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

Gonçalo M. Correia

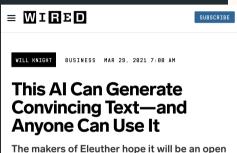
• Subset of machine learning that uses **neural networks**

- Subset of machine learning that uses neural networks
- Powerful tool for learning representations of any data

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

A robot wrote this entire article. Are you scared yet, human?

GPT-3



source alternative to GPT-3, the well-known

language program from OpenAI.

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Convincing Text— SCIENCE **Anvone Can Use It**

The makers of Eleuther hope it v source alternative to GPT-3, the language program from OpenAI

Danny's workmate is called GPT-3. You've probably read its work without realising it's an AI

ABC Science / By technology reporter James Purtill Posted Sat 28 May 2022 at 7:30pm



Are AI Systems About To Outperform Humans?

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Artificial intelligence beats eight world champions at bridge AI 'outperforms'

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Are AI Systems About T Outperform Humans?

robot wrote this

doctors bridge requires more human sk diagnosing breast cancer



Fergus Walsh Medical correspondent @BBCFergusWalsh

• Requires a lot of data

- Requires a lot of data
- Hard to understand and interpret reasons behind decisions

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- Hard to understand and interpret reasons behind decisions
- Requires a lot of computation



Forbes

ΔΙ

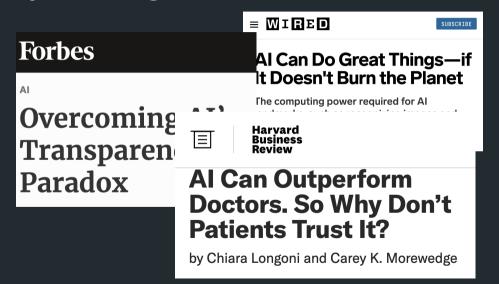
Overcoming AI's Transparency Paradox

WIRED

SUBSCRIBE

Al Can Do Great Things—if It Doesn't Burn the Planet

The computing power required for AI andmarks, such as recognizing images and defeating humans at Go, increased 300,000-fold from 2012 to 2018.



- A Simple and Effective Approach to APE with Transfer Learning
 - weak supervision
 - data-efficiency
 - Poster at ACL 2019

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 - learnable sparsity
 - compactness
 - Spotlight paper at NeurIPS 2020

Table of Contents

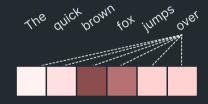
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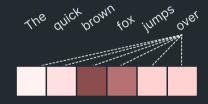
Future Work and Conclusions

What if... Attention is all you need?



What if... Attention is all you need?

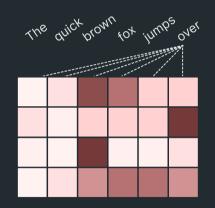
Key idea: Let's mainly use attention mechanisms!



What if... Attention is all you need?

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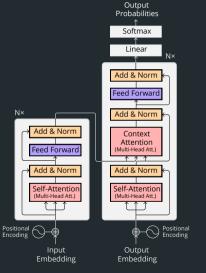
 Do attention with multiple heads (i.e. attention mechanisms in parallel)



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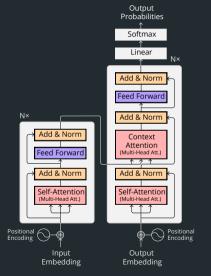
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- ... and do it through several layers
- Inspiration for big general-purpose models like BERT and GPT-3!

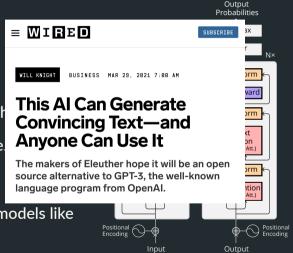


A bit of context on Transformers

What if... Attention is all you need?

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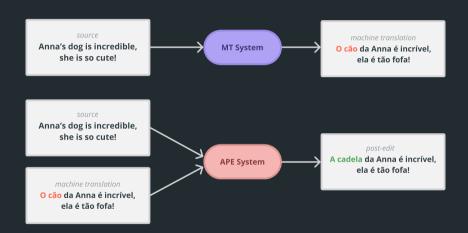
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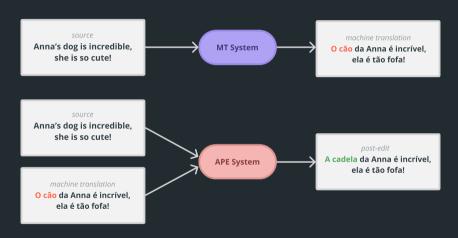


Embedding

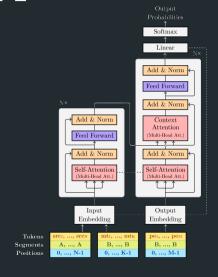
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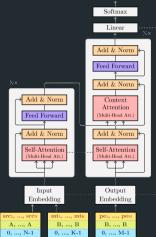


Challenge: APE data is very scarce! Need to create artificial data.



Key idea: Use BERT to do APE



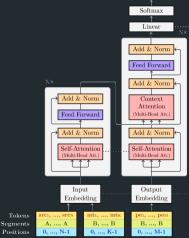




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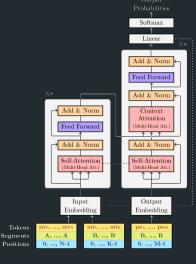
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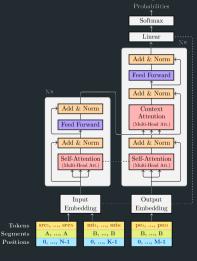
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- We introduced an effective method to use BERT in a generation task (APE)



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



model (data size)	TER↓	BLEU†
mt baseline	24.48	62.49

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Table of Contents

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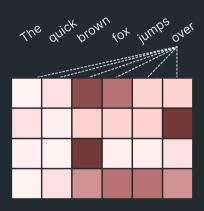
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Getting to know attention heads better

Attention heads may aid visualization but they are completely dense.

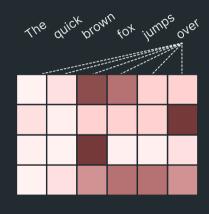


Getting to know attention heads better

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Our solution is to bet on sparsity:

- for interpretability
- for discovering linguistic structure
- for efficiency

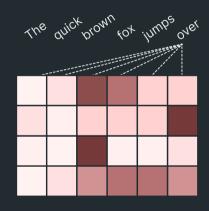


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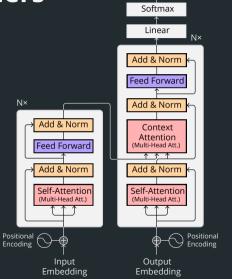
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In each attention head:

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



(Vaswani et al., 2017)

Output

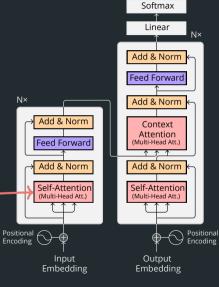
Probabilities

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Attention in three places:

• Self-attention in the encoder



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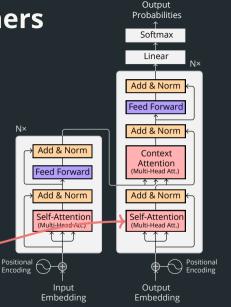
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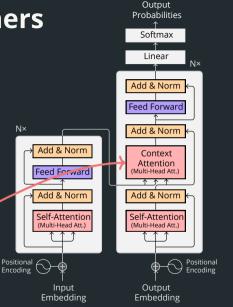
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Attention in three places:

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



(Vaswani et al., 2017)

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:

$$[\mathbf{softmax}(z)]_i := \frac{\exp(z_i)}{\sum_j \exp(z_j)}$$

What is softmax?

Softmax exponentiates and normalizes:

$$[\mathbf{softmax}(z)]_i := \frac{\exp(z_i)}{\sum_j \exp(z_j)}$$

It's fully dense: softmax(z) > 0

Parametrized by $\alpha \geq 0$:

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• Argmax corresponds to $\alpha \to \infty$

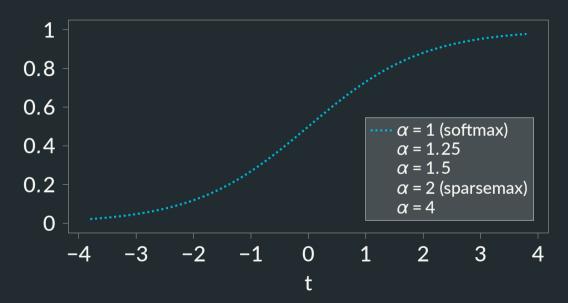
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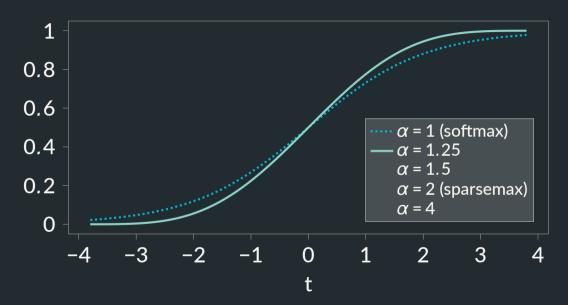
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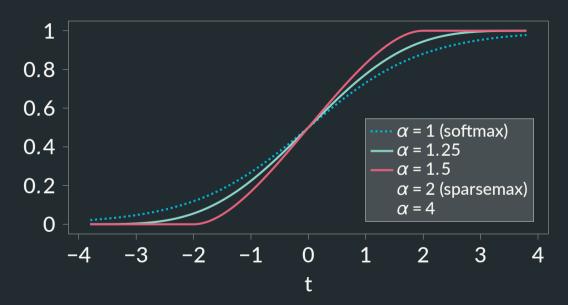
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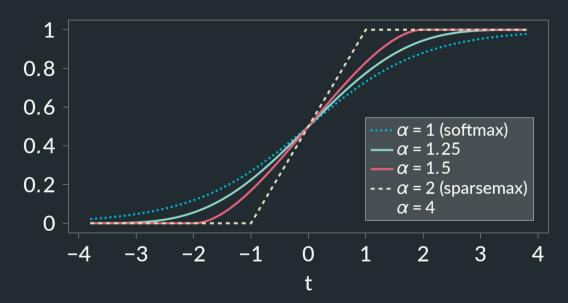
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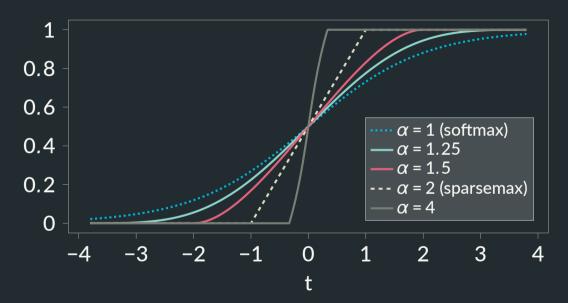
Key result: can be sparse for $\alpha > 1$, propensity for sparsity increases with α .





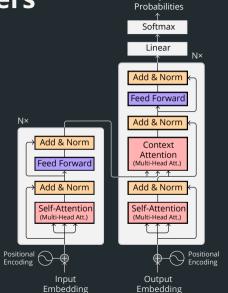






Output

Transformers

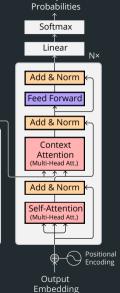


Transformers

Attention in three places:

Self-attention in the encoder

6 layers \times 8 attention heads = 48



Output

Add & Norm

Feed Forward

Add & Norm

Self-Attention

(Multi-Head Att.)

N×

Positional C

Encoding

Transformers

Attention in three places:

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

6 layers \times 8 attention heads = 48 + 48

N× Add & Norm Feed Forward Add & Norm Self-Auention (Multi-Head Att.) Positional C Encoding Input

Embedding

Embedding

Output Probabilities

Transformers

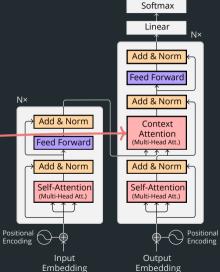
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+48

+48 = 144



Learning α

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Key contribution:

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



Learning α

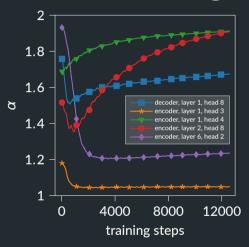
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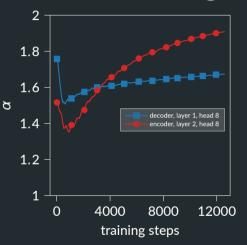


Not trivial! Requires implicit differentiation

Trajectories of α during training

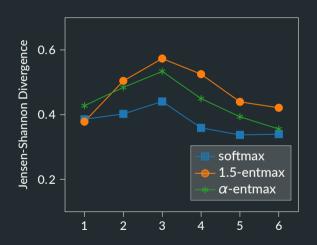


Trajectories of α during training



Some heads choose to start dense before becoming sparse.

Head Diversity per Layer

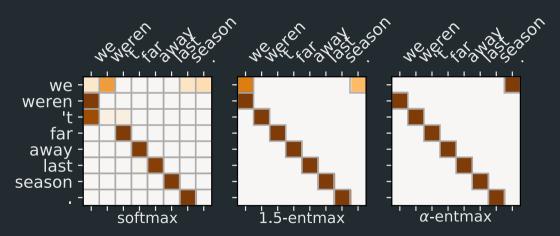


Head Diversity per Layer



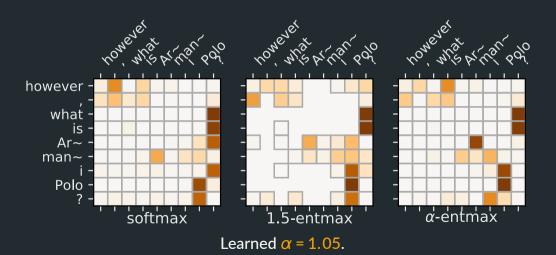
Specialized heads are important as seen in Voita et al. (2019)!

Previous position head



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

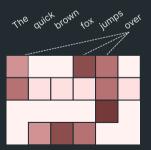
Interrogation-detecting head



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

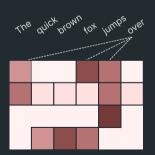
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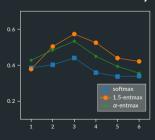


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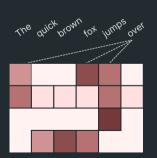


reduced head redundancy

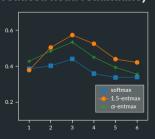


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adaptive sparsity



reduced head redundancy



clearer head roles

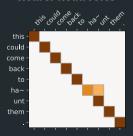


Table of Contents

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We focus on latent variables z that are

We focus on latent variables z that are discrete



We focus on latent variables z that are discrete or structured



We focus on latent variables z that are discrete or structured $\pi(z|x,\theta)$: distribution over possible z



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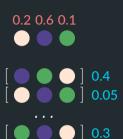
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 $\pi(z|x,\theta)$: distribution over possible z

 $\ell(x, z; \theta)$: downstream loss: ELBO, Log-Likelihood, (...)

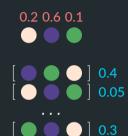


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To train, we need to compute the following expectation:



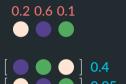
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$$\mathcal{L}_{x}(\boldsymbol{\theta}) = \sum_{z \in \mathcal{T}} \pi(z|x, \boldsymbol{\theta}) \, \ell(x, z; \boldsymbol{\theta})$$



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$$\mathcal{L}_{x}(\boldsymbol{\theta}) = \sum_{z \in \mathcal{Z}} \pi(z|x, \boldsymbol{\theta}) \; \ell(x, z; \boldsymbol{\theta})$$

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



We focus on latent variables z that are discrete or structured

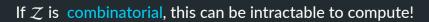
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0.2 0.6 0.1 0 0 0 0 0.4 [0 0 0] 0.05

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Current solutions

Using emergent communication as example



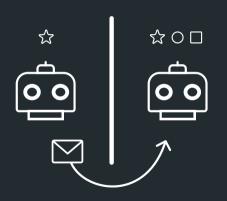


Method	success (%)	# messages
Monte Carlo		
Marginalization		

Current solutions

Using emergent communication as example





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Monte Carlo		
Marginalization		

\bowtie	Method	success (%)	# messages
	Monte Carlo		
	Marginalization		

\subseteq	\subseteq
\square	

Method	success (%)	# messages
Monte Carlo		
Marginalization Dense	93.37 ±0.42	256



Method	success (%)	# messages
Monte Carlo SFE	33.05 ±2.84	1
Marginalization Dense	93.37 ±0.42	256



Method	success (%)	# messages
Monte Carlo SFE SFE+	33.05 ±2.84 44.32 ±2.72	1 2
Marginalization Dense	93.37 ±0.42	256



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Monte Carlo SFE SFE+ Gumbel	33.05 ±2.84 44.32 ±2.72 23.51 ±16.19	1 2 1
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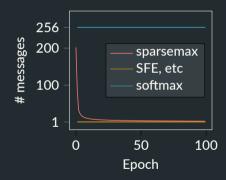


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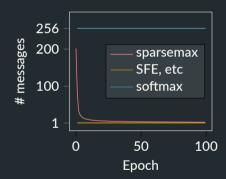
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Using emergent communication as example





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

We test our methods for models with discrete latent variables,

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Semi-Supervised VAE

We test our methods for models with discrete latent variables,

- Semi-Supervised VAE
- Emergent communication

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but also in models with an exponentially large set of \mathcal{Z} ,

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Bit-vector VAE

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- Emergent communication

but also in models with an exponentially large set of \mathcal{Z} ,

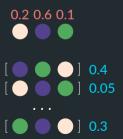
Bit-vector VAE

Our methods are top-performers and efficient!

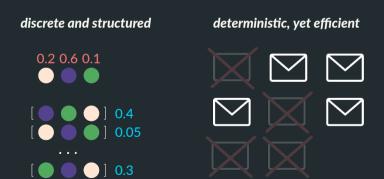
We introduce a new method to train compact latent variable models, using sparsity.

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discrete and structured



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Table of Contents

A Simple and Effective Approach to APE with Transfer Learning

Adaptively Sparse Transformers

Efficient Marg. of Discrete Latent Variables via Sparsity

Future Work and Conclusions

• Semi-supervised learning: data-efficiency and compactness

- Semi-supervised learning: data-efficiency and compactness
- Learning $\pi(z|x)$ without learning $\ell(x,z)$: compactness

- Semi-supervised learning: data-efficiency and compactness
- Learning $\pi(z|x)$ without learning $\ell(x,z)$: compactness
- Latent draft translations: transparency and compactness

Using learned sparsity and weak supervision we took steps to take neural models closer to version 2.0

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data-efficiency

model (data size)	BLEU↑
dual-source transformer (8M)	71.72
dual-source transformer (23K)	59.78
ours (23K)	70.66

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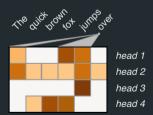


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better & efficient compactness



References I

- Child, Rewon, Scott Gray, Alec Radford, and Ilya Sutskever (2019). "Generating long sequences with sparse transformers". In: arXiv preprint arXiv:1904.10509.
- 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. NeurlPS. 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.
- Junczys-Dowmunt, Marcin and Roman Grundkiewicz (2018). "MS-UEdin Submission to the WMT2018 APE Shared Task: Dual-Source Transformer for Automatic Post-Editing". In: *Proceedings of WMT18*.
- Kyrillidis, Anastasios, Stephen Becker, Volkan Cevher, and Christoph Koch (2013). "Sparse projections onto the simplex". In: Proc. ICML.
- Lazaridou, Angeliki, Alexander Peysakhovich, and Marco Baroni (2017). "Multi-agent cooperation and the emergence of (natural) language". In: Proc. ICLR.
- Lee, Jihyung, WonKee Lee, Jaehun Shin, Baikjin Jung, Young-Kil Kim, and Jong-Hyeok Lee (2020). "POSTECH-ETRI's Submission to the WMT2020 APE Shared Task: Automatic Post-Editing with Cross-lingual Language Model". In: Proceedings of WMT.
- 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*.

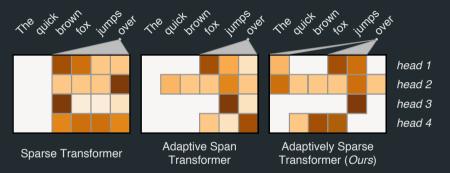
References II

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

Parameter sharing analysis

TER↓	BLEU↑
24.76	62.11
27.80	60.76
20.33	69.31
20.83	69.11
18.91	71.81
18.44	72.25
18.75	71.83
19.04	71.53
	24.76 27.80 20.33 20.83 18.91 18.44 18.75

Related Work: Other Sparse Transformers



Our model allows non-contiguous attention for each head.

Ω-Regularized Argmax

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

$$\operatorname{argmax}_{\Omega}(\mathbf{z}) \coloneqq \arg \max_{\mathbf{p} \in \Delta} \mathbf{z}^{\mathsf{T}} \mathbf{p} - \Omega(\mathbf{p})$$

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Is there something in-between?

BLEU Scores

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

BLEU Scores

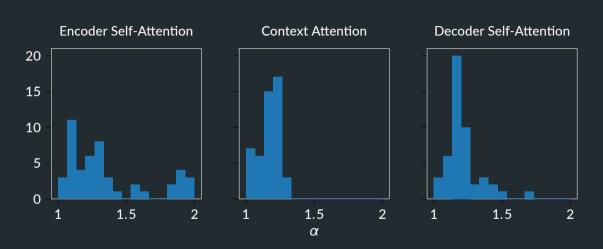
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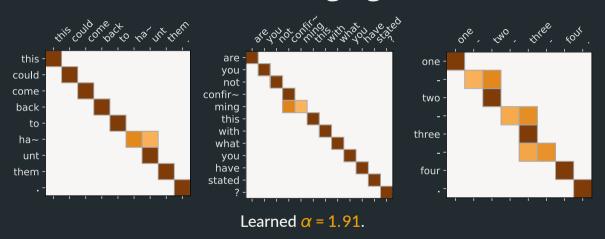
For analysis for other language pairs, see Appendix A.

Learned α



Bimodal for the encoder, mostly unimodal for the decoder.

Subword-Merging Head

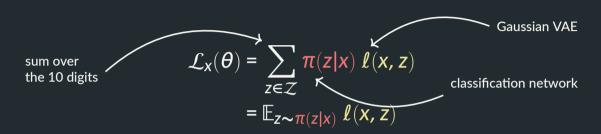


$$\mathcal{L}_{x}(\boldsymbol{\theta}) = \sum_{z \in \mathcal{Z}} \pi(z|x) \, \ell(x, z)$$
$$= \mathbb{E}_{z \sim \pi(z|x)} \, \ell(x, z)$$

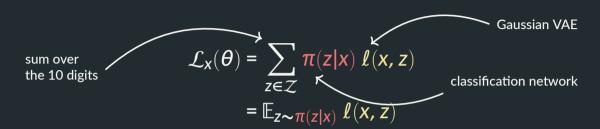
Semi-Supervised VAE on MNIST: z is one of 10 categories

$$\mathcal{L}_{X}(\boldsymbol{\theta}) = \sum_{\mathbf{z} \in \mathcal{Z}} \pi(\mathbf{z}|\mathbf{x}) \, \ell(\mathbf{x}, \mathbf{z})$$
 classification network
$$= \mathbb{E}_{\mathbf{z} \sim \pi(\mathbf{z}|\mathbf{x})} \, \ell(\mathbf{x}, \mathbf{z})$$

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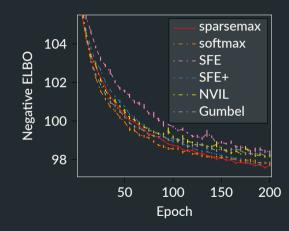


- Semi-Supervised VAE on MNIST: z is one of 10 categories
- Train this with 10% labeled data

Method	Accuracy (%)	Dec. calls
Monte Ca	rlo	
SFE	94.75±.002	1
SFE+	$96.53 \scriptstyle \pm .001$	2
NVIL	96.01 ±.002	1
Gumbel	95.46±.001	1
 Marginaliz	zation	
Dense	96.93±.001	10

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Marginaliz	zation	
Dense	$96.93 \pm .001$	10
Sparse	96.87±.001	1.01±0.01

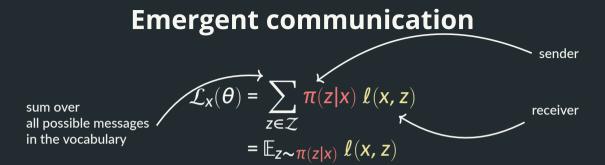
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$$\mathcal{L}_{x}(\theta) = \sum_{z \in \mathcal{Z}} \pi(z|x) \, \ell(x, z)$$
$$= \mathbb{E}_{z \sim \pi(z|x)} \, \ell(x, z)$$

Emergent communication $\mathcal{L}_{X}(\theta) = \sum_{z \in \mathcal{Z}} \pi(z|x) \, \ell(x,z)$ $= \mathbb{E}_{z \sim \pi(z|x)} \, \ell(x,z)$ sender $= \mathbb{E}_{z \sim \pi(z|x)} \, \ell(x,z)$

ullet receiver picks image from a set ${\mathcal V}$ based on message



- receiver picks image from a set V based on message
- images come from ImageNet

... but make it harder: |Z| = 256, |V| = 16

Method	success (%)	Dec. calls
Monte Carlo		
SFE	33.05 ± 2.84	1
SFE+	44.32 ±2.72	2
NVIL	37.04 ± 1.61	1
Gumbel	23.51 ± 16.19	1
ST Gumbel	27.42 ±13.36	1

Marginalization

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Limitations

- Mostly (and eventually) very sparse.
 But fully dense worst case.
- For the same reason, sparsemax cannot handle structured z.

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One solution: top-k sparsemax

$$k$$
-sparsemax(s) = $\underset{\boldsymbol{p} \in \Delta, \|\boldsymbol{p}\|_0 \le k}{\arg \min} \|\boldsymbol{p} - s\|_2^2$

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One solution: top-k sparsemax k-sparsemax(s) = arg min $\|p - s\|_2^2$

$$k\text{-sparsemax}(s) = \underset{\boldsymbol{p} \in \Delta, \|\boldsymbol{p}\|_0 \leq k}{\arg\min} \ \|\boldsymbol{p} - s\|_2^2$$

- Non-convex but easy: sparsemax over the k highest scores (Kyrillidis et al., 2013).
- Top-k oracle available for some structured problems.
- Certificate: if at least one of the top-k z gets p(z) = 0, k-sparsemax = sparsemax! thus, biased early on, but it goes away.





$$\mathcal{M} := \operatorname{conv} \left\{ \mathbf{a}_{z} : z \in \mathcal{Z} \right\}$$
$$= \left\{ \mathbf{A} \mathbf{p} : \mathbf{p} \in \Delta \right\}$$
$$= \left\{ \mathbb{E}_{Z \sim p} \mathbf{a}_{Z} : \mathbf{p} \in \Delta \right\}$$





• argmax arg max p^Ts
p∈∆





• argmax $\operatorname{arg\,max} \operatorname{p}^{\mathsf{T}} s$

$$\mathsf{MAP} \underset{\boldsymbol{\mu} \in \mathcal{M}}{\operatorname{arg\,max}} \boldsymbol{\mu}^\mathsf{T} \mathbf{t}$$





- $\operatorname{\mathsf{argmax}} \operatorname{\mathsf{argmax}} \operatorname{\mathsf{p}}^{\mathsf{T}} s$
- softmax $\underset{\boldsymbol{p} \in \Delta}{\operatorname{arg max}} \boldsymbol{p}^{\mathsf{T}} \boldsymbol{s} + \operatorname{H}(\boldsymbol{p})$





- argmax $\arg \max_{p \in \Delta} p^{\top} s$
- softmax $\arg \max_{\boldsymbol{p} \in \Delta} \boldsymbol{p}^{\mathsf{T}} \boldsymbol{s} + \mathrm{H}(\boldsymbol{p})$

MAP
$$\underset{\boldsymbol{\mu} \in \mathcal{M}}{\operatorname{arg \, max}} \boldsymbol{\mu}^{\mathsf{T}} t$$

marginals $\underset{\boldsymbol{\mu} \in \mathcal{M}}{\operatorname{marginals}} \operatorname{arg\,max} \boldsymbol{\mu}^{\mathsf{T}} \mathbf{t} + \widetilde{\operatorname{H}}(\boldsymbol{\mu})$





- argmax $\operatorname{arg\,max} \operatorname{p}^{\mathsf{T}} s$ $\operatorname{p} \in \Delta$
- softmax $\arg \max_{p \in \Delta} p^{\mathsf{T}} s + \mathrm{H}(p)$
- sparsemax $\arg \max_{p \in \Delta} p^{\top} s 1/2 ||p||^2$

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- softmax $\arg \max_{p \in \Delta} p^{\mathsf{T}} s + \mathrm{H}(p)$
- sparsemax $\arg \max_{p \in \Delta} \overline{p}^{\mathsf{T}} s \frac{1}{2} ||p||^2$

MAP
$$\underset{\boldsymbol{\mu} \in \mathcal{M}}{\operatorname{max}} \boldsymbol{\mu}^{\mathsf{T}} t$$

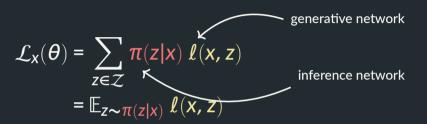
marginals $\underset{\boldsymbol{\mu} \in \mathcal{M}}{\operatorname{marginals}} \mathbf{\mu}^{\mathsf{T}} \mathbf{t} + \widetilde{\mathbf{H}}(\boldsymbol{\mu})$

SparseMAP $\underset{\boldsymbol{\mu} \in \mathcal{M}}{\arg\max} \boldsymbol{\mu}^{\mathsf{T}} t - \frac{1}{2} \|\boldsymbol{\mu}\|^2 \bullet$





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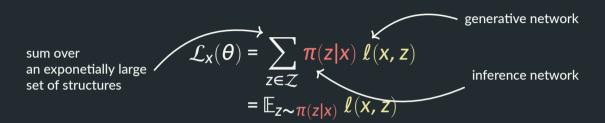


• VAE where z is a collection of D bits

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inference network

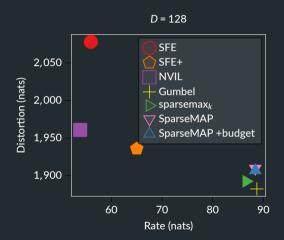
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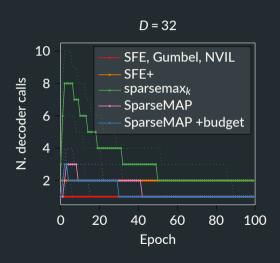
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Method	D = 32	D = 128
Monte Carlo		
SFE	3.74	3.77
SFE+	3.61	3.59
NVIL	3.65	3.60
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