Attention

Vojtěch Jindra

Outline

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2) The intuition behind attention
3) Transformer
4) Set Transformer
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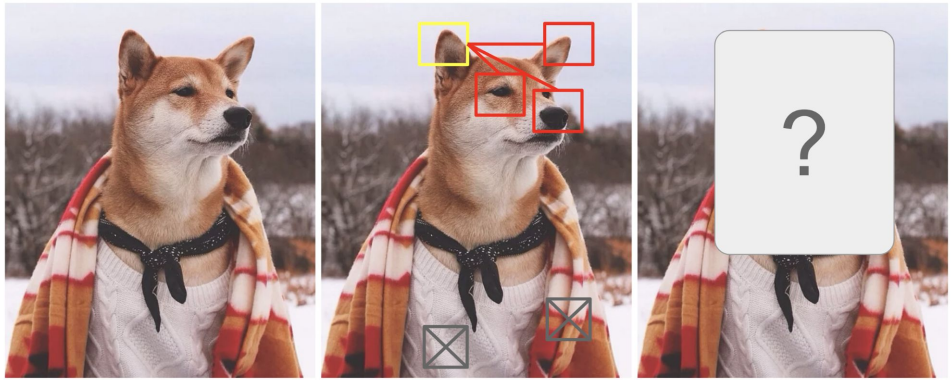
Motivation

- Initially used to improve seq2seq[1] models
- The idea of attention has spread to other applications as well
  - Neural Machine Translation (seq2seq)[2]
  - Speech recognition[3]
  - Graph attention networks[4]
  - Recommender systems[5]
  - Self-driving cars[6]
- Seq2seq models generate outputs iteratively from start of the sequence to its end
- With long sequences, the model tends to put less attention towards the start of the sequence
- Attention calculates a similarity vector between words to tell the model when to focus on what words

The intuition behind attention

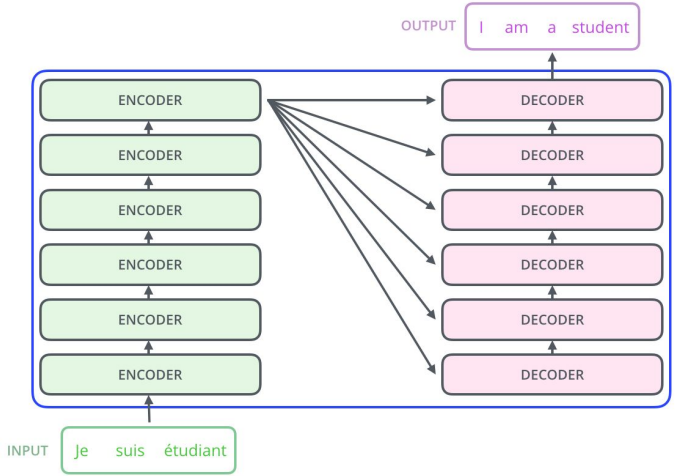
- Humans tend to put more attention towards words they want to translate in a sentence
  - When translating the sentence “Dude, look here!” to spanish (“¡Tío, mira aquí!”), one will put more attention towards the relationship between “Dude” and “Tío” than “Dude” and “aquí”
- Similarly, when figuring out what a picture is about, we put more more attention towards specific treats
  - When trying to classify if an animal is a dog, we will put more attention towards the dog-like features (e.g. ears) rather than to the general animal-like features (e.g. eyes)

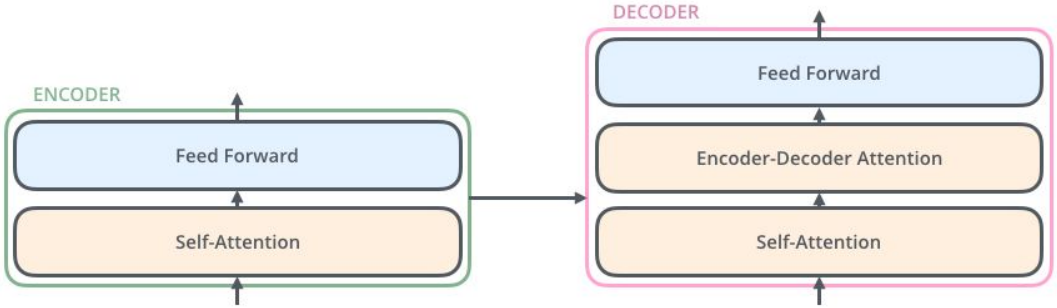


https://lilianweng.github.io/lil-log/2018/06/24/attention-attention.html

Transformer

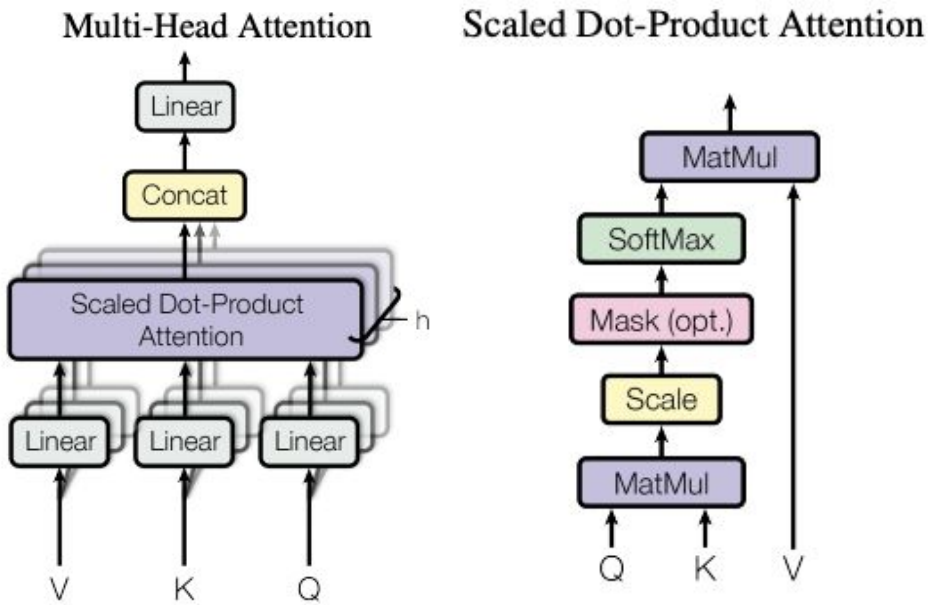
- The seq2seq with attention blackbox is called a Transformer
- Transformer is composed out of a stack of encoders and decoders (originally six of each)
- Inputs go sequentially through the encoders and then from the last encoder to each decoder
- Each encoder is composed of a self-attention component and a feed-forward NN
- Each decoder is composed of self-attention component, encoder-decoder attention component and a feed-forward NN





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

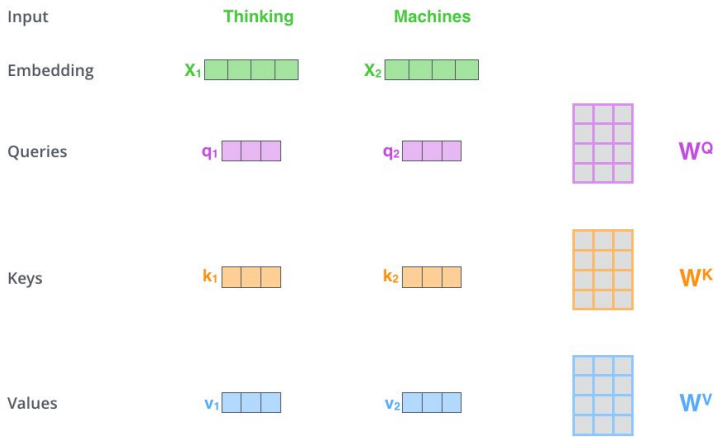
Self-attention in detail



https://arxiv.org/pdf/1706.03762.pdf

Query, key and value vectors

- Embedded input vectors are transformed into query, key and value vectors by multiplication with query, key and value weight matrices respectively



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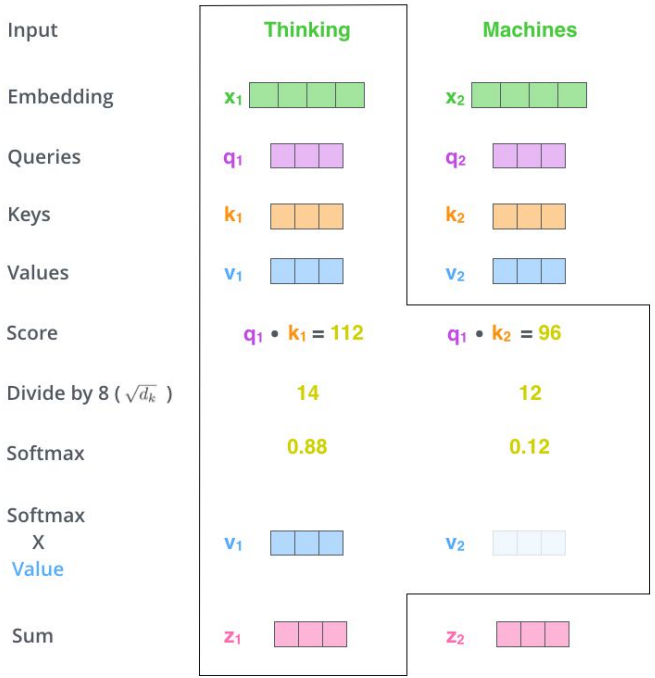
Scoring

- Each word is then compared to every other word to obtain scores between all words by multiplying the query vectors with the key vectors and normalizing them
- Each score is then multiplied with the value vector (to diminish irrelevant words) and then all the value vectors are summed and sent to the next encoder



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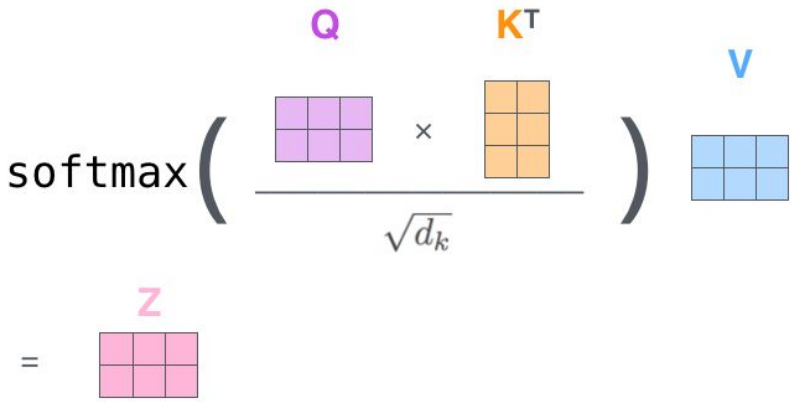
Attention as matrix multiplication

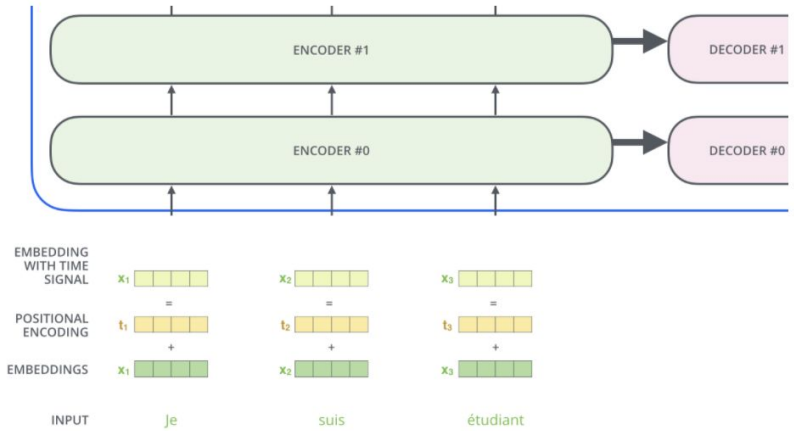
- Q^*K^T to produce scores
- Normalization of scores
- Softmax to get probabilities
- Multiply by V to get final score



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

Positional encoding

- We need to describe the position of each word in the sentence
- The Transformer adds a vector to each word's embedding
  - The vector follows a certain pattern about its position that the model learns



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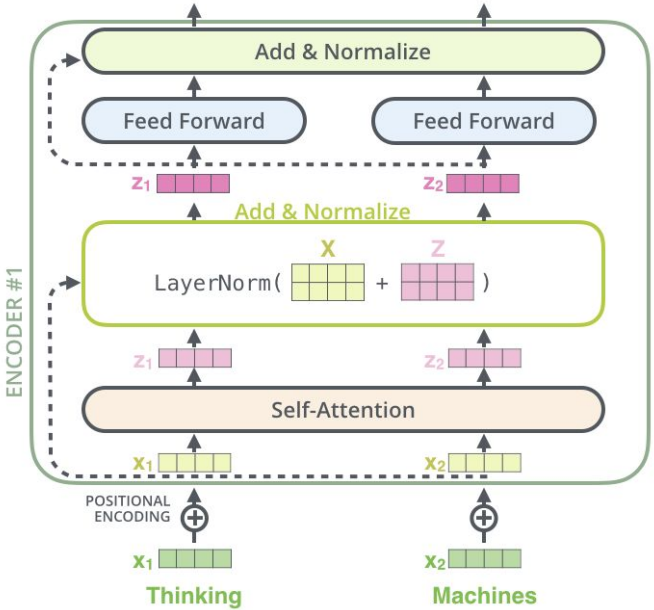
Residuals

- Each sub-layer in each encoder has a residual connection around it
- Therefore, sub-layers are followed by layer normalization layers



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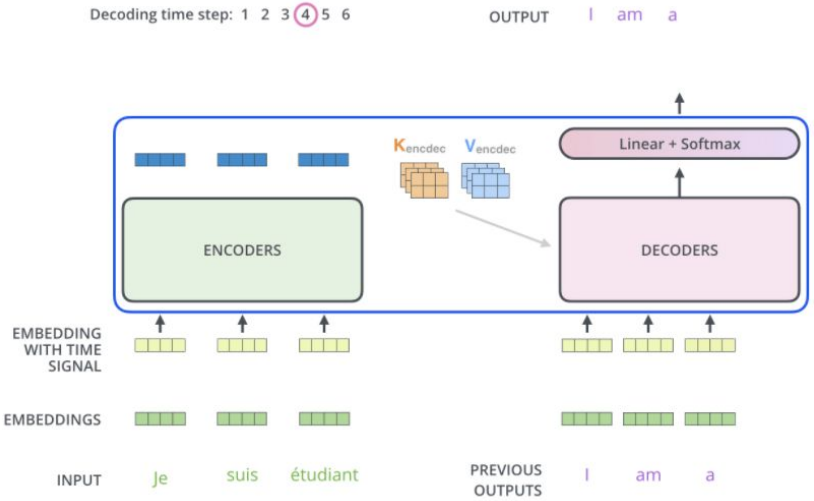
Layer Normalization

- Extension of Batch Normalization
- Batch Normalization is theoretically done on the mean and standard deviation of the whole dataset, which is impractical
- Instead, in practice the current mini-batch is used as an estimator of the mean and standard deviation
- Which puts constraint on the size of the mini-batch
- Layer Normalization overcomes the drawbacks by computing the mean and standard deviation on the current layer

Decoding

- Decoding works in a very similar way to encoding
- The last encoder passes its output to each decoder
  - There, it serves as the key and value matrices
- Query matrix is the output of the decoder one layer below
- Self-attention in the decoders are only allowed to attend to earlier position in the output sequence (which is solved with masking out the illegal connections)



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Converting outputs into a word

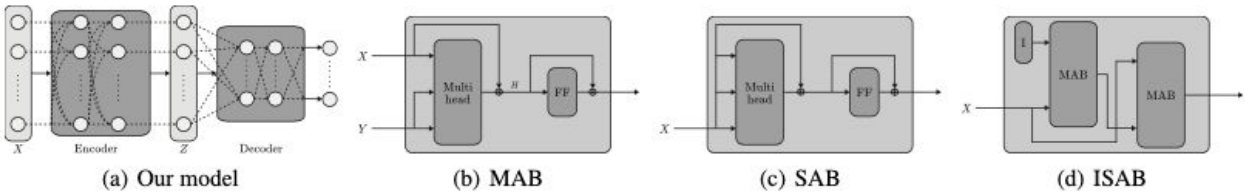
- Final layer after encoding and decoding is a feed-forward NN with a softmax layer
- The NN projects the output vectors into a logits vector that represents the whole english (for example) vocabulary
- The softmax layer produces a probability for each logit to be the final word
- The final word is simply the one with the highest probability

The loss function

- Input and output are probability distributions
- Kullback-Leibler divergence used to compare both distributions
- Each probability distribution is represented by a vector of the vocabularies
- Each word has a different probability distribution
    - “I” will have a distribution with “I” having the highest probability
    - “Am” will have a distribution with “am” having the highest probability
- This is plausible because the words are predicted one by one

Set Transformer

- Set Transformer[10] adjusts Transformer for sets that are required to be permutation invariant
- Presents a number of Set Attention Blocks
- Presents a parametrized pooling function that can adapt to the problem at hand
- Doesn't use positional encoding



https://arxiv.org/pdf/1810.00825.pdf

Multi-head Attention Block

- MAB(X, Y)
- Performs Multi-head attention between two input vectors and learnable parameters
- First vector is used as the query vector and second vector as both key and value vectors

$$\mathrm{MAB}(X, Y) = \mathrm{LayerNorm}(H + \mathrm{rFF}(H)), \tag{6}$$

$$\text{where } H = \mathrm{LayerNorm}(X + \mathrm{Multihead}(X, Y, Y; \omega)), \tag{7}$$

https://arxiv.org/pdf/1810.00825.pdf

Set Attention Block

- SAB(X) = MAB(X, X)
- Basically performs self-attention on given set X
- The output of SAB contains information about pairwise interactions among the elements of X
- Therefore, multiple SABs can be stacked to encode higher order interactions
- However, SAB has a quadratic complexity, which could be a problem for large sets

Induced Set Attention Block

- ISAB(X) = MAB(X, MAB(I, X))
- Inducing points I are trainable parameters of lower dimension
- MAB(I, X) attends the inducing points to the input set X
- Then again the first set is ran through MAB with X to produce the result
- The idea is to project X into a lower dimension, and then reconstruct it
- Unlike SAB's O(n^2) complexity, ISAB has O(nm) complexity, where m is typically a small number

Pooling by Multihead Attention

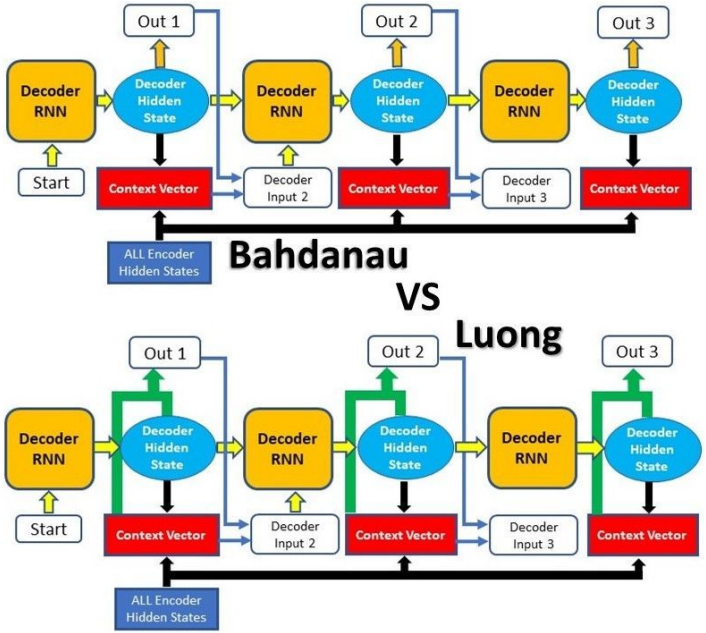
- $PMA_k(Z) = MAB(S, rFF(Z))$
- S is a set of k learnable seed vectors
- Output of PMA is a set of k items
- Those k seed vectors are then ran through SAB to further model the interactions
- $SAB(PMA_k(Z))$
- This has been shown only empirically that it increases the performance

Broad categories of attention mechanism

- Self-attention[7]
  - Relating different positions of the same input sequence
- Global/Soft[8]
  - Attending to the entire input state space
- Local/Hard[9]
  - Attending to a part of the input state space (e.g. a part of an image)
  - Predicts a single position and then computes a context vector in a window around that position

Popular attention mechanisms

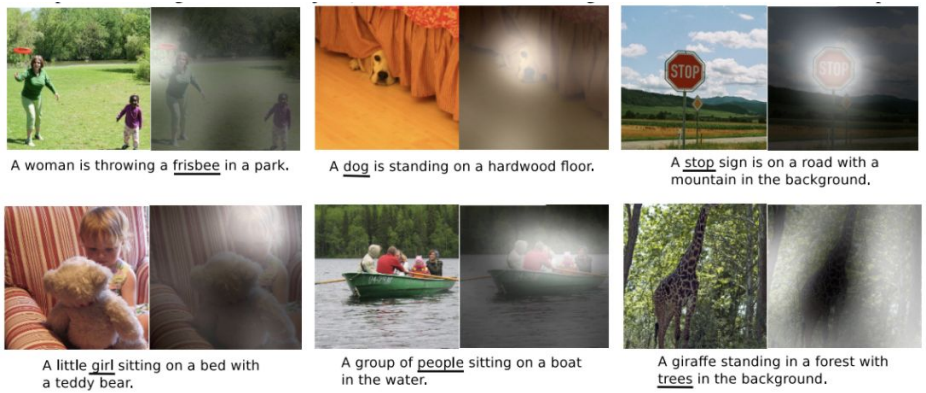
- General: score(s_t, h_i) = $s_t^T W_a h_i$ where W_a is a trainable weight matrix
- Dot-Product: score(s_t, h_i) = $s_t^T h_i$
- Scaled Dot-Product: score(s_t, h_i) = $s_t^T h_i$ / √n
- Content-based attention: score(s_t, h_i) = cos($s_t^T h_i$)



https://blog.floydhub.com/attention-mechanism/

Application: Image Captioning

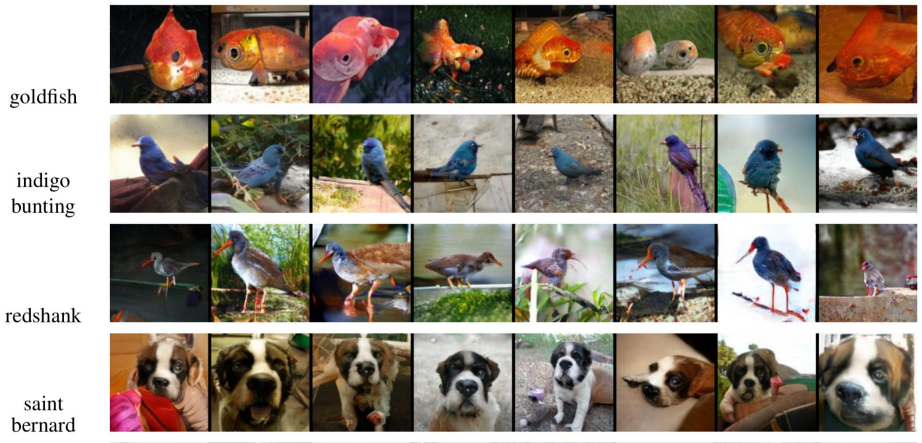
- Show, Attend and Tell: Neural Image Caption Generation with Visual Attention
- Attempts to align the input image and output word
- Captions are aligned with specific parts of the image, highlighting the relevant objects



https://lilianweng.github.io/lil-log/2018/06/24/attention-attention.html#born-for-translation

Application: Image Generation

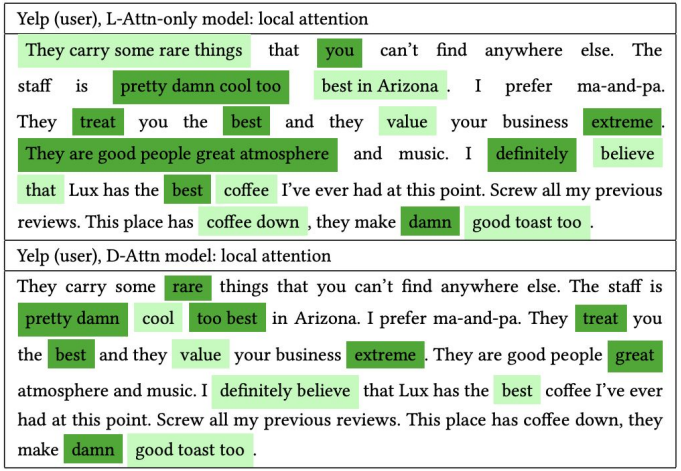
- Self-Attention Generative Adversarial Networks



https://arxiv.org/pdf/1805.08318.pdf

Application: Sentiment Analysis/Recommender Systems

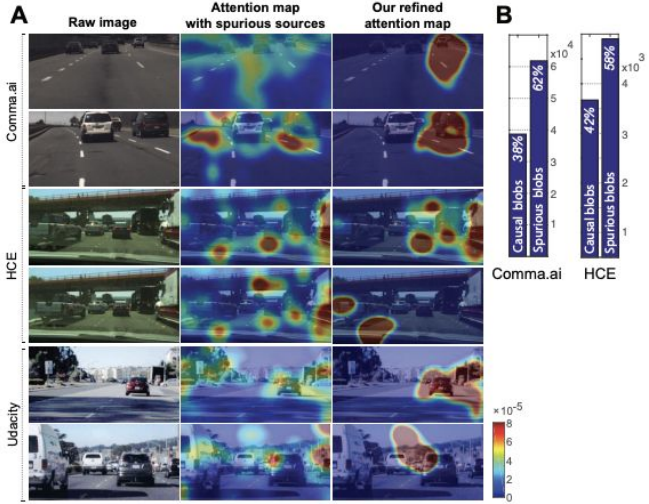
- Interpretable Convolutional Neural Networks with Dual Local and Global Aention for Review Rating Prediction
- Predicts importance of a ward in a sentence
- From that, builds up a recommender system



https://dl.acm.org/doi/10.1145/3109859.3109890

Application: Self-driving cars

- [Interpretable Learning for Self-Driving Cars by Visualizing Causal Attention]
- Uses local attention to spot places of a self-driving car's interest



https://arxiv.org/pdf/1710.10903.pdf

Demo

https://colab.research.google.com/github/tensorflow/tensor2tensor/blob/master/tensor2tensor/notebooks/hello_t2t.ipynb#scrollTo=OJKU36QAfqOC

Further reading

- https://jalammar.github.io/illustrated-transformer/
- https://lilianweng.github.io/lil-log/2018/06/24/attention-attention.html
- https://buomsoo-kim.github.io/attention/2020/01/01/Attention-mechanism-1.md/
- https://blog.floydhub.com/attention-mechanism/
- https://icml.cc/media/Slides/icml/2019/halla(10-09-15)-10-15-45-4343-a_tutorial_on.pdf

References

[1] Sequence to Sequence Learning with Neural Networks

[2] Attention Is All You Need

[3] Attention-Based Models for Speech Recognition

[4] Graph Attention Networks

[5] Multi-Pointer Co-Attention Networks for Recommendation

[6] Interpretable Learning for Self-Driving Cars by Visualizing Causal Attention

[7] Long Short-Term Memory-Networks for Machine Reading

[8] Show, Attend and Tell: Neural Image Caption Generation with Visual Attention

[9] Effective Approaches to Attention-based Neural Machine Translation

[10] Set Transformer: A Framework for Attention-based Permutation-Invariant Neural Networks

Thanks for your attention!