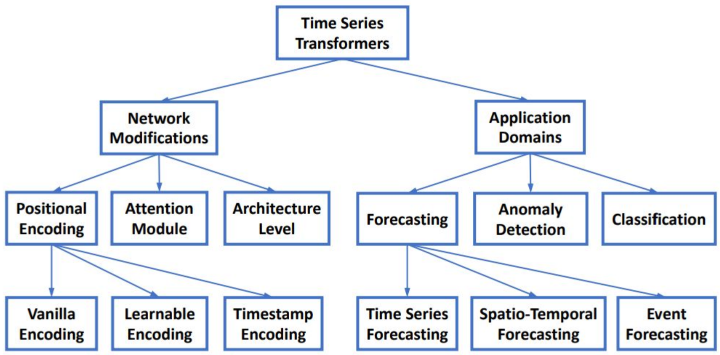


Figure 1: Taxonomy of Transformers for time series modeling from the perspectives of network modifications and application domains.

“Transformers in Time Series: A Survey” paper, by Wen et al. [2023]

Figure 1 from the “Transformers in Time Series: A Survey” paper, by Wen et al. -> https://arxiv.org/pdf/2202.07125.pdf ; https://github.com/qingsongedu/time-series-transformers-review

Mini-GPT Qualitative Results

Trained on DKRZ server:

```
WARWICK:
Mine eyes have bands the cause of block.

RICHARD:
Up Montague, and in the opin stroke,
Her hath hand with the sharp of Edward's care.

RICHARD:
But repetitor of thy brothers are postless of fight
Thy in habit wars, for presumpting Bishop's wrongs.

WARWICK:
And live peace, thou know'st what of Henry William come?

SOMERSET:
The which such debt sworns, giving loood of loving men:
Ere ye he suspicious, turns the devour death?
And spurn my kning bead of love to his friends,
I'ld up their witten in a wolvesse slay,
Standing from that in chiefes the befalls!

Second Murderer:
The talts, and did stand and call the surping lass;
More weightily in a jarent air,
More than my years, and being toilous,
Making weep and from mine head annest,
Courage of their rotten foot and tithe,
You cannot speak love the frown of y hands
The stread on my terrich! Valia, my dam:
More passion clergine of those first black ears:
Come, bring puling impositials that which
Rome or Rather's busine bow: this
```

`Also, checkout -> https://www.nytimes.com/interactive/2023/04/26/upshot/gpt-from-scratch.html`

On DKRZ server.

Training on GPU

```
Every 2.0s: nvidia-smi

Tue Jul 11 10:20:59 2023
+---------------------------------------------------------------------------------------+
| NVIDIA-SMI 535.54.03              Driver Version: 535.54.03    CUDA Version: 12.2     |
|-----------------------------------------+----------------------+----------------------+
| GPU  Name                 Persistence-M | Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp   Perf          Pwr:Usage/Cap |         Memory-Usage | GPU-Util  Compute M. |
|                                         |                      |               MIG M. |
|=========================================+======================+======================|
|   0  NVIDIA A100-SXM4-40GB          Off | 00000000:03:00.0 Off |                    0 |
| N/A   69C    P0             244W / 400W |   4355MiB / 40960MiB |     98%      Default |
|                                         |                      |             Disabled |
+-----------------------------------------+----------------------+----------------------+
|   1  NVIDIA A100-SXM4-40GB          Off | 00000000:44:00.0 Off |                    0 |
| N/A   49C    P0              63W / 400W |      8MiB / 40960MiB |      0%      Default |
|                                         |                      |             Disabled |
+-----------------------------------------+----------------------+----------------------+
|   2  NVIDIA A100-SXM4-40GB          Off | 00000000:84:00.0 Off |                    0 |
| N/A   48C    P0              59W / 400W |      8MiB / 40960MiB |      0%      Default |
|                                         |                      |             Disabled |
+-----------------------------------------+----------------------+----------------------+
|   3  NVIDIA A100-SXM4-40GB          Off | 00000000:C4:00.0 Off |                    0 |
| N/A   48C    P0              59W / 400W |      8MiB / 40960MiB |      0%      Default |
|                                         |                      |             Disabled |
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+---------------------------------------------------------------------------------------+
| Processes:                                                                            |
|  GPU   GI   CI        PID   Type   Process name                            GPU Memory |
|        ID   ID                                                             Usage      |
|=======================================================================================|
|    0   N/A  N/A    126312      G   /usr/libexec/Xorg                            23MiB |
|    0   N/A  N/A   1883655      C   python                                     4308MiB |
+---------------------------------------------------------------------------------------+
```


On DKRZ server.

Transformer Hyperparameters

```
# hyperparameters
batch_size = 64 # how many independent sequences will we process in parallel?
block_size = 256 # what is the maximum context length for predictions?
max_iters = 5000
eval_interval = 500
learning_rate = 3e-4
device = 'cuda' if torch.cuda.is_available() else 'cpu'
eval_iters = 200
n_embd = 384
n_head = 6
n_layer = 6
dropout = 0.2
```


Code reproduced using https://github.com/karpathy/ng-video-lecture on DKRZ server

Train Info Logs

```
10.788929 M parameters
step 0: train loss 4.2221, val loss 4.2306
step 500: train loss 1.7550, val loss 1.9111
step 1000: train loss 1.3907, val loss 1.6016
step 1500: train loss 1.2679, val loss 1.5275
step 2000: train loss 1.1857, val loss 1.4956
step 2500: train loss 1.1227, val loss 1.4960
step 3000: train loss 1.0720, val loss 1.4844
step 3500: train loss 1.0207, val loss 1.4968
step 4000: train loss 0.9595, val loss 1.5057
step 4500: train loss 0.9102, val loss 1.5299
step 4999: train loss 0.8607, val loss 1.5576
```

Starts to overfit

On DKRZ server.

Takeaways

➢ Transformers are powerful neural networks that **borrow the best ideas** from prior models in the AI ecosystem and **combine them together for a synergistic effect**.

➢ **Self-attention** and **Feed-Forward MLP** are the major conceptual components of a Transformer block.

➢ **Self-attention** is essentially a **communication graph** where tokens exchange **information stored in channels** amongst themselves.

➢ The **Feed-Forward MLP** is used for the **computation phase to learn embeddings**.

➢ **Residual connections** and **pre- / post-normalization** are other important attributes to help towards successful training and faster convergence.

References

- Slide 3: https://towardsdatascience.com/the-differences-between-artificial-and-biological-neural-networks-a8b46db828b7
- Slide 4, 5, 6: http://cs231n.stanford.edu/slides/2019/cs231n_2019_lecture04.pdf
- Slide 7, 8: https://towardsdatascience.com/neural-networks-backpropagation-by-dr-lihi-gur-arie-27be67d8fdce
- Slide 9: https://towardsdatascience.com/recurrent-neural-networks-rnns-3f06d7653a85
- Slide 10, 11: https://medium.com/towards-data-science/illustrated-guide-to-lstms-and-gru-s-a-step-by-step-explanation-44e9eb85bf21
- Slide 12: https://medium.com/@RaghavPrabhu/understanding-of-convolutional-neural-network-cnn-deep-learning-99760835f148
- Slides 13, 14, 17, 20, 21 Transformer components were taken from "Attention is all you need" paper, by Vaswani et al.
- Slide 19: "Swin Transformer V2: Scaling Up Capacity and Resolution" paper, by Liu et al.
- Slide 22: https://arstechnica.com/science/2018/12/move-over-alphago-alphazero-taught-itself-to-play-three-different-games/
- Slide 26: https://odsc.com/blog/reinforcement-learning-with-ppo/
- Slide 27: "An image is worth 16x16 words: Transformers for image recognition at scale" paper, by Dosovitskiy et al.
- Slide 28: "Swin Transformer: Hierarchical Vision Transformer using Shifted Windows" paper, by Liu et al.
- Slide 29: https://en.wikipedia.org/wiki/Short-time_Fourier_transform#/media/File:Spectrogram-19thC.png
- Slide 30: "Transformers in Time Series: A Survey" paper, by Wen et al.

Appendix: Self-Attention Snippet Version 1

```
# Version 1:
# We want x[b,t] = mean_{i<=t} x[b,i]
xbow = torch.zeros((B,T,C))
for b in range(B):
   for t in range(T):
       xprev = x[b,:t+1] # (t,C)
       xbow[b,t] = torch.mean(xprev, 0)

print(x[0])
print(xbow[0])
```

```
torch.Size([4, 8, 2])
tensor([[ 1.9269,  1.4873],
        [ 0.9007, -2.1055],
        [ 0.6784, -1.2345],
        [-0.0431, -1.6047],
        [-0.7521,  1.6487],
        [-0.3925, -1.4036],
        [-0.7279, -0.5594],
        [-0.7688,  0.7624]])
tensor([[ 1.9269,  1.4873],
        [ 1.4138, -0.3091],
        [ 1.1687, -0.6176],
        [ 0.8657, -0.8644],
        [ 0.5422, -0.3617],
        [ 0.3864, -0.5354],
        [ 0.2272, -0.5388],
        [ 0.1027, -0.3762]])
```

Appendix: Self-Attention Snippet Version 2

```python
# Version 1
# We want x[b,t] = mean_{i<=t} x[b,i]
xbow = torch.zeros((B,T,C))
for b in range(B):
    for t in range(T):
        xprev = x[b,:t+1] # (t,C)
        xbow[b,t] = torch.mean(xprev, 0)
print(x[0])
print(xbow[0])

# Version 2
wei = torch.tril(torch.ones(T, T))
wei = wei / wei.sum(1, keepdim=True)
xbow2 = wei @ x # (B, T, T) @ (B, T, C) --->
(B, T, C)
print("Are xbow and xbow2 the same? -> ",
torch.allclose(xbow, xbow2))
```

```
torch.Size([4, 8, 2])
tensor([[ 1.9269,  1.4873],
        [ 0.9007, -2.1055],
        [ 0.6784, -1.2345],
        [-0.0431, -1.6047],
        [-0.7521,  1.6487],
        [-0.3925, -1.4036],
        [-0.7279, -0.5594],
        [-0.7688,  0.7624]])
tensor([[ 1.9269,  1.4873],
        [ 1.4138, -0.3091],
        [ 1.1687, -0.6176],
        [ 0.8657, -0.8644],
        [ 0.5422, -0.3617],
        [ 0.3864, -0.5354],
        [ 0.2272, -0.5388],
        [ 0.1027, -0.3762]])
Are xbow and xbow2 the same? ->  True
```

Appendix: Self-Attention Snippet Version 3

```python
# Version 2
wei = torch.tril(torch.ones(T, T))
wei = wei / wei.sum(1, keepdim=True)
xbow2 = wei @ x # (B, T, T) @ (B, T, C) --->
(B, T, C)
print("Are xbow and xbow2 the same? -> ",

# Version 3: using Softmax
tril = torch.tril(torch.ones(T,T))
wei = torch.zeros((T,T))
wei = wei.masked fill(tril == 0,
float('-inf'))
wei = F.softmax(wei, dim=-1)
xbow3 = wei @ x
print("Are xbow/xbow2 equal to xbow3? -> ",
torch.allclose(xbow, xbow3))
```

```
torch.Size([4, 8, 2])
tensor([[ 1.9269,  1.4873],
        [ 0.9007, -2.1055],
        [ 0.6784, -1.2345],
        [-0.0431, -1.6047],
        [-0.7521,  1.6487],
        [-0.3925, -1.4036],
        [-0.7279, -0.5594],
        [-0.7688,  0.7624]])
tensor([[ 1.9269,  1.4873],
        [ 1.4138, -0.3091],
        [ 1.1687, -0.6176],
        [ 0.8657, -0.8644],
        [ 0.5422, -0.3617],
        [ 0.3864, -0.5354],
        [ 0.2272, -0.5388],
        [ 0.1027, -0.3762]])
Are xbow/xbow2 equal to xbow3? ->  True
```