Lecture 6

Attention & Transformers

Part 1: Pooling: Fixed vs. Adaptive

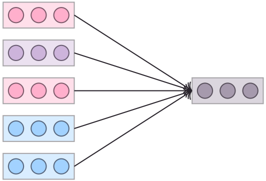
Machine Learning for Structured Data

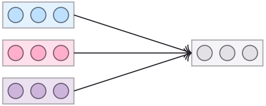
Vlad Niculae · LTL, UvA · https://vene.ro/mlsd

1. Pooling: Fixed vs. Adaptive
2. Hierarchical Attention
3. Self-Attention
4. Transformers

Let's talk about pooling.

$$\mathbf{z} = \text{AveragePool}(\mathbf{z}_1, \ldots, \mathbf{z}_n) := \frac{1}{n}\sum_{j=1}^{n} \mathbf{z}_i$$





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Combine n input vectors into one single output vector,
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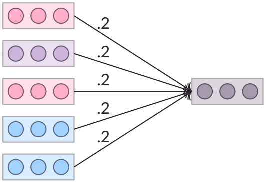
Used to get one representation of a variable-size set or sequence.

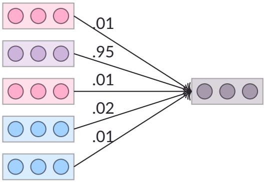
Combine n input vectors into one single output vector,
with equal contribution.

But what if some of the inputs should contribute more than others?

Weighted Average Pooling

$$\boldsymbol{z} = \sum_i \alpha_i \boldsymbol{z}_i, \quad \text{where} \quad \alpha_i \geq 0, \sum_i \alpha_i = 1$$





The weights $\boldsymbol{\alpha}$ control the relative importance of the inputs.

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But how to come up with these weights?
How to decide what's important in a given context?

Attention

Key idea: have a representation of the "context" as a vector $\boldsymbol{q} \in \mathbb{R}^d$.

Then, say the importance of $\boldsymbol{z}_i$ is proportional to its alignment ($\sim$ angle) to $\boldsymbol{q}$:

$$\alpha_i = \underbrace{\frac{\exp(\boldsymbol{q} \cdot \boldsymbol{z}_i)}{\sum_j \exp(\boldsymbol{q} \cdot \boldsymbol{z}_j)}}_{[\mathrm{softmax}([\boldsymbol{q}\cdot\boldsymbol{z}_1,\ldots,\boldsymbol{q}\cdot\boldsymbol{z}_n])]_i} \quad ; \qquad \mathrm{Attn}(\boldsymbol{q}; \boldsymbol{z}_1, \ldots, \boldsymbol{z}_n) := \sum_i \alpha_i \boldsymbol{z}_i.$$

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This is the basic **attention mechanism**:

Pool a bunch of vectors, with varying weights,
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What could be the context?

- Could be just a static learned parameter.
- If training on multiple tasks or domains, $\boldsymbol{q}$ can be an embedding of the domain.
- In machine translation (say EN→NL), $\boldsymbol{z}_i$ are the EN words,
  $\boldsymbol{q}$ can be an embedding of the last NL word predicted (one by one).

Attention In Math And Code

$$\alpha_i = \underbrace{\frac{\exp(\boldsymbol{q} \cdot \boldsymbol{z}_i)}{\sum_j \exp(\boldsymbol{q} \cdot \boldsymbol{z}_j)}}_{[\mathrm{softmax}([\boldsymbol{q}\cdot\boldsymbol{z}_1,\ldots,\boldsymbol{q}\cdot\boldsymbol{z}_n])]_i}$$

$$\boldsymbol{z} = \sum_i \alpha_i \boldsymbol{z}_i$$

```
words = [21, 79, 14]  # indices
emb = Embedding(vocab_sz, dim)
# optionally add RNN, CNN, whatever

Z = emb(words)  # (3 × dim)

q = randn(dim)  # (random context)

s = Z @ q
# [-.3, -1.0, 1.8]

alpha = softmax(s, dim=0)
# [.10, .05, .85]

z = alpha @ Z  # (dim)
```

Attention and Expressivity

Attention by itself doesn't make a model more expressive: intuitively, all the same "information" is there in a uniform average too.

But it provides a sort of "shortcut": it makes it easier to represent useful functions.

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Attention & Transformers

Part 2: Hierarchical Attention

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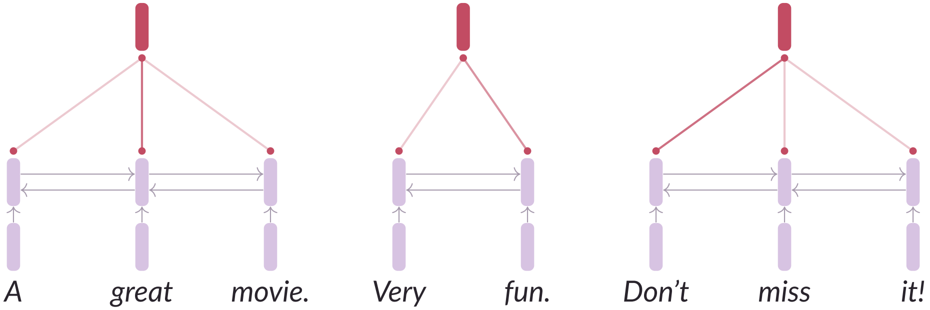
Hierarchical Attention

Encode and pool each sentence separately, then repeat over the sentence vectors.



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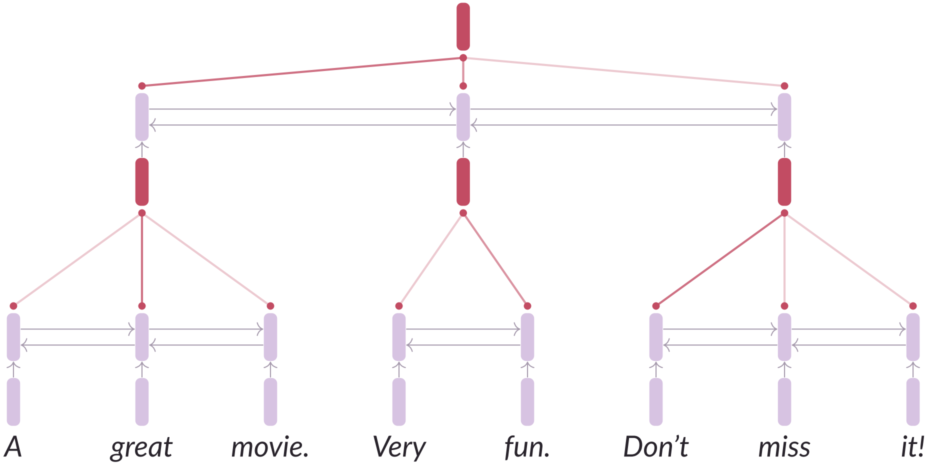

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Key-Value Attention

Attention resembles set lookup:

Soft lookup (attention):

$$s_j = \boldsymbol{q} \cdot \boldsymbol{z}_j$$

$$\boldsymbol{\alpha} = \text{softmax}(\boldsymbol{s})$$

$$\text{return } \textstyle\sum_i \boldsymbol{\alpha}_i \boldsymbol{z}_i$$

Hard set lookup (by similarity):

$$s_j = \boldsymbol{q} \cdot \boldsymbol{z}_j$$

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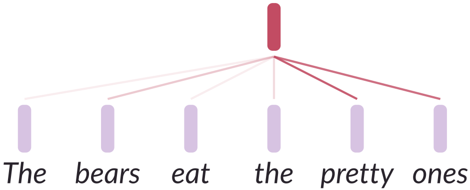
If we only have item embeddings $\boldsymbol{z}_1, \ldots, \boldsymbol{z}_n$, we can learn a key/value "views":

$$\boldsymbol{k}_i = \boldsymbol{W}_K^\top \boldsymbol{z}_i$$
$$\boldsymbol{v}_i = \boldsymbol{W}_V^\top \boldsymbol{z}_i$$

Self-Attention



Can we represent an item (word) as a combination of items relevant to it? (i.e., the item is itself the context)

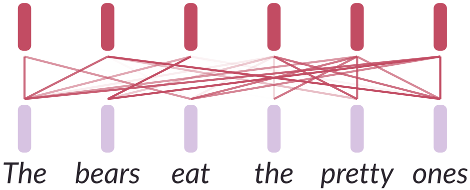
If we had $K = V = Q = Z$ we would always retrieve the item itself.

```
z_out = []

K = Z @ Wk  # (n x dim)
V = Z @ Wv  # (n x dim)
Q = Z @ Wq  # (n x dim)

for i in range(n):
  zi = softmax(K @ Q[i]) @ V
  z_out.append(zi)
```

Self-Attention



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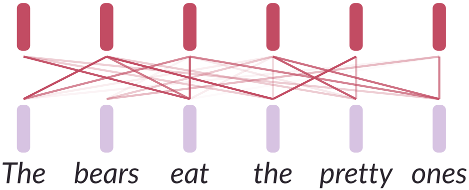


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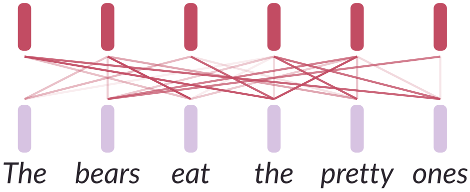


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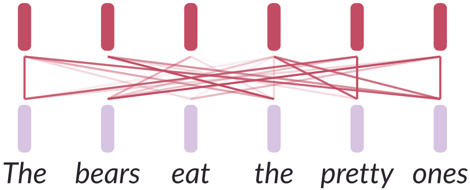


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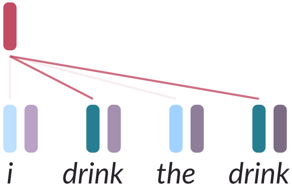
So, by default, self-attention **is unaware of sequential order**. (Unlike CNN or RNN encoders!)

Self-Attention for Sequences: Positional Embeddings



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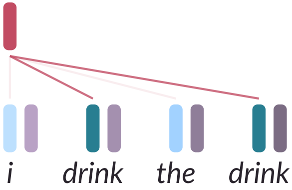

Add to each input vector an "offset" vector that encodes (only) the position in the sequence.

$\tilde{\boldsymbol{z}}_i = \boldsymbol{z}_i + \boldsymbol{p}_i$

Output now depends on the order: if permuting by σ, $\tilde{\boldsymbol{z}}_i = \boldsymbol{z}_{\sigma(i)} + \boldsymbol{p}_i$.

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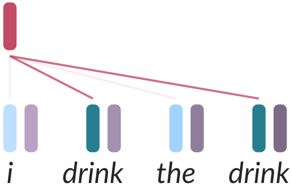

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Positional embeddings can be

1. fixed: e.g., based on trig functions of i.
2. learned: i.e., a separate `torch.nn.Embedding(num_embeddings=max_len)` through which we embed the sequence of position indices $(0, 1, 2, \ldots, n-1)$.

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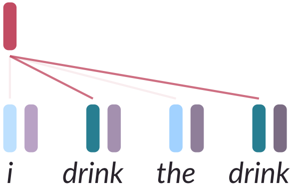
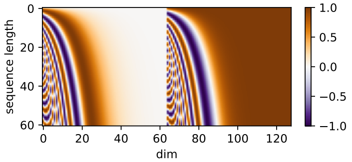


fixed sinusoidal embeddings:



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2. learned: i.e., a separate `torch.nn.Embedding(num_embeddings=max_len)` through which we embed the sequence of position indices $(0, 1, 2, \ldots, n-1)$.

(2) is easier to code, but (1) can generalize to sequences seen in training, due to its fixed pattern.

Self-Attention for Graphs

But hey: maybe permutation equivariance is sometimes a good thing!

For instance, for **graph neural networks!**

Remember in GNN we computed the message from neighbors as a sum:

$$\boldsymbol{m}_i = \sum_{j \in N(i)} \boldsymbol{z}_j$$

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Instead, self-attention over neighbors:

$$\alpha_{ij} = \frac{\exp(\boldsymbol{q}_i \cdot \boldsymbol{k}_j)}{\sum_{j' \in N(i)} \exp(\boldsymbol{q}_i \cdot \boldsymbol{k}_{j'})}$$
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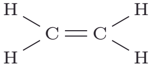
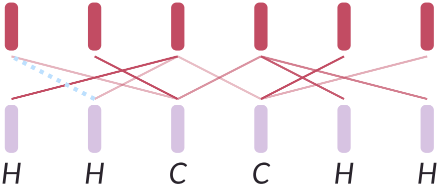
In other words: self-attention constrained by the adjacency structure

(no attention allowed where there is no edge)

Ethylene (C_2H_4): 



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Multi-Head Attention

Apply attention M times, independently, with different linear transformations to give different keys/vals/queries.

$$
\begin{aligned}
\boldsymbol{k}_i^{(m)} &= \boldsymbol{W}_K^{(m)\top} \boldsymbol{z}_i \\
\boldsymbol{v}_i^{(m)} &= \boldsymbol{W}_V^{(m)\top} \boldsymbol{z}_i \\
\boldsymbol{q}^{(m)} &= \boldsymbol{W}_Q^{(m)\top} \boldsymbol{q} \\
\boldsymbol{z}^{(m)} &= \mathrm{KeyValAttn}(\boldsymbol{q}, \boldsymbol{k}_{1,\ldots,n}^{(m)}, \boldsymbol{v}_{1,\ldots,n}^{(m)})
\end{aligned}
$$

and concatenate the outputs:

$$
\boldsymbol{z} = [\boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(M)}]
$$

Intuition: learn M different ways to look at the same set.

Multi-Head Attention In Code

$$\boldsymbol{k}_i^{(m)} = \boldsymbol{W}_K^{(m)\top} \boldsymbol{z}_i$$
$$\boldsymbol{v}_i^{(m)} = \boldsymbol{W}_V^{(m)\top} \boldsymbol{v}_i$$
$$\boldsymbol{q}^{(m)} = \boldsymbol{W}_Q^{(m)\top} \boldsymbol{q}$$
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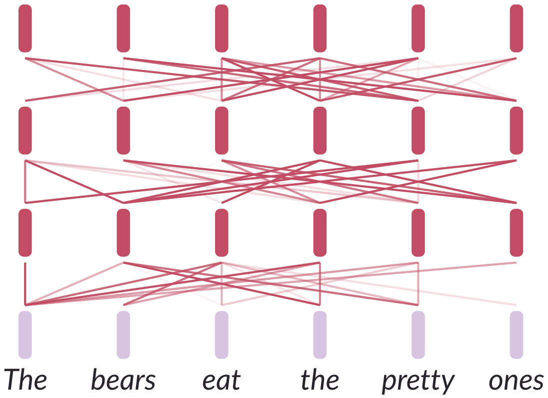
$$\boldsymbol{z} = [\boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(M)}]$$

```
zms = []

for m in range(M):
  Km = Z @ Wk[m]
  Vm = Z @ Wv[m]
  qm = q @ Wq[m]

  zm = softmax(Km @ qm) @ Vm
  zms.append(zm)

z = cat(zms)
```

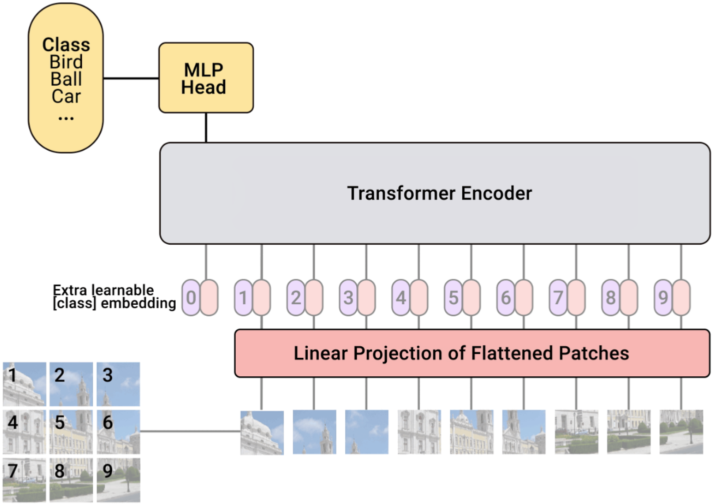
Transformer

Stacked multi-head attention (+ some annoying details like LayerNorm)



- Combines some of the strengths of CNN and RNN:
- Global even without much depth: every output depends on every input.
- Parallelizable: each position and each head can be computed separately. (still one layer at a time)
- Sequence-aware thanks to positional embeddings.

Vision Transformer (ViT)



Source: Google blog https://ai.googleblog.com/2020/12/transformers-for-image-recognition-at.html ©Dosovitskiy, Houlsby, Weissenborn, et al.

Wrapping Up

- Transformers are very popular right now. Important to understand why.
- All things being equal, my (and my friends') experience is that they are **harder to train** than RNNs and CNNs.
- But their parallelizable nature lets them make best use of today's best supercomputing hardware!
- It's not that two Transformer layers > two GRU layers.
  But, we can train deeper Transformers faster and longer (on more data), and currently this looks like the better trade-off.
  This will probably change!