Learnable Sparsity and Weak Supervision for Data-efficient, Transparent, and Compact Neural Models

Gonçalo M. Correia

Jury: André Martins, Mário Figueiredo, Ivan Titov, Wilker Aziz, Isabel Trancoso

Deep learning successes

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- Subset of machine learning that uses **neural networks**

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- Powerful tool for learning representations of any data

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- Powerful tool for learning representations of any data
- Remarkable results

Deep learning successes

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Deep learning successes

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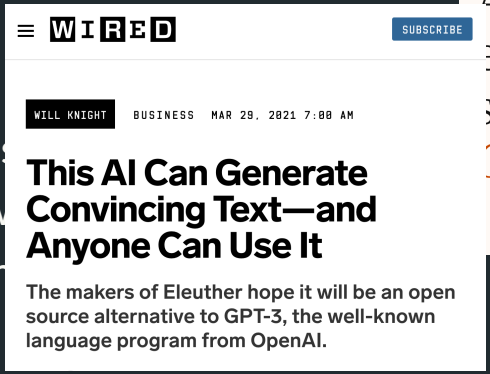

Deep learning successes

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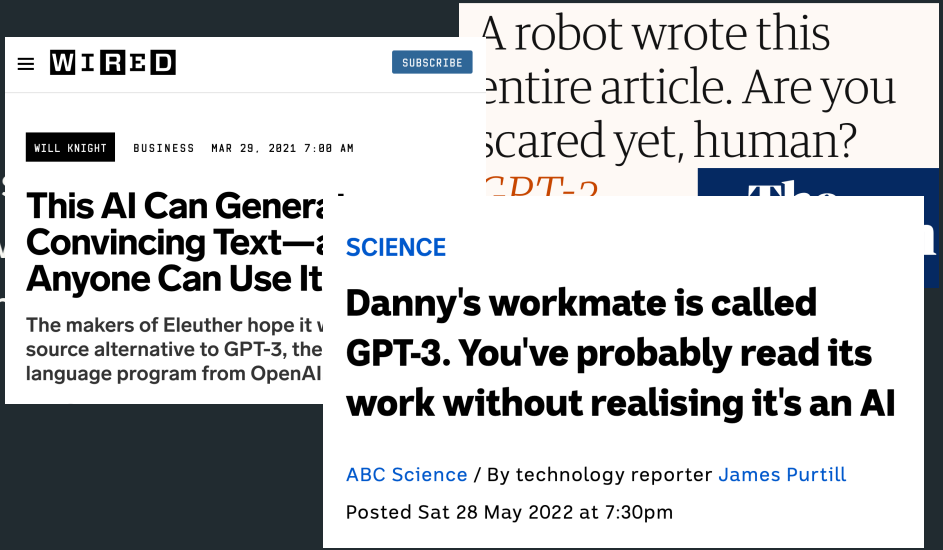

Deep learning successes

- Subs
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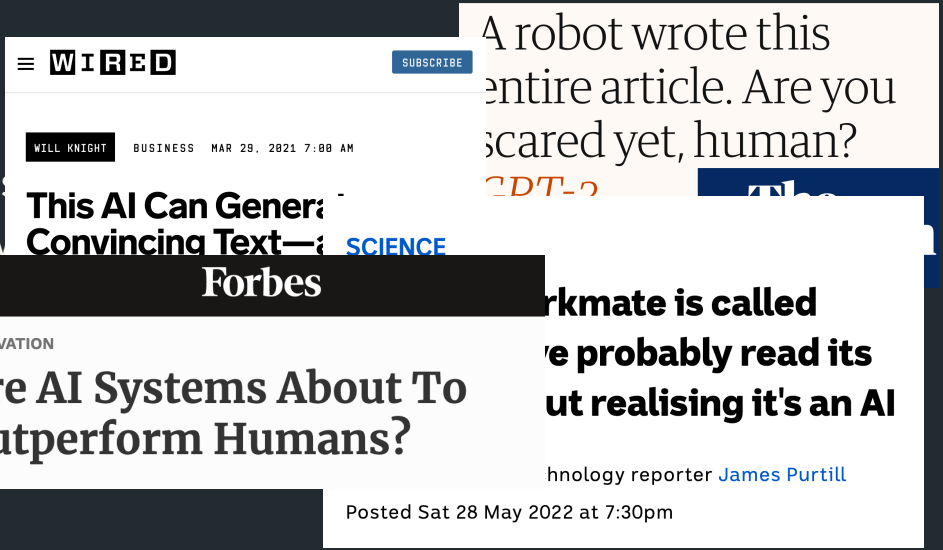
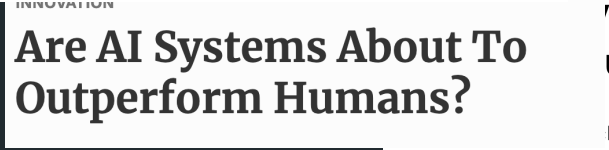
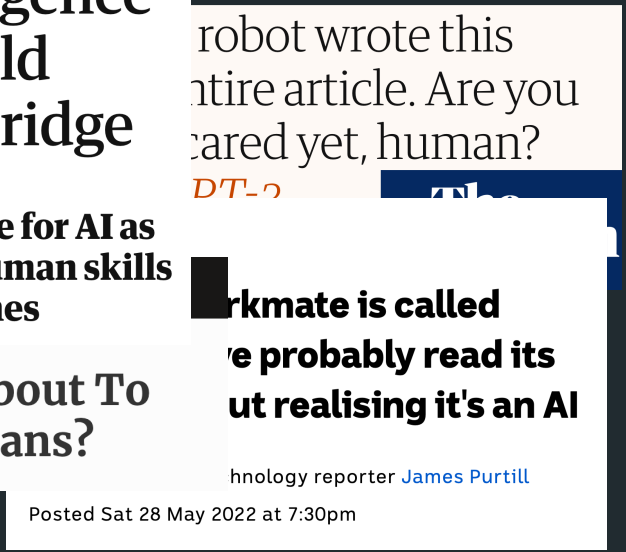
- F



Deep learning successes





Deep learning successes

Artificial intelligence beats eight world champions at bridge

Victory marks milestone for AI bridge requires more human sk than other strategy games

INNOVATION

Are AI Systems About T Outperform Humans?

Posted Sa

robot wrote this

AI 'outperforms' doctors diagnosing breast cancer

Fergus Walsh
Medical correspondent
@BBCFergusWalsh

Deep learning limitations and drawbacks

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- Requires a lot of data

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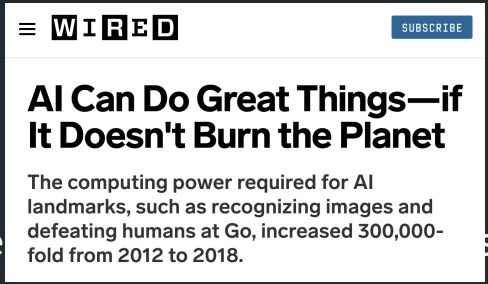

Deep learning limitations and drawbacks

- Req
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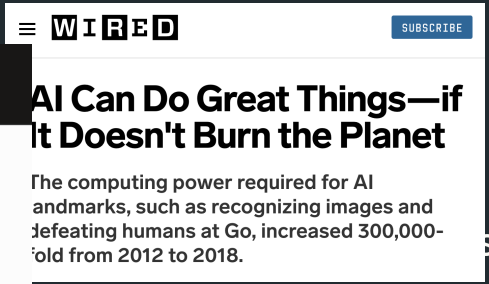

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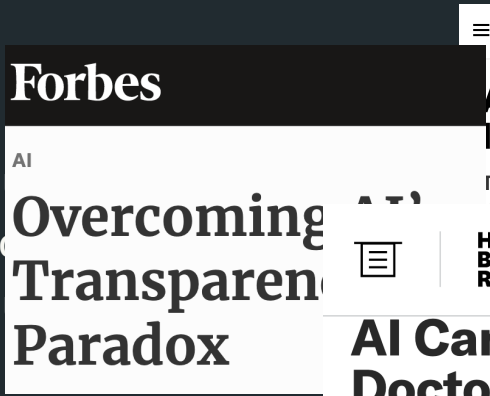

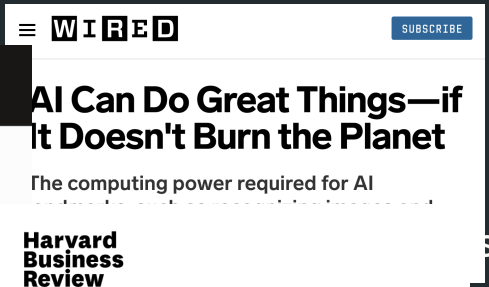

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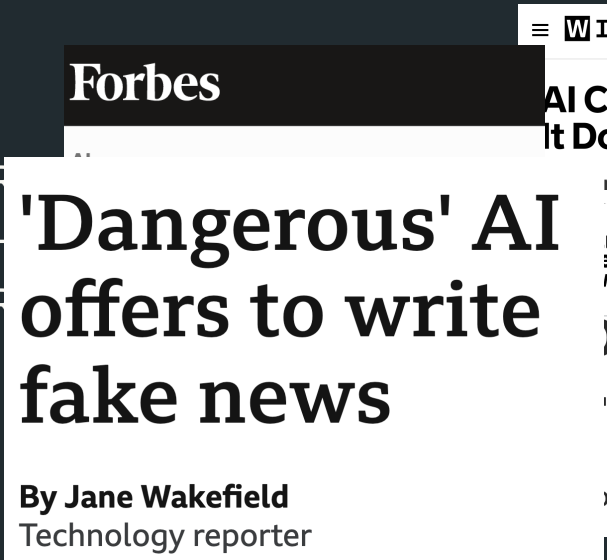

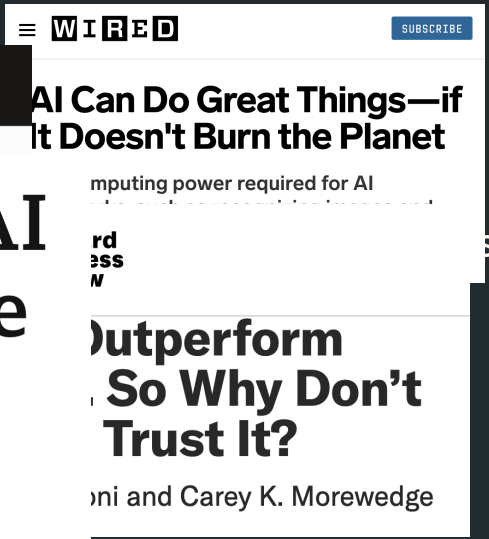

sions

Key concepts of this thesis

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Learnable Sparsity and **Weak Supervision**
for **Data-efficient**, **Transparent**, and **Compact**
Neural Models

Published work of this thesis

(Correia and Martins, 2019)

Published work of this thesis

- Automatic Post-Editing using weak supervision for data-efficiency (ACL)

(Correia, Niculae, and Martins, 2019)

Published work of this thesis

- Automatic Post-Editing using weak supervision for data-efficiency (ACL)
- Letting transformer learn sparsity of its attentions for transparency (EMNLP)

(Correia, Niculae, Aziz, and Martins, 2020)

Published work of this thesis

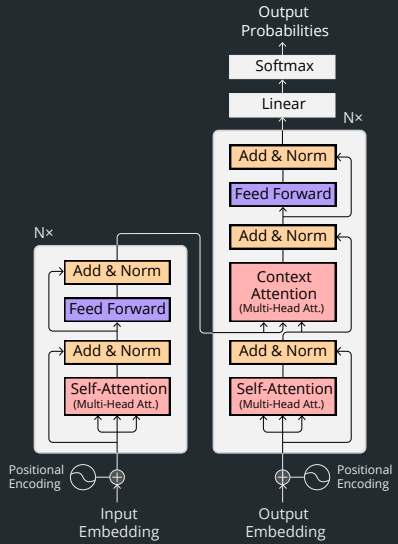
- Automatic Post-Editing using weak supervision for data-efficiency (ACL)
- Letting transformer learn sparsity of its attentions for transparency (EMNLP)
- General strategy for efficiently training discrete latent variable models, to have compactness (NeurIPS)

Table of Contents

(Vaswani et al., 2017)

A bit of context on transformers

What if... Attention is all you need?



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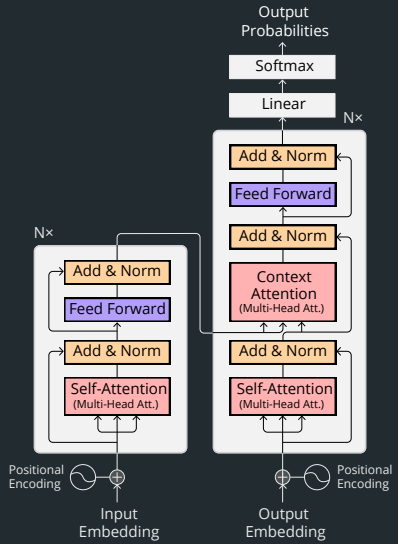
Key idea: Instead of Recurrent Neural Networks (RNNs), let's use attention mechanisms!



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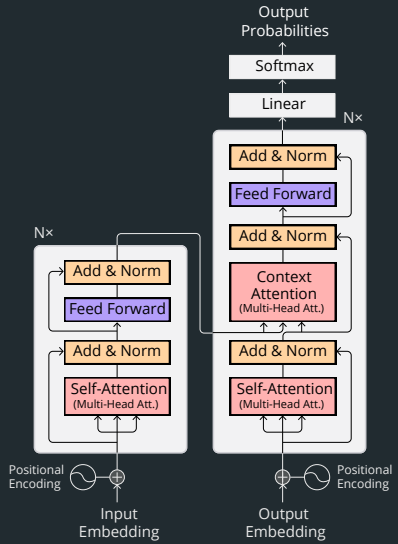

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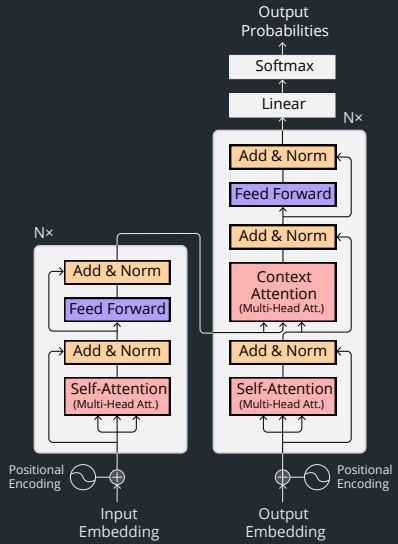

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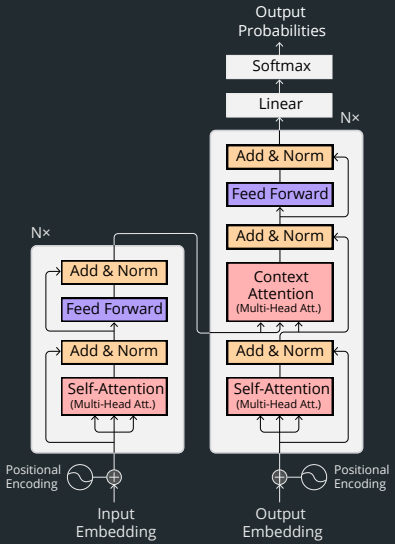


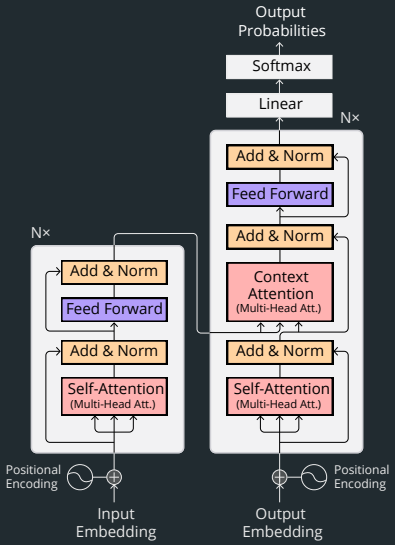
(Devlin et al., 2019)

A bit of context on transformers

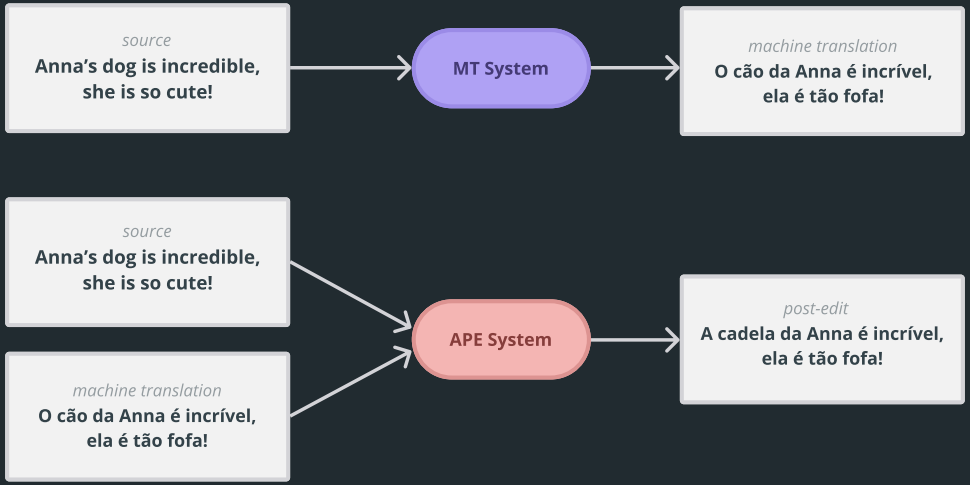
What if... Attention is all you need?

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

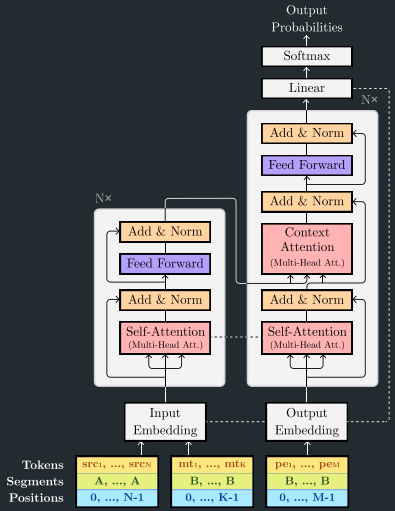
- In place of the RNNs, use self-attention
- Do this with multiple heads (i.e. attention mechanisms in parallel)
- ... and do it through several layers
- Inspiration for big general-purpose models like BERT!



What is APE?

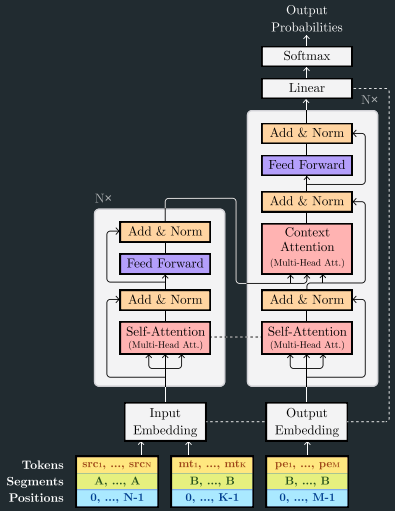

source
Anna's dog is incredible, she is so cute!
MT System
machine translation
O cão da Anna é incrível, ela é tão fofa!
source
Anna's dog is incredible, she is so cute!
machine translation
O cão da Anna é incrível, ela é tão fofa!
APE System
post-edit
A cadela da Anna é incrível, ela é tão fofa!

BERT for APE


Output Probabilities
Softmax
Linear
N×
Add & Norm
Feed Forward
Add & Norm
Context Attention
(Multi-Head Att.)
Add & Norm
Self-Attention
(Multi-Head Att.)
N×
Add & Norm
Feed Forward
Add & Norm
Self-Attention
(Multi-Head Att.)
Input Embedding
Output Embedding
Tokens
Segments
Positions
src1, ..., srcN
A, ..., A
0, ..., N-1
mt1, ..., mtK
B, ..., B
0, ..., K-1
pe1, ..., peM
B, ..., B
0, ..., M-1

BERT for APE

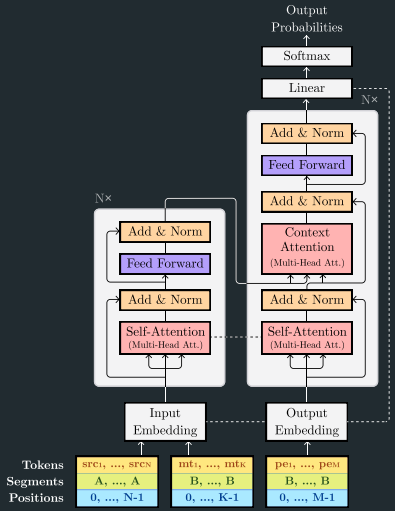
Key idea: Use BERT to do APE



BERT for APE

Key idea: Use BERT to do APE

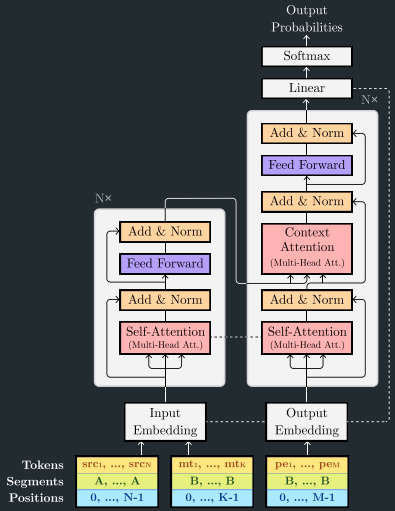
- Prior to this work, BERT was mainly used for simple classification tasks



BERT for APE

Key idea: Use BERT to do APE

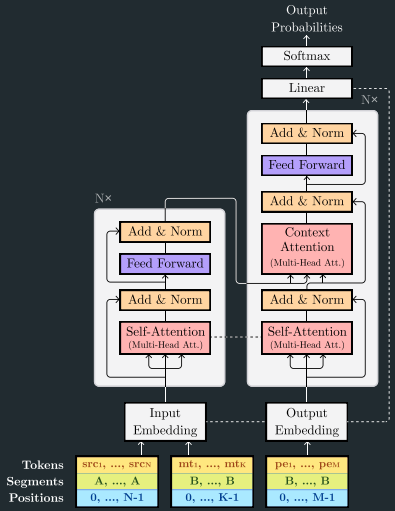
- Prior to this work, BERT was mainly used for simple classification tasks
- We introduced an effective method to use BERT in a generation task (APE)



BERT for APE

Key idea: Use BERT to do APE

- Prior to this work, BERT was mainly used for simple classification tasks
- We introduced an effective method to use BERT in a generation task (APE)
- Smart parameter sharing between encoder and decoder



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Getting to know attention heads better

Attention heads may aid visualization but they are completely dense.

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Our solution is to bet on sparsity:

- for interpretability
- for discovering linguistic structure
- for efficiency

Getting to know attention heads better

Attention heads may aid visualization but they are completely dense.

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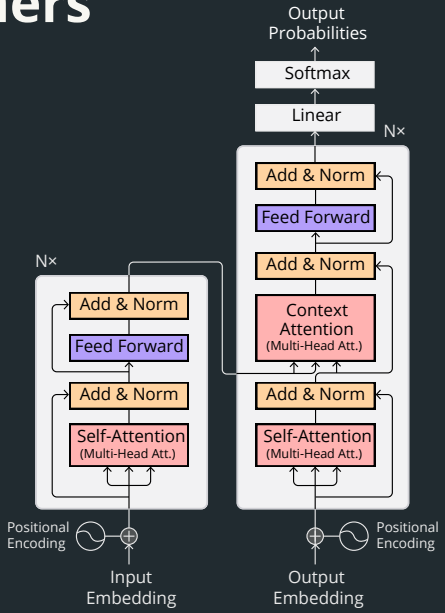
- for interpretability
- for discovering linguistic structure
- for efficiency

(Vaswani et al., 2017)

Transformers

In each attention head:

$$\bar{\mathbf{V}} = \mathbf{softmax}\left(\frac{\mathbf{Q}\mathbf{K}^\top}{\sqrt{d_k}}\right)\mathbf{V}.$$



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Transformers

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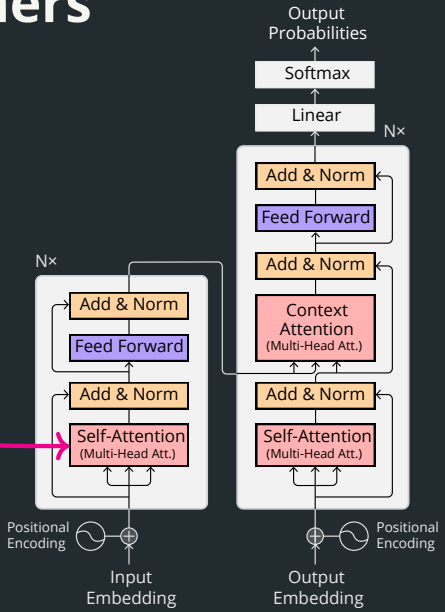
Attention in three places:

- Self-attention in the encoder



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Attention in three places:

- Self-attention in the encoder
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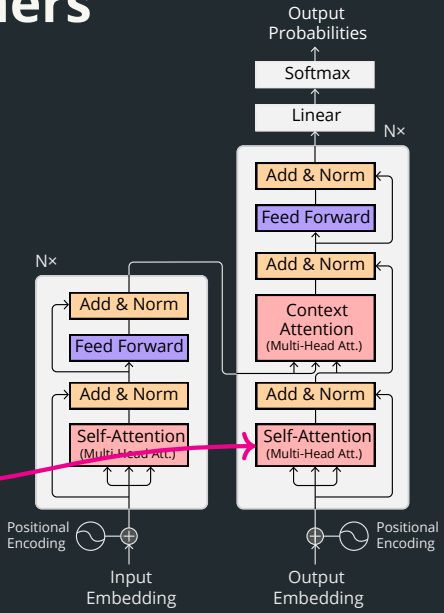

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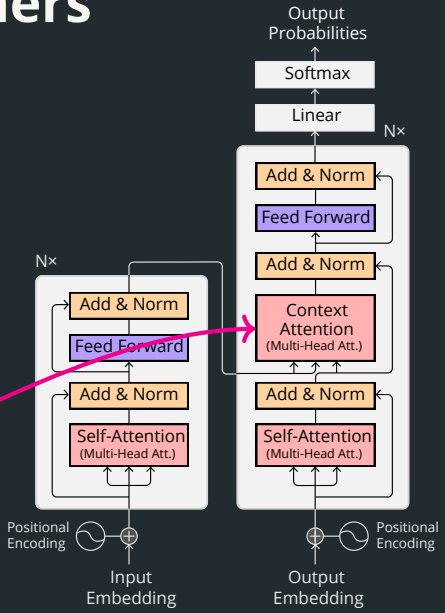
Transformers

In each attention head:

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

Attention in three places:

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



Sparse Transformers

Sparse Transformers

Key idea: replace softmax in attention heads by a sparse normalizing function! 🙌

Adaptively Sparse Transformers

Key idea: replace softmax in attention heads by a sparse normalizing function! 🙌

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

What is softmax?

Softmax exponentiates and normalizes:

$$\textbf{softmax}(z_i) := \frac{\exp(z_i)}{\sum_j \exp(z_j)}$$

What is softmax?

Softmax exponentiates and normalizes:

$$\textbf{softmax}(z_i) := \frac{\exp(z_i)}{\sum_j \exp(z_j)}$$

It's fully dense: $\textbf{softmax}(z) > 0$

(Peters et al., 2019)

α-Entmax

Parametrized by $\alpha \geq 0$:

(Peters et al., 2019)

α-Entmax

Parametrized by $\alpha \geq 0$:

- **Argmax** corresponds to $\alpha \rightarrow \infty$

(Peters et al., 2019)

α-Entmax

Parametrized by $\alpha \geq 0$:

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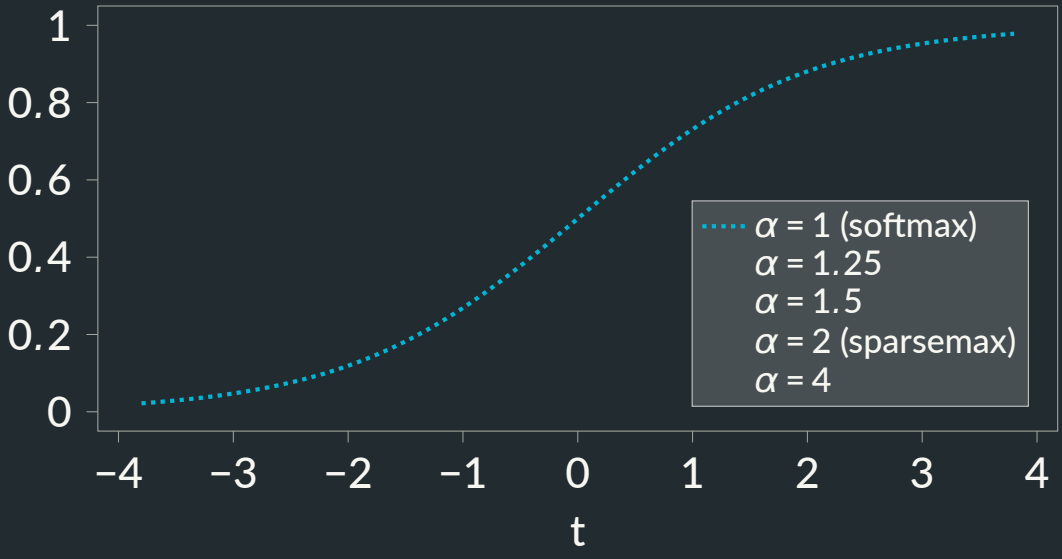
α-Entmax

Parametrized by $\alpha \geq 0$:

- **Argmax** corresponds to $\alpha \to \infty$
- **Softmax** amounts to $\alpha \to 1$
- **Sparsemax** amounts to $\alpha = 2$.

Key result: **can be sparse for** $\alpha > 1$, propensity for sparsity increases with α.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0.4
0.2
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−4
−3
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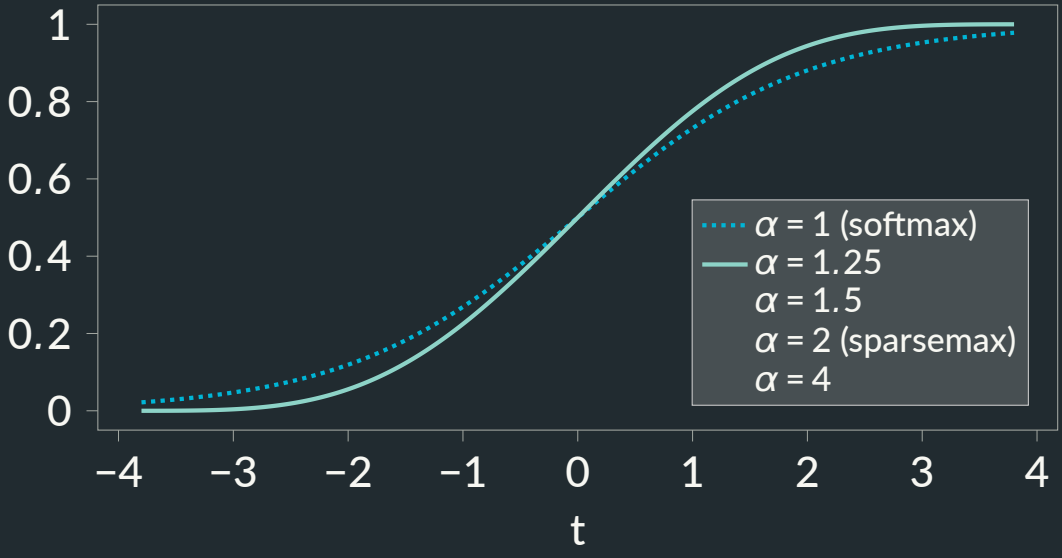
t
α = 1 (softmax)
α = 1.25
α = 1.5
α = 2 (sparsemax)
α = 4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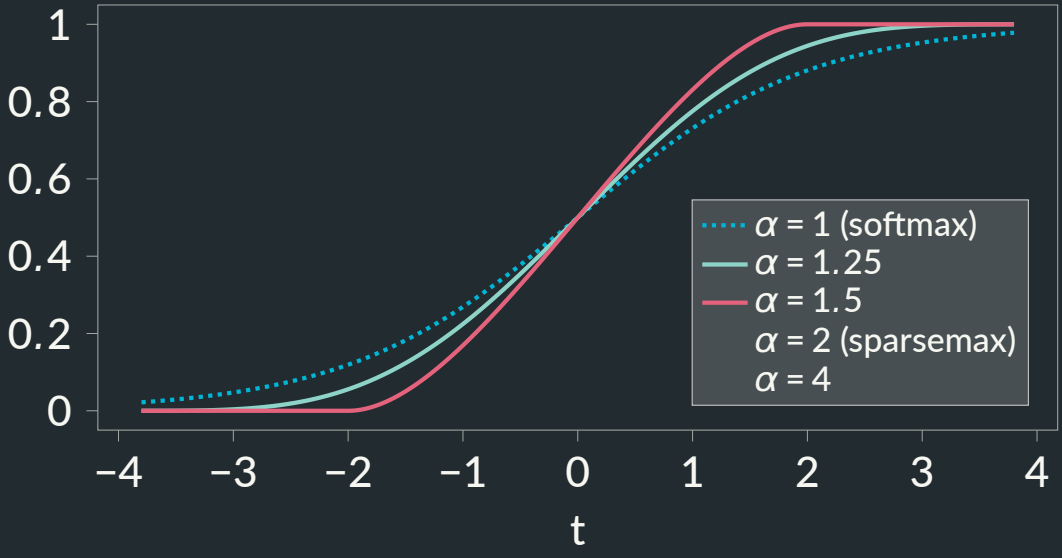
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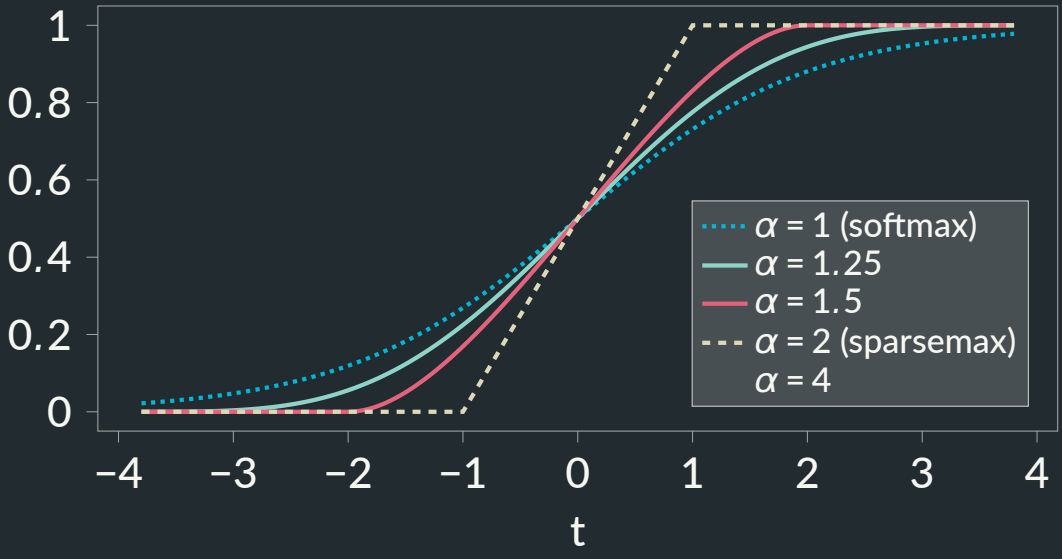
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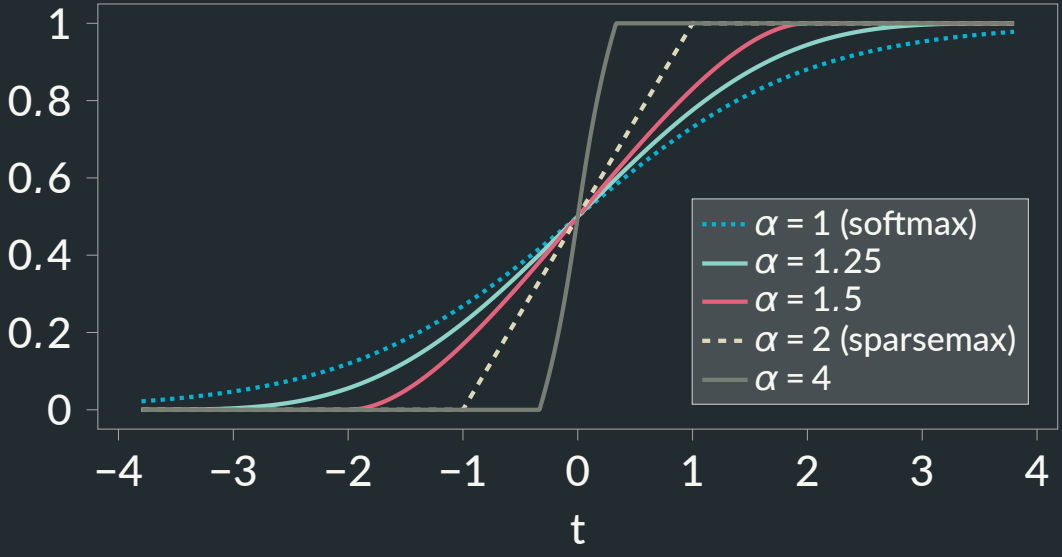
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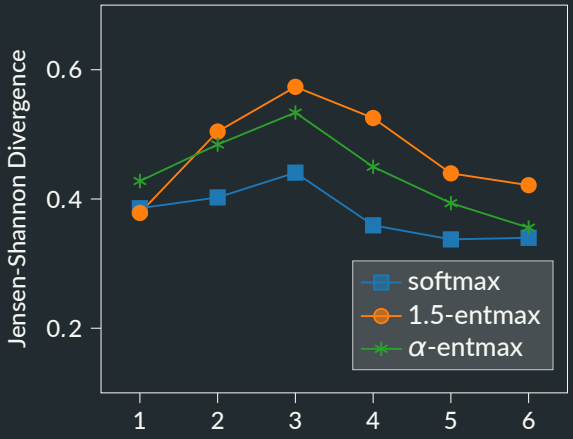
Learning α

Learning α

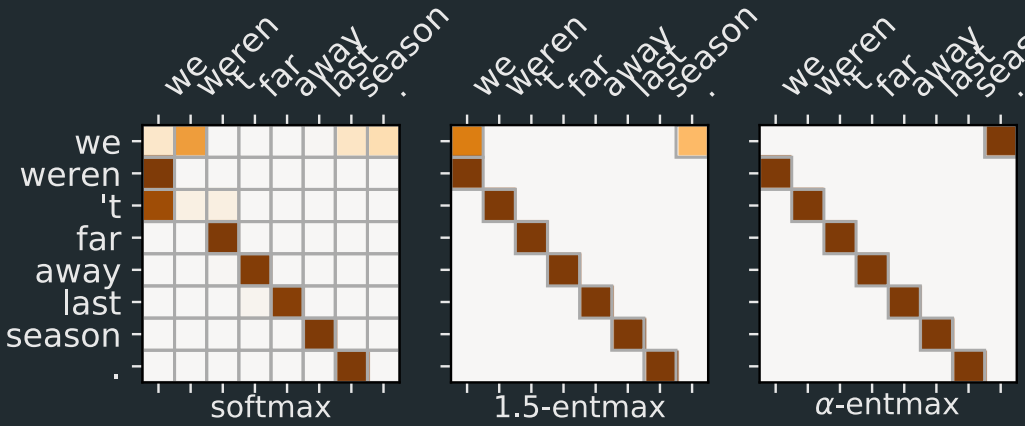
Key contribution:

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

Head Diversity per Layer

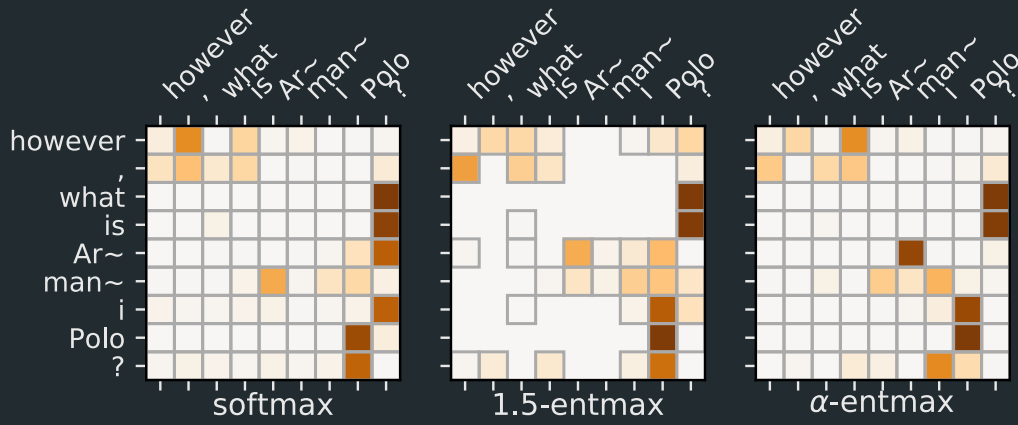


Previous Position Head



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

Interrogation-Detecting Head



Learned $\alpha = 1.05$.

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Latent Variable Models

Latent variable z can be

Latent Variable Models

Latent variable z can be continuous

Source: Bouges et al., 2013

Latent Variable Models

Latent variable z can be continuous, discrete

Source: valleyeyecareaz.com

Latent Variable Models

Latent variable z can be continuous, discrete, or structured

Source: Liu et al., 2015

Training Discrete or Structured Latent Variable Models

Latent variable z can be

Training Discrete or Structured Latent Variable Models

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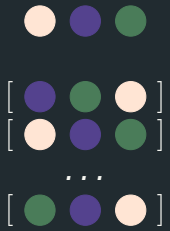
Training Discrete or Structured Latent Variable Models

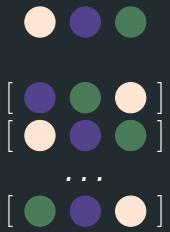
Latent variable z can be discrete or structured



Training Discrete or Structured Latent Variable Models

Latent variable z can be discrete or structured

$\pi(z|x, \theta)$: distribution over possible z



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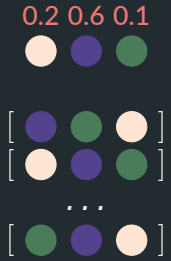

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If $\mathcal{Z}$ is large, this sum can get very expensive due to $\ell(x, z; \theta)$! 😱

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If $\mathcal{Z}$ is combinatorial, this can be intractable to compute! 😱 😱 😱

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New option: use sparsity! 🙌

no need for sampling → no variance
no relaxation into the continuous space

Taking a step back...

Does the expectation over possible z need to be expensive?

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$$\begin{aligned}\mathcal{L}_x(\theta) &= \sum_{z \in \mathcal{Z}} \pi(z|x, \theta)\, \ell(x, z; \theta) \\ &= \pi(z_1|x, \theta)\, \ell(x, z_1; \theta) + \pi(z_2|x, \theta)\, \ell(x, z_2; \theta) + \ldots \\ &+ \pi(z_i|x, \theta)\, \ell(x, z_i; \theta) + \ldots + \pi(z_N|x, \theta)\, \ell(x, z_N; \theta)\end{aligned}$$

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Usually we normalize π with softmax $\propto \exp(s) \Rightarrow \pi(z_i\,|x, \theta) > 0$

(Martins and Astudillo, 2016; Niculae et al., 2018)

Sparse normalizers

We use sparsemax, top-k sparsemax and SparseMAP to allow efficient marginalization

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$$\mathcal{L}_x(\theta) = \sum_{z \in \mathcal{Z}} \pi(z|x, \theta)\, \ell(x, z; \theta)$$
$$= \pi(z_1|x, \theta)\, \ell(x, z_1; \theta) + \underbrace{\pi(z_2|x, \theta)}_{=0}\, \ell(x, z_2; \theta) + \dots$$
$$+ \pi(z_i|x, \theta)\, \ell(x, z_i; \theta) + \dots + \underbrace{\pi(z_N|x, \theta)}_{=0}\, \ell(x, z_N; \theta)$$

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$$+ \pi(z_i|x, \theta)\, \ell(x, z_i; \theta) + \ldots + \underbrace{\pi(z_N|x, \theta)}_{=0}\, \cancel{\ell(x, z_N; \theta)}$$

No need for computing $\ell(x, z; \theta)$ for all $z \in \mathcal{Z}$!

Results

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Our methods are top-performers and efficient!

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References I

- Bouges, Pierre, Thierry Chateau, Christophe Blanc, and Gaëlle Loosli (Dec. 2013). “Handling missing weak classifiers in boosted cascade: application to multiview and occluded face detection”. In: *EURASIP Journal on Image and Video Processing* 2013, p. 55. DOI: 10.1186/1687-5281-2013-55.
- Correia, Gonçalo M, Vlad Niculae, and André FT Martins (2019). “Adaptively sparse transformers”. In: *Proc. EMNLP*.
- Correia, Gonçalo M. and André F. T. Martins (July 2019). “A Simple and Effective Approach to Automatic Post-Editing with Transfer Learning”. In: *Proceedings of the 57th Annual Meeting of the Association for Computational Linguistics*. Florence, Italy: Association for Computational Linguistics, pp. 3050–3056. DOI: 10.18653/v1/P19-1292. URL: https://www.aclweb.org/anthology/P19-1292.
- Correia, Gonçalo M., Vlad Niculae, Wilker Aziz, and André F. T. Martins (2020). “Efficient Marginalization of Discrete and Structured Latent Variables via Sparsity”. In: *Proc. NeurIPS*. URL: https://arxiv.org/abs/2007.01919.
- Devlin, Jacob, Ming-Wei Chang, Kenton Lee, and Kristina Toutanova (2019). “BERT: Pre-training of deep bidirectional transformers for language understanding”. In: *Proc. NAACL-HLT*.
- Liu, Ziwei, Ping Luo, Xiaogang Wang, and Xiaoou Tang (Dec. 2015). “Deep Learning Face Attributes in the Wild”. In: *Proceedings of International Conference on Computer Vision (ICCV)*.
- 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*.

References II

- Niculae, Vlad, André FT Martins, Mathieu Blondel, and Claire Cardie (2018). “SparseMAP: Differentiable sparse structured inference”. In: *Proc. of ICML*.
- 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*.
- 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*.