## Transformers

## Transformers

1. Attention
2. Multi-head Attention
3. Transformer Block
4. Other Modules
5. Models

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## Transformers

## Attention

- Attention is the primary mechanic used in the transformer network.


## Transformers

## Attention

- Attention is the primary mechanic used in the transformer network.
- A lot models use it in a range of ways.


## Transformers

## Attention

"An attention function can be described as mapping a query and a set of key-value pairs to an output, where the query, keys, values, and output are all vectors. The output is computed as a weighted sum of the values, where the weight assigned to each value is computed by a compatibility function of the query with the corresponding key."

# Transformers 

Attention: Working Example
the cat danced $\rightarrow$ die Katze tanzte

## Transformers

Attention: Working Example

## the cat danced $\rightarrow$ die Katze tanzte

Assume that we have generated the first two words, and now are trying to generate: "tanzte".

# Transformers 

Attention: Working Example
the cat danced $\rightarrow$ die Katze tanzte
the cat danced

The input words are the keys K and the values V .

## Transformers

Attention: Working Example

## the cat danced $\rightarrow$ die Katze tanzte

The words generated so far are the queries Q .

## Transformers

## Attention: Working Example

Q: die Katze

K : the cat danced

V: the cat danced
[

$$
\begin{array}{ll}
{[-1.0,} & -2.5],
\end{array} \quad \# \text { q1: die }
$$

]
[

$$
\begin{array}{ll}
{[-2.0,} & -4.0],
\end{array} \begin{array}{ll}
{[-2.5,} & \text { \# k1: the } \\
{[4.5],} & \text { \# k2: cat } \\
{[4.5,} & 2.5]
\end{array}
$$

]
[

$$
\begin{array}{ll}
{[-2.0,} & -4.0],
\end{array} \quad \text { \# v1: the }
$$

]

## Transformers

Attention: Working Example

- Note: the keys and the values correspond 1:1.


## Transformers

## Attention: Working Example

- Note: the keys and the values correspond 1:1.
- They don't have to be the same (although in the transformer models they always are.)


## Transformers

## Attention: Working Example

- Note: the keys and the values correspond 1:1.
- They don't have to be the same (although in the transformer models they always are.)
- In fact, the queries, keys, and values can all be the same vectors. This is self-attention.





## Transformers

 Scaled Dot-Product Attention

## Transformers

## Attention: Working Example

```
def scaled-dot-product-attention(Q,K,V):
    # Q : N x D_1
    # K : M x D_1
    # V : M x D_2
    # -> N x D_2
    scores = Q • K.T # N x M
    scaled = scores / sqrt(D_1) # N x M
    alpha = softmax(scores) # N x M
    out = alpha • V # N x d_2
```

```
Q = [
```

Q = [
[-1.0, -2.5], \# q1: die
[-1.0, -2.5], \# q1: die
[4.0, 3.0], \# q2: Katze
[4.0, 3.0], \# q2: Katze
]

```
]
```

```
K.T = [
```

K.T = [
[-2, -2.5, 4.5], \# k1: the
[-2, -2.5, 4.5], \# k1: the
[-4, -0.5, 2.5], \# k2: cat
[-4, -0.5, 2.5], \# k2: cat
\# k3: danced

```
        # k3: danced
```


## Transformers

## Attention: Working Example

```
def scaled-dot-product-attention(Q,K,V):
    # Q : N x D_1
    # K : M x D_1
    # V : M x D_2
    # -> N x D_2
    scores = Q • K.T # N x M
    scaled = scores / sqrt(D_1) # N x M
    alpha = softmax(scores) # N x M
    out = alpha • V # N x d_2
scores = [
    [
        (-1.0 * -2.0 + -2.5 * -4.0),
        (-1.0 * -2.5 + -2.5 * -0.5),
        (-1.0 * 4.5 + -2.5 * 2.5),
    ],
    [
        ( 4.0 * -2.0 + 3.0 * -4.0),
        (4.0 * -2.5 + 3.0 * -0.5),
        (4.0 * 4.5 + 3.0 * 2.5),
    ],
]
```


## Transformers

## Attention: Working Example

```
def scaled-dot-product-attention(Q,K,V):
    # Q : N x D_1
    # K : M x D_1
    # V : M x D_2
    # -> N x D_2
    scores = Q • K.T # N x M
    scaled = scores / sqrt(D_1) # N x M
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    out = alpha • V # N x d_2
scores = [
```



## Transformers

## Attention: Working Example

```
def scaled-dot-product-attention(Q,K,V):
    # Q : N x D_1
    # K : M x D_1
    # V : M x D_2
    # -> N x D_2
    scores = Q • K.T # N x M
    scaled = scores / sqrt(D_1) # N x M
    alpha = softmax(scores) # N x M
    out = alpha • V # N x d_2
scores = [
```



## Transformers

## Attention: Working Example

```
def scaled-dot-product-attention(Q,K,V):
    # Q : N x D_1
    # K : M x D_1
    # V : M x D_2
    # -> N x D_2
    scores = Q • K.T # N x M
    scaled = scores / sqrt(D_1) # N x M
    alpha = softmax(scores) # N x M
    out = alpha • V # N x d_2
scores = [
    [\mp@code{12.00, 3.75, -10.75 ],}
```

Each index in this NxM matrix represents the compatibility between query $n$ and key $m$.

## Transformers

## Attention: Working Example

```
def scaled-dot-product-attention(Q,K,V):
    # Q : N x D_1
    # K : M x D_1
    # V : M x D_2
    # -> N x D_2
    scores = Q • K.T # N x M
    scaled = scores / sqrt(D_1) # N x M
    alpha = softmax(scores) # N x M
    out = alpha • V # N x d_2
scores = [
    [rrrrer, 3.75, -10.75 ],
```

Each index in this NxM matrix represents the compatibility between query $n$ and key $m$.

## Transformers

## Attention: Working Example

```
def scaled-dot-product-attention(Q,K,V):
    # Q : N x D_1
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    # V : M x D_2
    # -> N x D_2
    scores = Q • K.T # N x M
    scaled = scores / sqrt(D_1) # N x M
    alpha = softmax(scores) # N x M
    out = alpha • V # N x d_2
scores = [
    [\mp@code{12.00, 3.75, -10.75 ],}
```

Each index in this NxM matrix represents the compatibility between query $n$ and key $m$.

## Transformers

## Attention: Working Example

```
def scaled-dot-product-attention(Q,K,V):
    # Q : N x D_1
    # K : M x D_1
    # V : M x D_2
    # -> N x D_2
    scores = Q • K.T # N x M
    scaled = scores / sqrt(D_1) # N x M
    alpha = softmax(scores) # N x M
    out = alpha • V # N x d_2
scores = [
    [ 12.00, 3.75, -10.75 ],
    [-20.00, -11.50, 25.50 ]]
scaled = [
    [ 4.0000, 1.2500, -3.5833],
    [-6.6667, -3.8333, 8.5000]]
```


## Transformers

## Attention: Working Example

```
def scaled-dot-product-attention(Q,K,V):
    # Q : N x D_1
    # K : M x D_1
    # V : M x D_2
    # -> N x D_2
    scores = Q • K.T # N x M
    scaled = scores / sqrt(D_1) # N x M
    alpha = softmax(scores) # N x M
    out = alpha • V # N x d_2
scaled = [
    [ 4.0000, 1.2500, -3.5833],
    [-6.6667, -3.8333, 8.5000]]
```

The motivation for scaling the product is that the dot product gets larger as the dimensionality gets larger: the variance of the dot-product of 0-1 random variables is the length of the vector.

## Transformers

## Attention: Working Example

```
def scaled-dot-product-attention(Q,K,V):
    # Q : N x D_1
    # K : M x D_1
    # V : M x D_2
    # -> N x D_2
    scores = Q • K.T # N x M
    scaled = scores / sqrt(D_1) # N x M
    alpha = softmax(scores) # N x M
    out = alpha • V # N x d_2
scaled = [
    [ 4.0000, 1.2500, -3.5833],
    [-6.6667, -3.8333, 8.5000]]
```

When the values are large, the gradients of the softmax will be small (which can hurt learning).

## Transformers

Softmax

$$
\frac{e^{x_{i}}}{\sum_{j} e^{x_{j}}}
$$

## Transformers

## Attention: Working Example

```
def scaled-dot-product-attention(Q,K,V):
    # Q : N x D_1
    # K : M x D_1
    # V : M x D_2
    # -> N x D_2
    scores = Q • K.T # N x M
    scaled = scores / sqrt(D_1) # N x M
    alpha = softmax(scores) # N x M
    out = alpha • V # N x d_2
scaled = [
    [ 4.0000, 1.2500, -3.5833],
    [-6.6667, -3.8333, 8.5000]]
alpha = [
    [0.94, 0.06, 0.00],
    [0.00, 0.00, 0.99]
]
```


## Transformers

## Attention: Working Example

```
def scaled-dot-product-attention(Q,K,V):
    # Q : N x D_1
    # K : M x D_1
    # V : M x D_2
    # -> N x D_2
    scores = Q • K.T # N x M
    scaled = scores / sqrt(D_1) # N x M
    alpha = softmax(scores) # N x M
    out = alpha • V # N x d_2
scaled = [
    [ 4.0000, 1.2500, -3.5833],
    [-6.6667, -3.8333, 8.5000]]
alpha = [
    [0.94, 0.06, 0.00],
    [0.00, 0.00, 0.99]
]
```


## Transformers

## Attention: Working Example

```
def scaled-dot-product-attention(Q,K,V):
    # Q : N x D_1
    # K : M x D_1
    # V : M x D_2
    # -> N x D_2
    scores = Q • K.T # N x M
    scaled = scores / sqrt(D_1) # N x M
    alpha = softmax(scores) # N x M
    out = alpha • V # N x d_2
out = [
        (0.94* -2.0 + 0.06* -2.5 + 0.00 * 4.5),
        (0.00 * -4.0 + 0.00 * -0.5 + 0.99 * 2.5),
    ],
        (0.94 * -2.0 + 0.06 * -2.5 + 0.00 * 4.5),
        (0.00 * -4.0 + 0.00 * -0.5 + 0.99 * 2.5),
    ]
]
```


## Transformers

## Attention: Working Example

```
def scaled-dot-product-attention(Q,K,V):
    ..
    out = alpha • V
    # N x d_2
```

$$
\begin{aligned}
& \text { out }=[ \\
& \quad[-2.02, \\
& {[4.3 .78]} \\
& {[49,} \\
& 2.49]]
\end{aligned}
$$



## Transformers

## Attention: Working Example

```
def scaled-dot-product-attention(Q,K,V):
    ..
    out = alpha • V
    # N x d_2
```

```
out = [
    \([-2.02,-3.78]\),
    [ 4.49, 2.49]]
```

- Thus, each query is mapped to a linear combination of the values.
- Note: the weight of each value depends on the compatibility between the corresponding key and query.


## Transformers

Attention: Working Example


## Transformers

## Attention

"An attention function can be described as mapping a query and a set of key-value pairs to an output, where the query, keys, values, and output are all vectors. The output is computed as a weighted sum of the values, where the weight assigned to each value is computed by a compatibility function of the query with the corresponding key."


## Transformers

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2. Multi-head Attention
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## Transformers

Multi-head Attention Intuition

- No parameters in scaled dot-product attention.


## Transformers

Multi-head Attention Intuition

- No parameters in scaled dot-product attention.
- Thus, to influence how we attend the vectors, downstream functions have to be updated.


# Transformers 

Multi-head Attention Intuition

- Dot-product isn't flexible; it's difficult to attend to different aspects of a representation.


# Transformers <br> Multi-head Attention Intuition 

- Dot-product isn't flexible; it's difficult to attend to different aspects of a representation.
- How can we get the model to attend differently based upon the context?


## $\mathrm{U}_{\mathrm{a}}$ q.v $\uparrow$

Multi-Head Attention





## Transformers

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## Transformers Transformer Block

1. Input embedding.


## Transformers Transformer Block

1. Input embedding.
2. Position encodings are element-wise added to the embeddings.


Inputs

## Transformers Transformer Block

1. Input embedding.
2. Position encodings are element-wise added to the embeddings.
3. Stacked transformer blocks.


## Transformers Transformer Block

You may have noticed: there are two modules in the block we haven't covered.


## Transformers

1. Attention
2. Multi-head Attention
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## Transformers

## Positional Encoding

- Positional Encodings are meant to replace the ordering information lost (as all the vectors are operated on in parallel).
- These could directly learned; but the authors opt for a "simpler" approach.


## Transformers

Positional Encoding


## Transformers

## Positional Encoding

the cat danced


$$
\begin{array}{ll}
{[-2,-4],} & \text { \# v1: the } \\
{[-2.5,-0.5],} & \text { \# v2: cat } \\
{[4.5,2.5]} & \text { \# v3: danced }
\end{array}
$$

## Transformers <br> Positional Encoding


[
[0, ... 0], \# v1: the
[0, ... 0], \# v2: cat
[0, ... 0] \# v3: danced
]

## Transformers

## Positional Encoding

Encoded Empty Embeddings

[
[0, ... 0], \# v1: the
[0, ... 0], \# v2: cat
[0, ... 0] \# v3: danced
]

## Transformers

## Positional Encoding

Encoded Empty Embeddings

[
[0, ... 0], \# v1: the
[0, ... 0], \# v2: cat
[0, ... 0] \# v3: danced
]

## Transformers Positional Encoding



## Transformers

## Add \& Norm

## def add-norm(sublayer, x): return LayerNorm(x + sublayer(x))

- Sub-layer connection between the input of the layer and the output of the layer.
- This structure has been used in a wide range of networks; its effective at "stabilizing the gradient", and letting us build deeper networks.
"Highway networks." arXiv preprint arXiv:1505.00387 (2015).

He, Kaiming, et al. "Deep residual learning for image recognition." Proceedings of the IEEE conference on computer vision and pattern recognition. 2016.

## Transformers

## Add \& Norm

```
def add-norm(sublayer, x):
    return LayerNorm(x + sublayer(x))
```

"While the traditional plain neural architectures become increasingly difficult to train with increasing network depth (even with variance-preserving initialization), our experiments show that optimization of highway networks is not hampered even as network depth increases to a hundred layers."

## Transformers

## Add \& Norm

def add-norm(sublayer, x): return LayerNorm(x + sublayer(x))

- This is layer normalization across the residual connection between the input and the output of the sublayer (e.g. multi-head attention).
- It's similar to batch-normalization, except that all variables are normalized per layer.


## Transformers

## Add \& Norm

```
def add-norm(sublayer, x):
    return LayerNorm(x + sublayer(x))
```

"Layer normalization is very effective at stabilizing the hidden state dynamics in recurrent networks. Empirically, we show that layer normalization can substantially reduce the training time compared with previously published techniques."

Ba, Jimmy Lei, Jamie Ryan Kiros, and Geoffrey E. Hinton. "Layer
normalization." arXiv preprint arXiv:1607.06450 (2016).
https://pytorch.org/docs/stable/nn.html\#layernorm

## Transformers

Position-wise Feed Forward

$$
\operatorname{FFN}(x)=\sigma\left(x \cdot W_{1}+b_{1}\right) \cdot W_{2}+b_{2}
$$

## Transformers

## Transformer Block Recap



1. Attention is used for Self-Attention.
2. Transformers don't require the size of inputs to match or be padded.
3. The operations are all parallel across the inputs.

Input Embedding

Inputs

## Transformers

1. Attention
2. Multi-head Attention
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## Transformers <br> Models

Transformer Encoder-Decoder (T-ED)<br>Transformer Decoder<br>Generative Pre-Training<br>Generative Pre-Training<br>Bidirectional Transformers<br>(T-D)<br>(GPT-1)<br>(GPT-2)<br>(BERT)

## Transformers T-ED



## Transformers T-ED



## Transformers T-ED



## Transformers T-ED

The outputs (so-far) are embedded in the same way.


## Transformers T-ED

Self-attention starts each decoder block.


## Transformers T-ED

Next, attention between the encoded inputs and the encoded outputs, and the outputs are mapped to the inputs.


## Transformers T-ED



## Softmax

## $\uparrow$

Each output is produced auto-regressively.

Output Embedding

Outputs (shifted right)

Test / Live

# Transformers <br> Generating Outputs (Greedy) 

## Encoded Input



Input Embedding
<s> the cat danced <e>

# Transformers <br> Generating Outputs (Greedy) 

die
Output Embedding

<s> the cat danced <e>


## Transformers

Generating Outputs (Greedy)


# Transformers <br> Generating Outputs (Greedy) 

Katze
Output Embedding


Input Embedding
Output Embedding
<s> the cat danced <e>

## Transformers

Generating Outputs (Greedy)
Katze
Output Embedding


Input Embedding
<s> the cat danced <e>

## Transformers

Generating Outputs (Greedy)

<s> the cat danced <e>


# Transformers <br> Generating Outputs (Greedy) 

Output Embedding


Encoded Output
4
Transformer Decoder

Input Embedding
<s> the cat danced <e>

# Transformers <br> Generating Outputs (Greedy) 

<s> die Katze tantze <e>


Training

## Transformers T-ED

Output Probabilities
$\uparrow$

## Softmax

$\uparrow$
Linear

Two minor details: masking \& shifting.

# Transformers <br> Masked Training 



# Transformers <br> Masked Training 



# Transformers <br> Masked Training 



# Transformers <br> Masked Training 



# Transformers <br> Masked Training 



# Transformers <br> Masked Training 

| <s> | 1 | 0 | 0 | 0 |
| :---: | :---: | :---: | :---: | :---: |
| die | 1 | 1 | 0 | 0 |
| Katze | 1 | 1 | 1 | 0 |
| tantze | 1 | 1 | 1 | 1 |

## Transformers

## Attention: Working Example

```
def masked-self-attention(Q, mask):
    # Q : N x D_1
    # mask : N x N
    K = V = Q
    scores = Q • K.T # N x N
    scaled = scores / sqrt(D_1) # N x N
    masked = scores.masked_fill(
            mask == 0, -1e9)
    alpha = softmax(masked) # N x N
    out = alpha • V # N x d_2
Q = [[[1.0000, 1.0000], mask = [ [lll, 0, 0, 0], [1.0000, -2.5000], 
    [ 4.0000, 3.0000], [1, 1, 1, 0],
    [ 2.0000, -3.0000]] [1, 1, 1, 1]])
```


## Transformers

## Attention: Working Example

```
def masked-self-attention(Q, mask):
    # Q : N x D_1
    # mask : N x N
    K = V = Q
    scores = Q • K.T # N x N
    scaled = scores / sqrt(D_1) # N x N
    masked = scores.masked_fill(
        mask == 0, -1e9)
    alpha = softmax(masked) # N x N
    out = alpha • V # N x d_2
scores =}\mathrm{ tensor([ 
```


## Transformers

## Attention: Working Example

```
def masked-self-attention(Q, mask):
    # Q : N x D_1
    # mask : N x N
    K = V = Q
    scores = Q • K.T # N x N
    scaled = scores / sqrt(D_1) # N x N
    masked = scores.masked_fill(
        mask == 0, -1e9)
    alpha = softmax(masked) # N x N
    out = alpha • V # N x d_2
scaled = tensor(
    [[ 0.5000, -0.8750, 1.7500, -0.2500],
    [-0.8750, 1.8125, -2.8750, 1.3750],
    [ 1.7500, -2.8750, 6.2500, -0.2500],
    [-0.2500, 1.3750, -0.2500, 3.2500]])
```


## Transformers

## Attention: Working Example

```
def masked-self-attention(Q, mask):
    # Q : N x D_1
    # mask : N x N
    K = V = Q
    scores = Q • K.T # N x N
    scaled = scores / sqrt(D_1) # N x N
    masked = scores.masked_fill(
        mask == 0, -1e9)
    alpha = softmax(masked) # N x N
    out = alpha • V # N x d_2
```

masked $=$ tensor $($
[ [ 0.5000, -1e9, -1e9, -1e9],
[-0.8750, 1.8125, -1e9, -1e9],
[ 1.7500, -2.8750, 6.2500, -1e9],
$[-0.2500,1.3750,-0.2500,3.2500]])$

## Transformers

## Attention: Working Example

```
def masked-self-attention(Q, mask):
    # Q : N x D_1
    # mask : N x N
    K = V = Q
    scores = Q • K.T # N x N
    scaled = scores / sqrt(D_1) # N x N
    masked = scores.masked_fill(
        mask == 0, -1e9)
    alpha = softmax(masked) # N x N
    out = alpha • V # N x d_2
```

Thus, as we generate the output for the first query, there is no compatibility between it and subsequent queries (and so on).
masked = tensor(
[ $\left[\begin{array}{lll}0.5000, & -1 e 9, & -1 e 9, ~-1 e 9], ~\end{array}\right.$
[-0.8750, 1.8125, -1e9, -1e9],
[ 1.7500, -2.8750, 6.2500, -1e9],
$[-0.2500,1.3750,-0.2500,3.2500]])$

## Transformers

## Attention: Working Example

```
def masked-self-attention(Q, mask):
    # Q : N x D_1
    # mask : N x N
    K = V = Q
    scores = Q • K.T # N x N
    scaled = scores / sqrt(D_1) # N x N
    masked = scores.masked_fill(
        mask == 0, -1e9)
    alpha = softmax(masked) # N x N
    out = alpha • V # N x d_2
alpha = tensor([[
    [1.0000, 0.0000, 0.0000, 0.0000],
    [0.0000, 1.0000, 0.0000, 0.0000],
    [0.0000, 0.0000, 1.0000, 0.0000],
    [0.0000, 0.0006, 0.0000, 0.9994]]])
```


## Transformers

## Attention: Working Example

```
def masked-self-attention(Q, mask):
    # Q : N x D_1
    # mask : N x N
    K = V = Q
    scores = Q • K.T # N x N
    scaled = scores / sqrt(D_1) # N x N
    masked = scores.masked_fill(
        mask == 0, -1e9)
    alpha = softmax(masked) # N x N
    out = alpha • V # N x d_2
out = [ 
```


## Transformers

## Attention: Working Example

```
def masked-self-attention(Q, mask):
    # Q : N x D_1
    # mask : N x N
    K = V = Q
    scores = Q · K.T # N x N
    scaled = scores / sqrt(D_1) # N x N
    masked = scores.masked_fill(
        mask == 0, -1e9)
    alpha = softmax(masked) # N x N
    out = alpha • V # N x d_2
```



## Transformers T-D



## Transformers GPT (1)

- This is the first model that uses a transformer uses LM as pre-training for future use.
- T-D blocks are used as encoders, and then a single weight matrix is learned on top for finetuned tasks (at most 3 epochs of training).


## Transformers GPT (1)

- They continue to use the LM as an auxiliary loss which speeds up convergence.
- They demonstrate zero-shot capacity on many simple tasks (sentiment analysis).


# Transformers <br> GPT (2) 

- There are minor modifications to the transformer block, but it's basically just the T-D.
- Predominately, they only test on LM; they get SOTA on 7/8 datasets with zero-shot evaluation.


# Transformers <br> GPT (2) 

- They demonstrated some capacity for zero-shot learning in other tasks (including reading comprehension and question answering). Both results were impressive, but not close to SOTA.


## Transformers BERT

- Similar to GPT, but it is stacked T-E. - It used two pre-training tasks.


# Transformers BERT 

- The task is like LM, but instead the model has to predict words which were randomly masked.
- Like skip-thought vectors, they train the model to predict if two sentences should follow one another.






# Transformers <br> RNN Comparison 

## Transformers <br> RNNs

Parallel across inputs.
Sequential across inputs.

Constant path length from input to output.
Path length from output symbol to input depends on the length of the sequence, making it difficult to learn long range dependencies.

