Adaptively Sparse Transformers

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github.com/deep-spin/entmax goncalomcorreia.github.io

TL;DL (Too Long; Didn't Listen)

We replace the softmax function in Transformers with α-entmax, creating a model that is able to learn its own sparsity in each attention head.

(Bahdanau et al., 2015)

A bit of context... On Seq2Seq

United Nations elections end today

Slide Credit: Vlad Niculae

(Bahdanau et al., 2015)

A bit of context… On Seq2Seq

Encoder

(Bahdanau et al., 2015)

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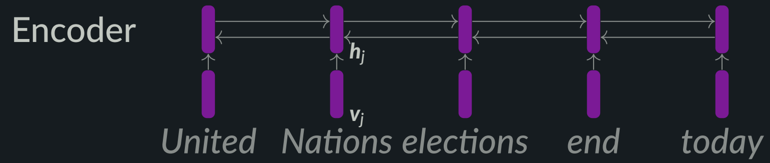

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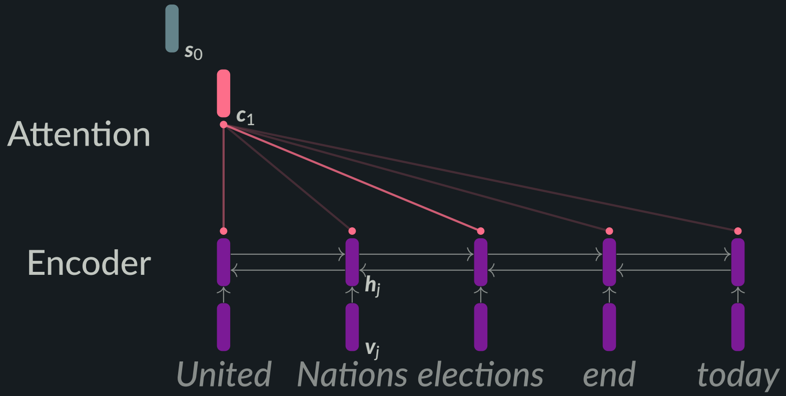

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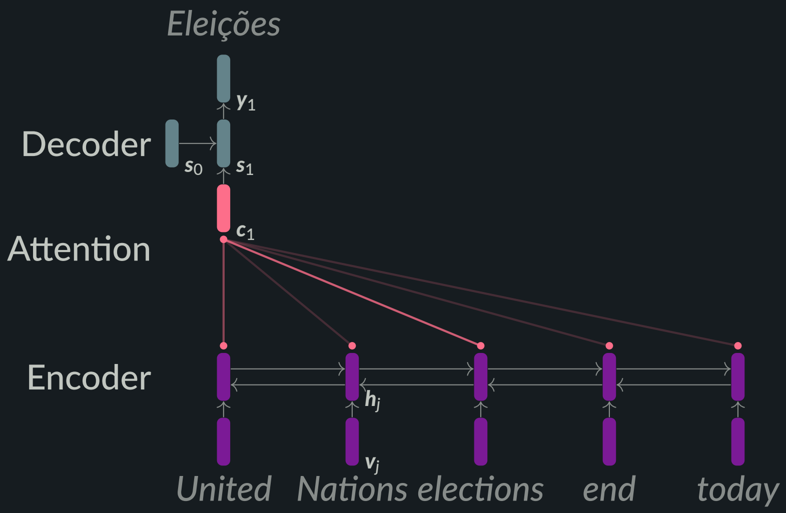

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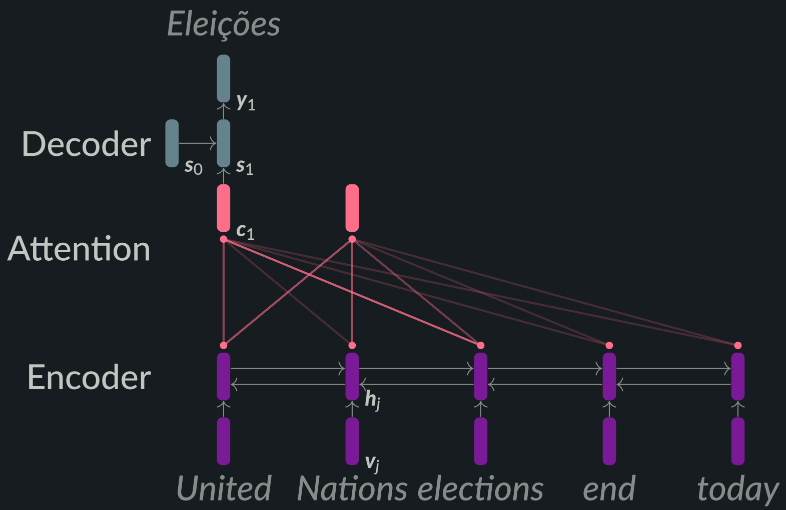

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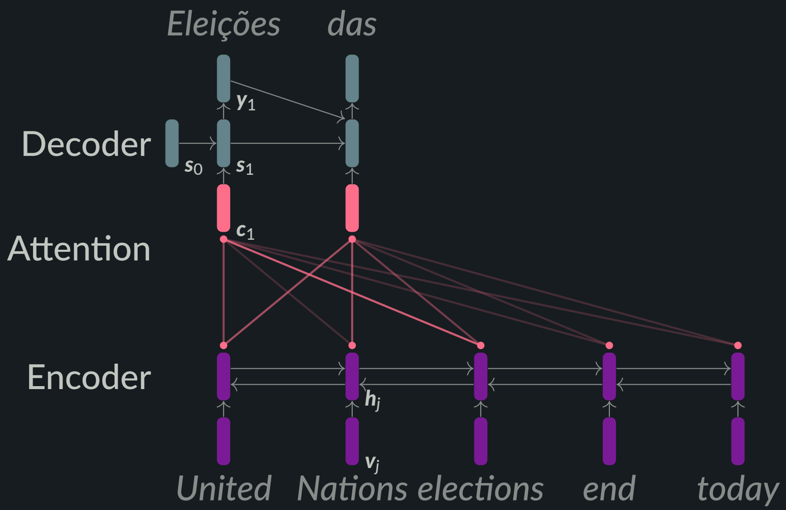

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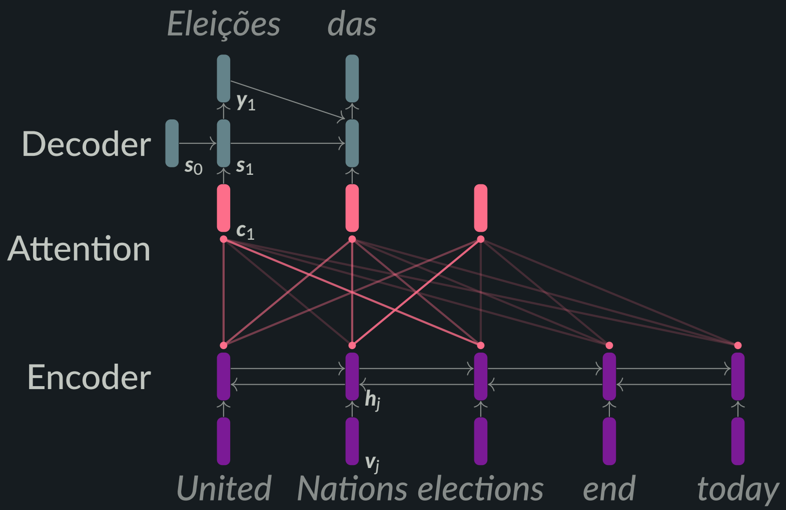

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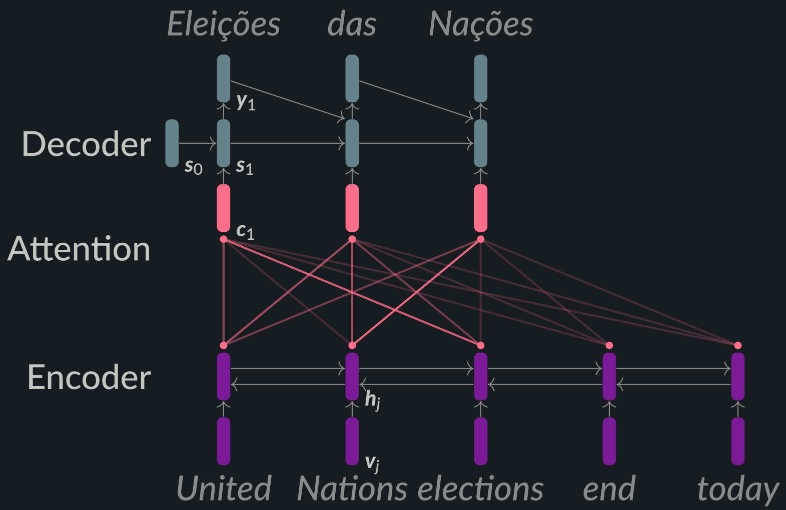

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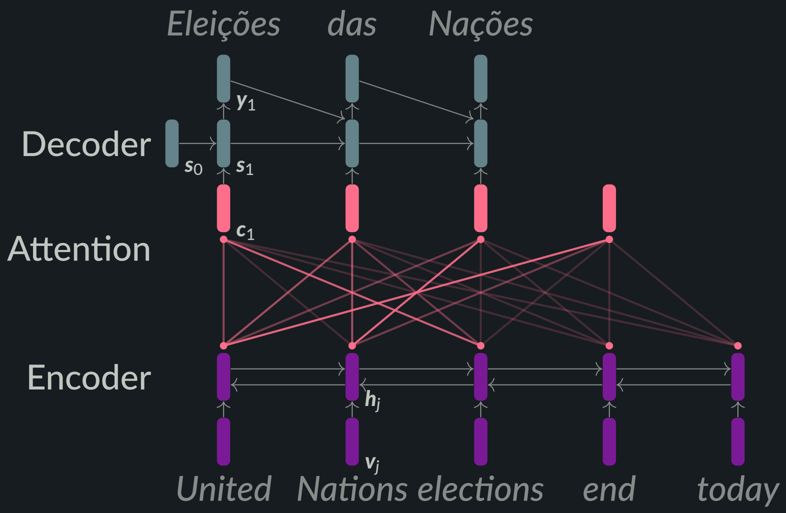

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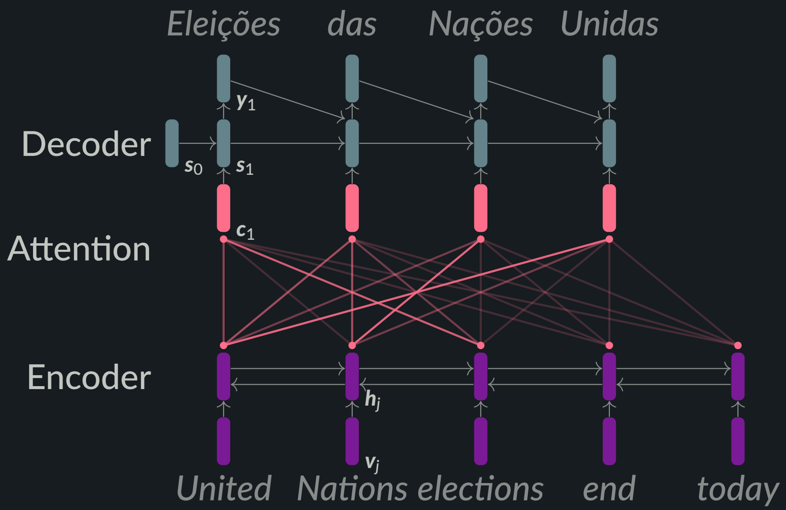


attention weights computed with *softmax*:

for some decoder state s_t, compute contextually weighted average of input c_t:

$$z_j = \boldsymbol{s}_t^\top \boldsymbol{W}^{(a)} \boldsymbol{h}_j$$

$$\pi_j = \operatorname{softmax}_j(\boldsymbol{z})$$

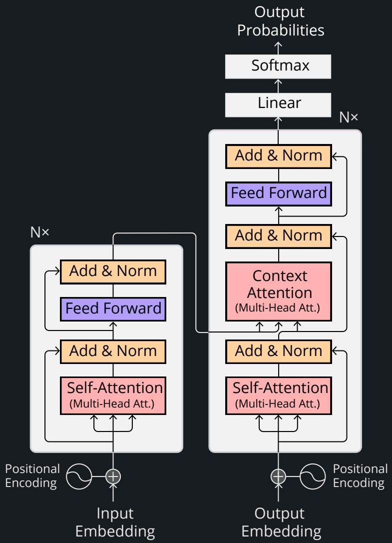
$$\boldsymbol{c}_t = \sum_j \pi_j \boldsymbol{h}_j$$

Slide Credit: Vlad Niculae

(Vaswani et al., 2017)

A bit of context… on Transformers

What if… Attention is all you need?



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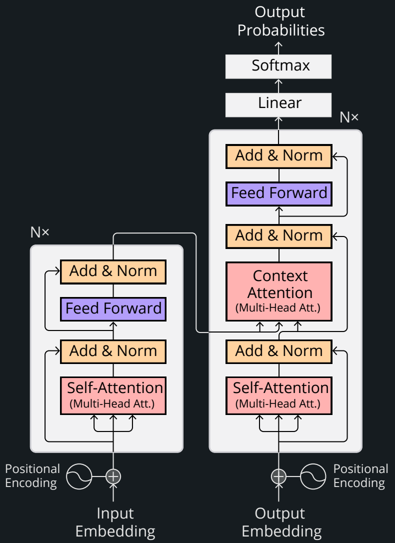
Key idea: Instead of Recurrent Neural Networks (RNNs), let's use attention mechanisms!



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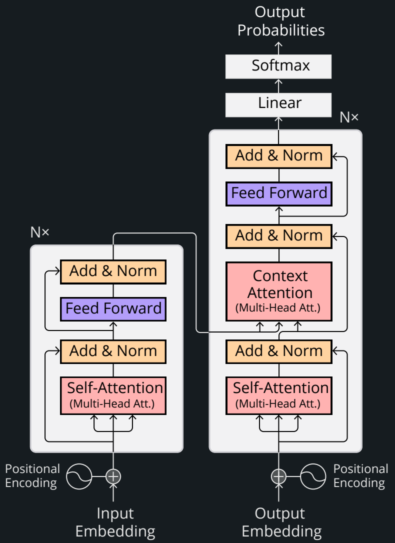

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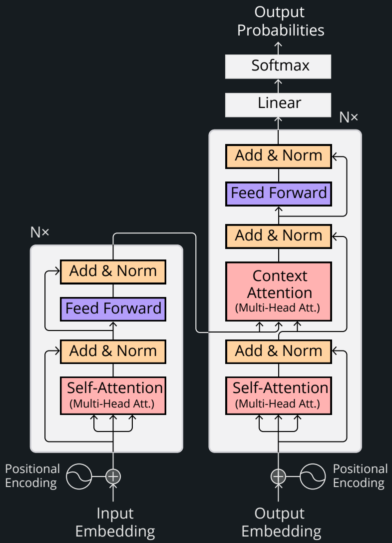

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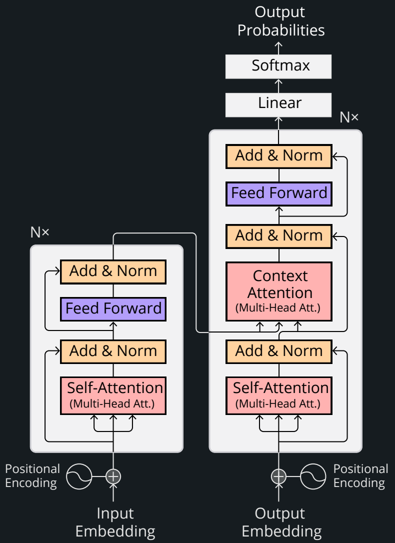
- ... and do it through several layers



Introduction

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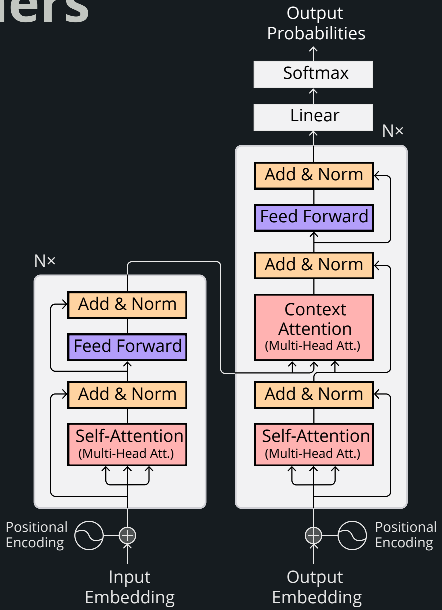
Transformers

In each attention head:

$$\bar{V} = \textbf{softmax}\left(\frac{QK^\top}{\sqrt{d_k}}\right)V.$$



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Attention in three places:

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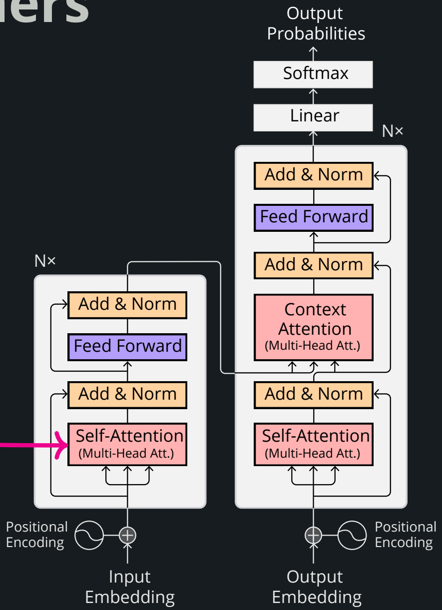

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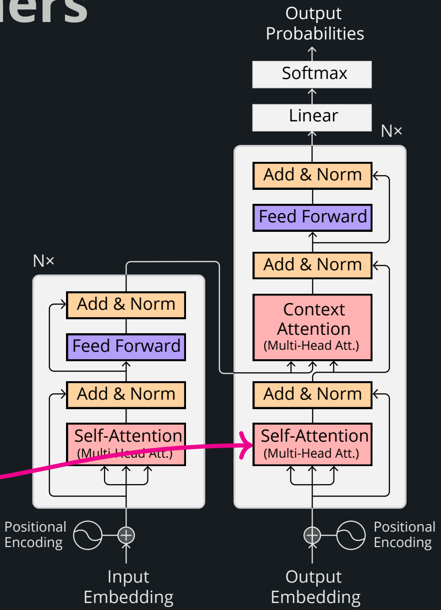

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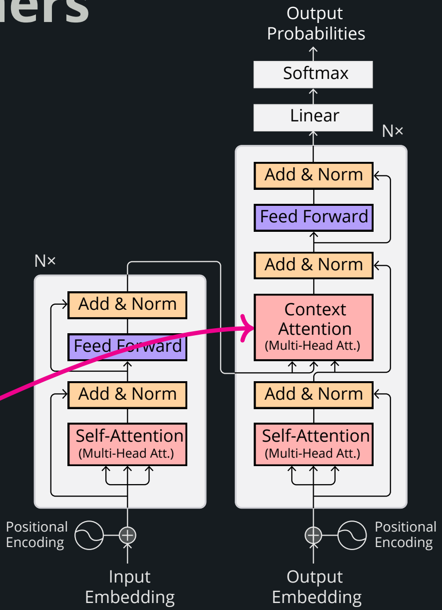
Transformers

In each attention head:

$$\bar{V} = \mathbf{softmax}\left(\frac{QK^{T}}{\sqrt{d_k}}\right)V.$$

Attention in three places:

- Self-attention in the encoder
- Self-attention in the decoder
- Contextual attention



Sparse Transformers

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Adaptively Sparse Transformers

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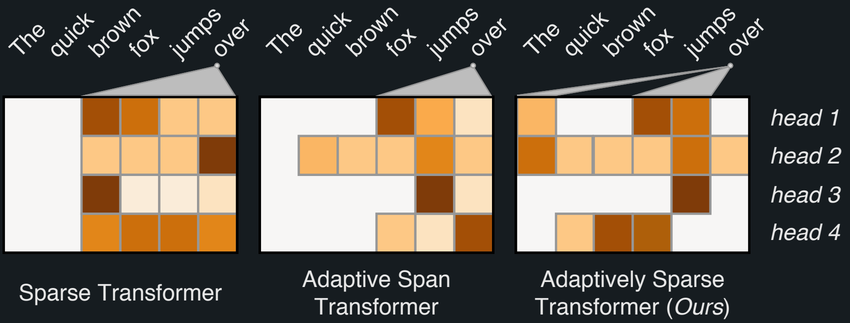
Another key idea: use a normalizing function that is adaptively sparse via a learnable α! 🙌 🙌 🙌

(Child et al., 2019; Sukhbaatar et al., 2019)

Related Work: Other Sparse Transformers



Our model allows non-contiguous attention for each head.

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- Retrieves a **one-hot vector** for the highest scored index.
- Sometimes used as hard attention, but not differentiable!

(Niculae and Blondel, 2017)

Ω-Regularized Argmax

For convex Ω, define the **Ω-regularized argmax transformation**:

$$\mathbf{argmax}_{\Omega}(\boldsymbol{z}) := \arg\max_{\boldsymbol{p} \in \triangle} \boldsymbol{z}^\top \boldsymbol{p} - \Omega(\boldsymbol{p})$$

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(Martins and Astudillo, 2016)

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Is there something in-between?

α-Entmax

Parametrized by $\alpha \geq 0$:

$$\Omega_\alpha(\boldsymbol{p}) := \begin{cases} \frac{1}{\alpha(\alpha-1)}\left(1 - \sum_{i=1}^{K} p_i^\alpha\right) & \text{if } \alpha \neq 1 \\ \sum_{i=1}^{K} p_i \log p_i & \text{if } \alpha = 1. \end{cases}$$

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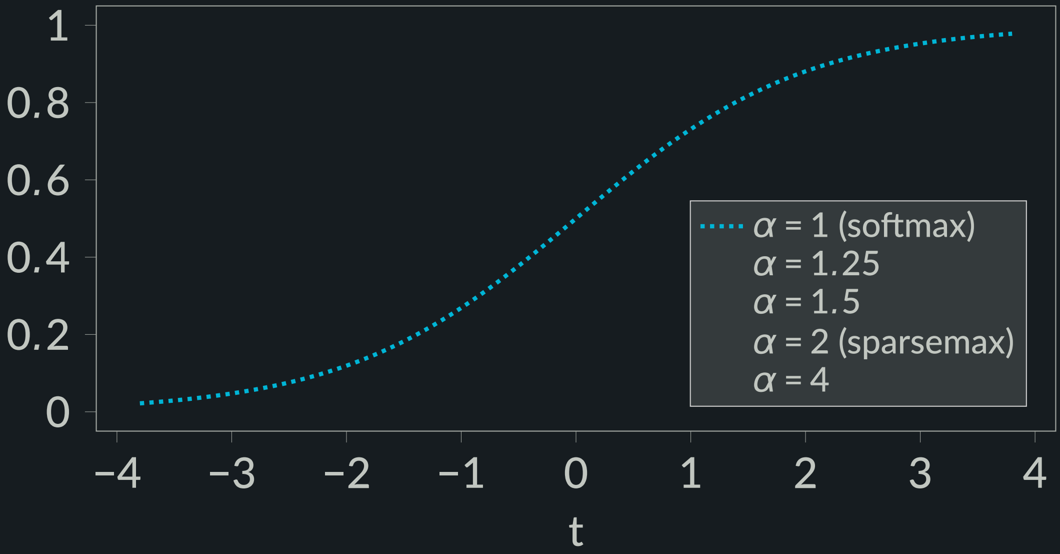
Key result: **can be sparse for** $\alpha > 1$, propensity for sparsity increases with α.



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α = 1 (softmax)
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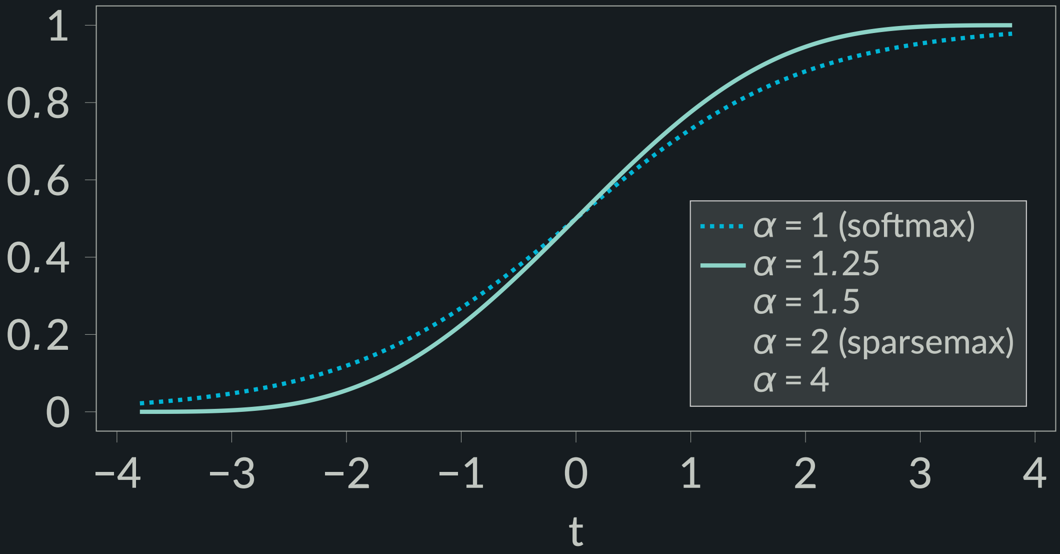
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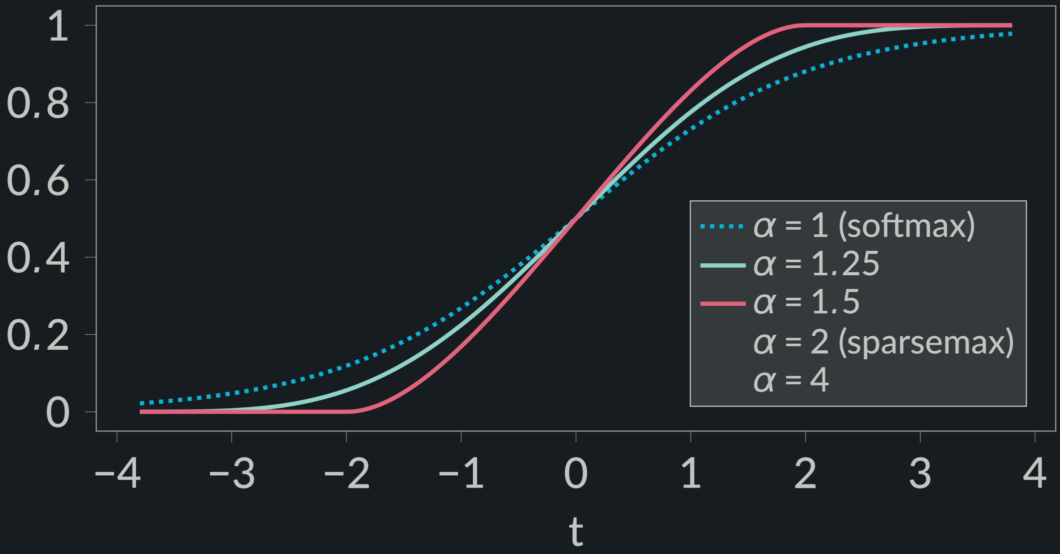

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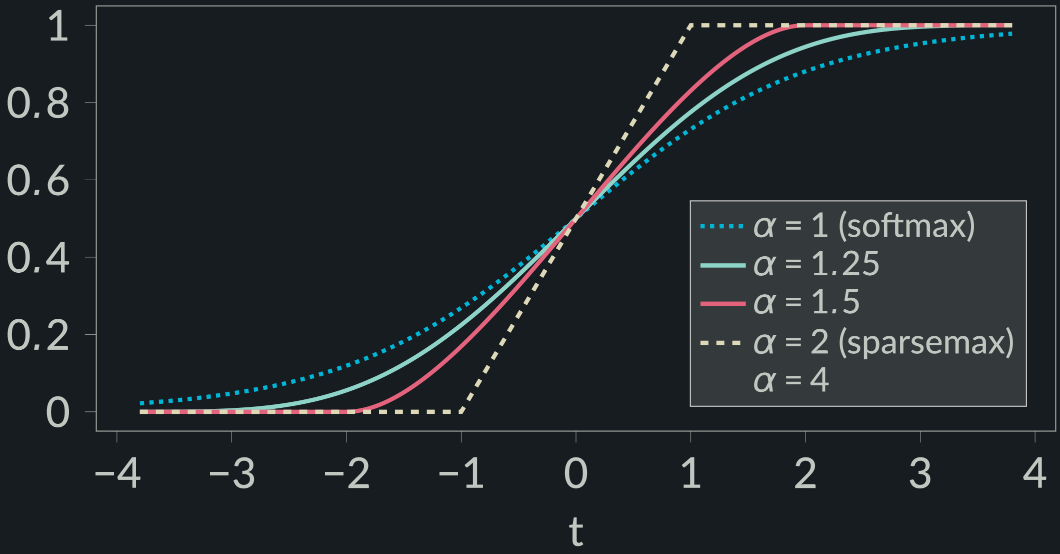
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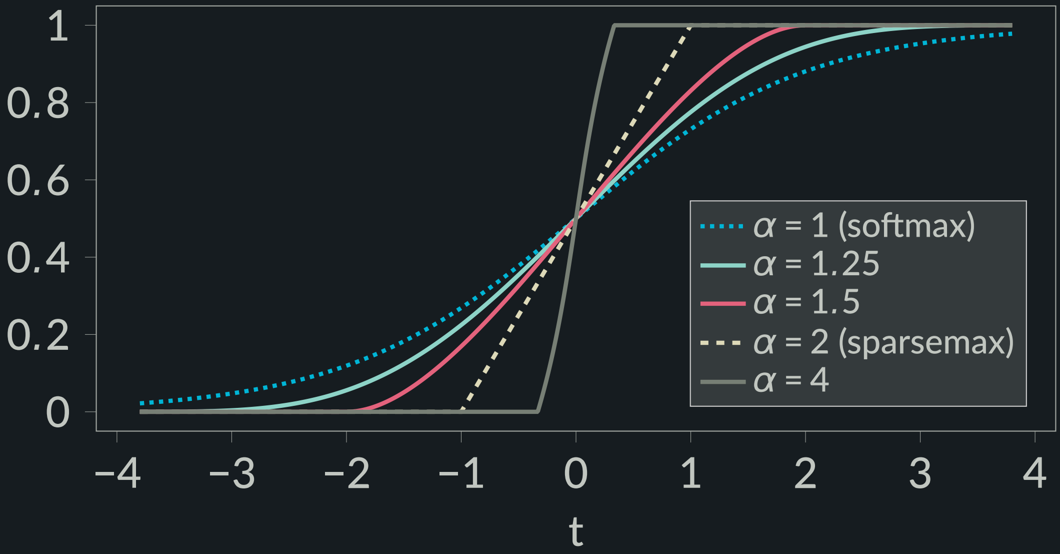
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Key contribution:

a closed-form expression for $\dfrac{\partial\, \alpha\text{-entmax}(\mathbf{z})}{\partial \alpha}$ 😱

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Requires argmin differentiation $\rightarrow$ see paper for details!

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Key co

a cl

:pip install entmax

Check `github.com/deep-spin/entmax`

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BLEU Scores

activation	de→en	ja→en	ro→en	en→de
softmax	29.79	21.57	32.70	26.02
1.5-entmax	29.83	22.13	33.10	25.89
α-entmax	29.90	21.74	32.89	26.93

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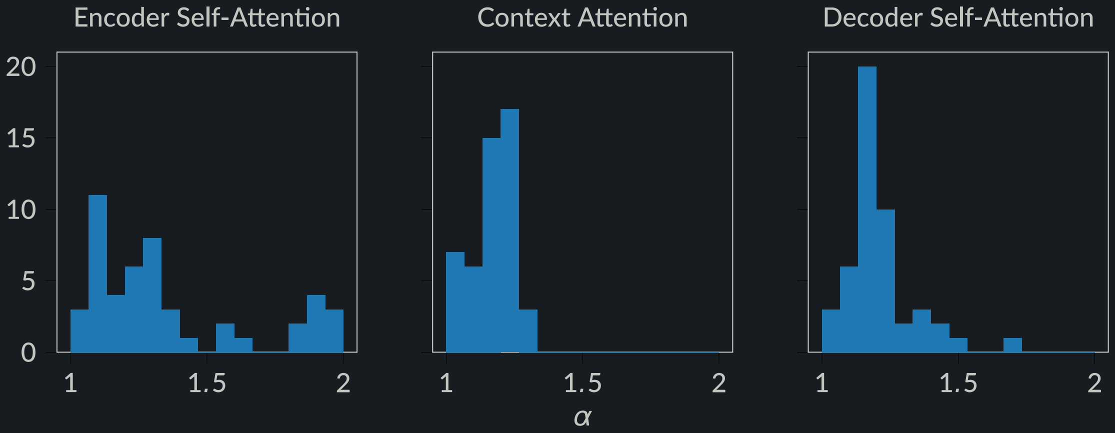
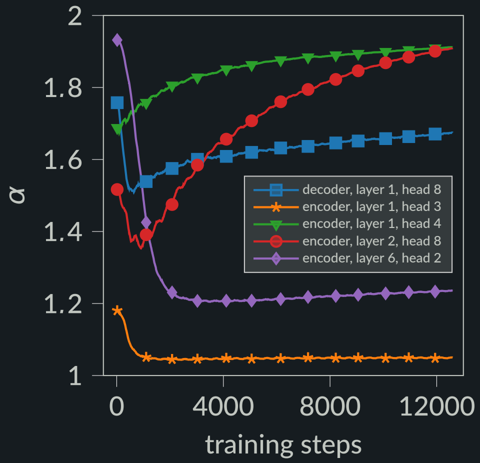
For analysis for other language pairs, see Appendix A.

Learned α



Bimodal for the encoder, mostly unimodal for the decoder.

Trajectories of α During Training



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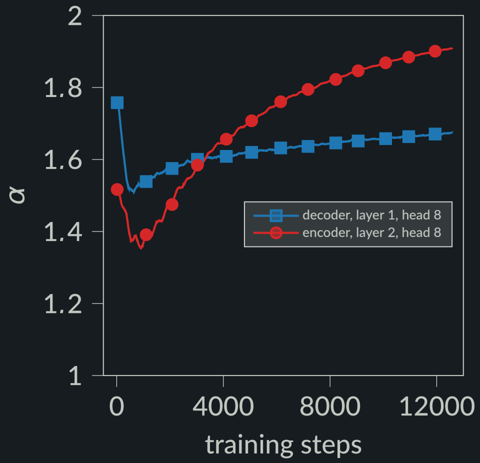
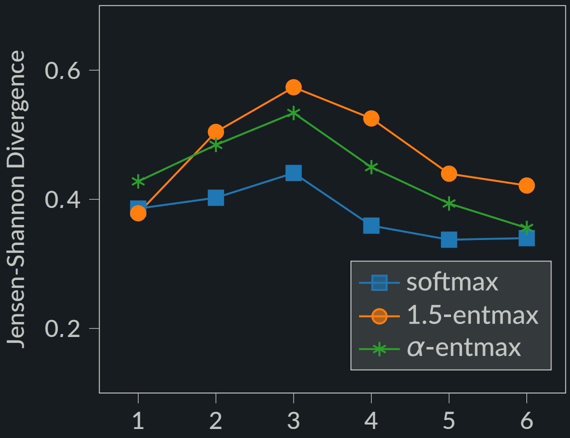


Some heads choose to start dense before becoming sparse.

Head Diversity per Layer



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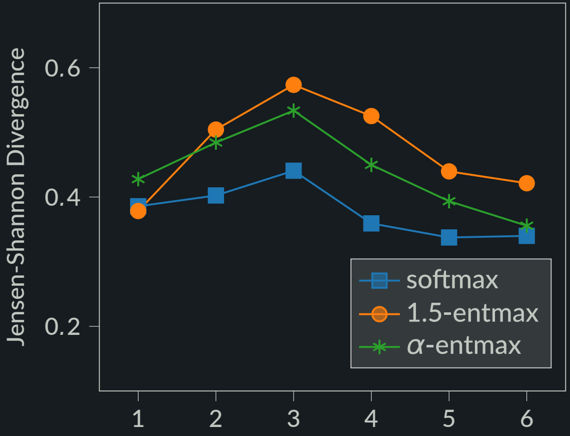
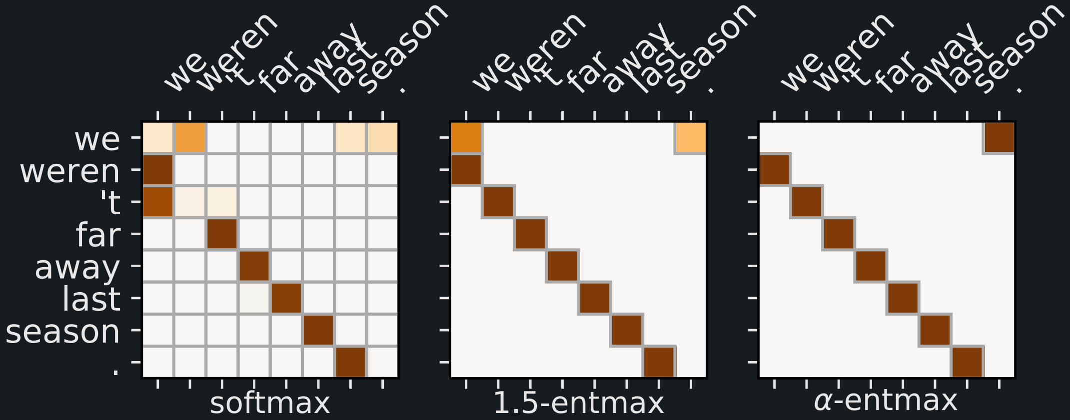


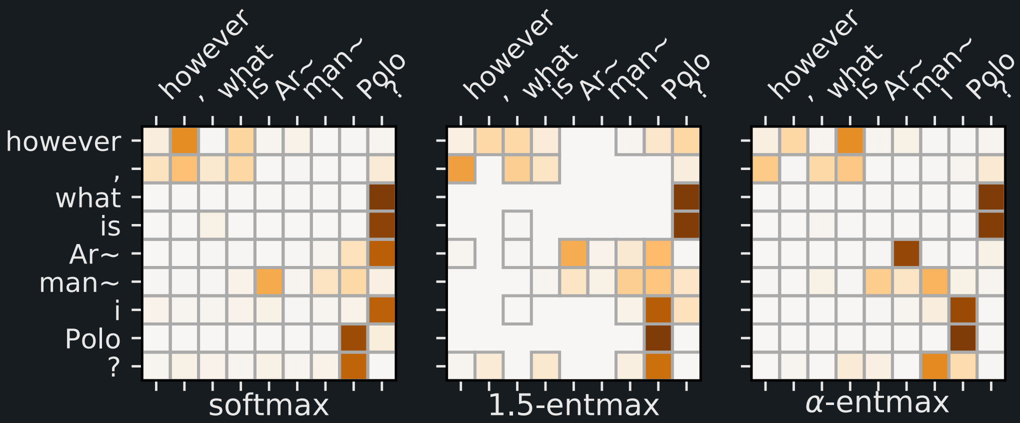
Specialized heads are important as seen in Voita et al. (2019)!

Previous Position Head



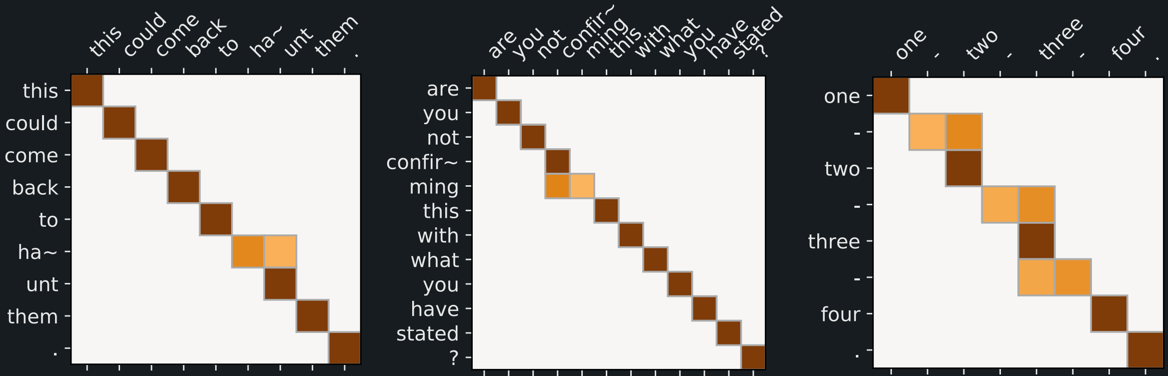
This head role was also found in Voita et al. (2019)! Learned $\alpha = 1.91$.

Interrogation-Detecting Head



Learned $\alpha = 1.05$.

Subword-Merging Head



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Key Takeaways

Introduce adaptive sparsity
for Transformers via α-entmax with a gradient learnable α.

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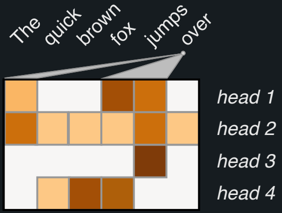
adaptive sparsity

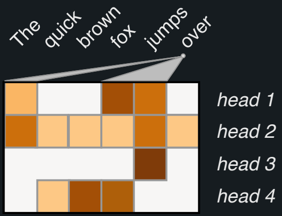


github.com/deep-spin/entmax goncalomcorreia.github.io

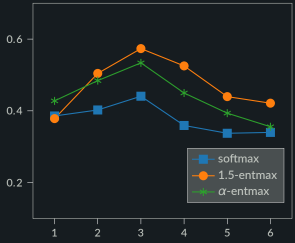
Key Takeaways

Introduce adaptive sparsity
for Transformers via α-entmax with a gradient learnable α.

adaptive sparsity



reduced head redundancy



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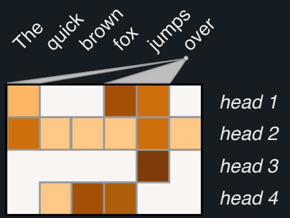
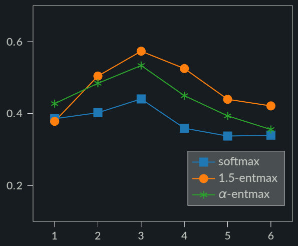
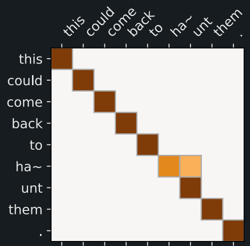


reduced head redundancy



clearer head roles



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Thank you!

Questions?

`:pip install entmax`

Check `github.com/deep-spin/entmax`

Acknowledgements

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References I

Bahdanau, Dzmitry, Kyunghyun Cho, and Yoshua Bengio (2015). “Neural machine translation by jointly learning to align and translate”. In: *Proc. of ICLR*.

Child, Rewon, Scott Gray, Alec Radford, and Ilya Sutskever (2019). “Generating long sequences with sparse transformers”. In: *arXiv preprint arXiv:1904.10509*.

Martins, André FT and Ramón Fernandez Astudillo (2016). “From softmax to sparsemax: A sparse model of attention and multi-label classification”. In: *Proc. of ICML*.

Niculae, Vlad and Mathieu Blondel (2017). “A Regularized Framework for Sparse and Structured Neural Attention”. In: *arXiv preprint arXiv:1705.07704*.

Peters, Ben, Vlad Niculae, and André F. T. Martins (2019). “Sparse Sequence-to-Sequence Models”. In: *Proceedings of the Annual Meeting of the Association for Computational Linguistics*.

Sukhbaatar, Sainbayar, Edouard Grave, Piotr Bojanowski, and Armand Joulin (2019). “Adaptive Attention Span in Transformers”. In: *arXiv preprint arXiv:1905.07799*.

Vaswani, Ashish, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N. Gomez, Lukasz Kaiser, and Illia Polosukhin (2017). “Attention Is All You Need”. In: *Proc. of NeurIPS*.

Voita, Elena, David Talbot, Fedor Moiseev, Rico Sennrich, and Ivan Titov (2019). “Analyzing multi-head self-attention: Specialized heads do the heavy lifting, the rest can be pruned”. In: *Proc. ACL*.