From Sparse Modeling to Sparse Communication in NLP

André Martins







TALN Récital 2021

André Martins (IST)

Sparse Communication

Our Amazing Team (December 2019, pre-COVID)



André Martins (IST)

DeepSPIN



- ERC starting grant (2018–23)
- Topics: deep learning, structured prediction, NLP
- More details: https://deep-spin.github.io



Old times: rule-based systems

Mid-90s ("empirical revolution"): statistical methods (HMMs, PCFGs, IBM models)

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Today: neural models, attention, transformers, ...

Structure, feature selection, and neural networks can go together!



model interpretability

(Slide from 2017)

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model interpretabilit

(Slide from 2017)

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Transformers Are Big Bulldozers



Very powerful, but highly overparametrized.

André Martins (IST)

This Talk: Bet on Sparsity

What's inside a bulldozer? Can we redesign its components?

Sparsity can be useful:

- for interpretability
- for discovering linguistic structure
- for efficiency
- for generating.



From Sparse Modeling ...

- Mostly used with linear models, lots of work in the 2000s
- Main idea: embed a sparse regularizer (e.g. l₁-norm) in the learning objective
- Irrelevant features get zero weight and can be discarded
- Extensions to structured sparsity (group-lasso, fused-lasso, etc.)

... to Sparse Communication:

- Mostly used with neural networks, most work after 2015
- Main idea: sparse neuron activations (biological plausibility)
- Predictions are triggered by a few neurons only (input-dependent)
- Example: ReLUs, dropout, sparse attention mechanisms

This Talk

An inventory of transformations that capture sparsity and structure:

- All differentiable (efficient forward and backward propagation)
- Adaptively sparse
- Can be used at hidden or output layers
- Effective in many NLP tasks.

Building block:



Sparse transformations from the Euclidean space to the simplex \triangle .

Outline

1 Sparse Attention Mechanisms

- Sparsemax and Entmax
- Adaptively Sparse Transformers
- Other Transformations

2 Sparse Losses

- Sparse Sequence-to-Sequence Models
- Entmax Sampling

3 Conclusions

Recap: Softmax and Argmax

Softmax exponentiates and normalizes:

$$\mathsf{softmax}(\pmb{z}) = rac{\mathsf{exp}(\pmb{z})}{\sum_{k=1}^{K}\mathsf{exp}(z_k)}$$

- **Fully dense:** $softmax(z) > 0, \forall z$
- Used both as a loss function (cross-entropy) and for attention.

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Argmax can be written as:

Retrieves a **one-hot vector** for the highest scored index.



(Same z = [1.0716, -1.1221, -0.3288, 0.3368, 0.0425])

- Argmax is an extreme case of sparsity, but it is **discontinuous**.
- Is there a sparse and differentiable alternative?



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- Argmax is an extreme case of sparsity, but it is **discontinuous**.
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Euclidean projection of z onto the probability simplex \triangle :

sparsemax(z) :=
$$\arg \min_{\boldsymbol{p} \in \Delta} \|\boldsymbol{p} - \boldsymbol{z}\|^2$$

= $\arg \max_{\boldsymbol{p} \in \Delta} \boldsymbol{z}^\top \boldsymbol{p} - \frac{1}{2} \|\boldsymbol{p}\|^2$.

- Likely to hit the boundary of the simplex, in which case sparsemax(z) becomes sparse (hence the name)
- End-to-end differentiable
- Forward pass: $O(K \log K)$ or O(K), (almost) as fast as softmax
- Backprop: sublinear, **better than softmax!**

Sparsemax in 2D and 3D

(Martins & Astudillo, 2016, ICML)



Sparsemax is piecewise linear, but asymptotically similar to softmax.

Ω -Regularized Argmax (Niculae & Blondel, 2017, NeurIPS)

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

$$\operatorname{argmax}_{\Omega}(oldsymbol{z}) := \operatorname{argmax}_{oldsymbol{p} \in riangle} oldsymbol{z}^{ op} oldsymbol{p} - \Omega(oldsymbol{p})$$

- Argmax corresponds to no regularization, $\Omega \equiv 0$
- Softmax amounts to entropic regularization, $\Omega(\mathbf{p}) = \sum_{i=1}^{K} p_i \log p_i$
- Sparsemax amounts to ℓ_2 -regularization, $\Omega(\boldsymbol{p}) = \frac{1}{2} \|\boldsymbol{p}\|^2$

Is there something in-between?

Entmax (Peters, Niculae & Martins, 2019, ACL)

Parametrized by $\alpha \geq 0$:

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

Related to Tsallis generalized entropies (Tsallis, 1988).

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

Key result: always sparse for $\alpha > 1$, sparsity increases with α

- Forward pass for general α can be done with a bissection algorithm
- Backward pass runs in sublinear time.

Entmax in 2D (Peters, Niculae & Martins, 2019, ACL)



$\alpha = 1.5$ is a sweet spot!

 Efficient exact algorithm (nearly as fast as softmax), smooth, and good empirical performance.

Pytorch code: https://github.com/deep-spin/entmax

Sparse Transformations (Peters, Niculae & Martins, 2019, ACL)



(Same z = [1.0716, -1.1221, -0.3288, 0.3368, 0.0425])

Example: Sparse Attention for Machine Translation

(Peters, Niculae & Martins, 2019, ACL)

- Selects source words when generating a target word (sparse alignments)
- Better interpretability
- Can also model fertility: constrained sparsemax (Malaviya, Ferreira & Martins, 2018, ACL)



Example: Sparse Attention for Explainability

(Treviso & Martins, 2020, BlackboxNLP)



- A classifier makes a prediction
- An "explainer" (embedded or not in the classifier) generates a sparse message that explains the classifier's decision
- The layperson receives the message and tries to guess the classifier's prediction (also called simulatability, forward simulation/prediction)
- Communication success rate: how often the two predictions match?

From Sparse Modeling to Sparse Communication

(Treviso & Martins, 2020, BlackboxNLP)

	Model interpretability	Prediction explainability			
Wrappers	 Forward selection Backward elimination (Kohavi & John, 1997) 	 Input reduction (Feng et al., 2018) Erasure (leave-one-out) (Li et al., 2016; Serrano & Smith, 2019) LIME (Ribeiro et al., 2016) 			
Filters	 PMI (Church & Hanks, 1990) recursive feature elimination (Guyon et al., 2002) 	 Input gradient (Li et al., 2016) LRP (Bach et al., 2015) top-k softmax attention 			
Embedded	 l₁-regularization (Tibshirani, 1996) elastic net (Zou & Hastie, 2005) 	 Stochastic attention (Xu et al., 2015; Lei et al., 2016; Bastings et al 2019) Sparse attention 			

Comparing Explainers

(Treviso & Martins, 2020, BlackboxNLP)

		SST		IMDB		AgNews		Yelp		SNLI	
Clf.	Explainer	CSR	ACC _L	CSR	ACC _L	CSR	ACC _L	CSR	ACC _L	CSR	ACC _L
C C C C _{ent} C _{sp}	Random Erasure Top- <i>k</i> gradient Top- <i>k</i> softmax Top- <i>k</i> 1.5-entmax Top- <i>k</i> sparsemax	69.41 80.12 79.35 84.18 85.23 85.23	70.07 81.22 79.24 82.43 83.31 81.93	67.30 92.17 86.30 93.06 93.32 93.34	66.67 88.72 83.93 89.46 89.60 89.57	92.38 97.31 96.49 97.59 97.29 95.92	91.14 95.41 94.86 95.61 95.67 94.48	58.27 78.72 70.54 81.00 82.20 82.50	53.06 68.90 62.86 70.18 70.78 70.99	75.83 77.88 76.74 78.66 80.23 82.89	68.74 70.04 69.40 71.00 73.39 74.76
C _{ent} C _{sp} C _{ber} C _{hk}	Selec. 1.5-entmax Selec. sparsemax n Bernoulli HardKuma	83.96 85.23 82.37 85.17	82.15 81.93 78.42 80.40	92.55 93.24 91.66 94.72	89.96 89.66 86.13 90.16	97.30 95.92 96.91 97.11	95.66 94.48 94.43 95.45	81.38 83.55 84.93 87.39	70.41 71.60 66.89 71.64	77.25 82.04 76.81 74.98	71.44 73.46 69.65 71.48

See paper for human experiments.

In general, attention > erasure \gg gradient methods (in terms of CSR).

Questions

- Which α to choose?
- The bigger the α , the higher propensity to sparsity.
- What if we have many attention heads, and we don't know how sparse we want each one to be?
- Can we learn α from data?

Transformer (Vaswani et al., 2017)

Attention in three places:

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

Multi-head attention: 6 layers, 8 attention heads (48 total).

Each head involves a query, a key, and a value matrix:

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



Figure 1: The Transformer - model architecture.

Adaptively Sparse Transformers

(Correia, Niculae & Martins, 2019, EMNLP)

Key idea: replace softmax in attention heads by α -entmax!

- Recall: α controls propensity to sparsity
- Learn each $\alpha \in [1, 2]$ adaptively!
- One α for each attention head and each layer.

Related Work: Other Sparse Transformers

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



Our model allows **non-contiguous** attention for each head, learned **adaptively**.

Accuracies and Learned α

(Correia, Niculae & Martins, 2019, EMNLP)



Bimodal for the encoder, mostly unimodal for the decoder.

Trajectories of α During Training

(Correia, Niculae & Martins, 2019, EMNLP)



Most heads become denser in the beginning, before converging.

Dense attention more beneficial while the network is still uncertain, becomes sparser as the network learns.

Previous Position Head

(Correia, Niculae & Martins, 2019, EMNLP)



Interrogation-Detecting Head

(Correia, Niculae & Martins, 2019, EMNLP)


Subword-Merging Head

(Correia, Niculae & Martins, 2019, EMNLP)



(Learned $\alpha = 1.91$)

Other Related Transformations

Constrained softmax (Martins & Kreutzer, 2017, EMNLP),

Constrained sparsemax (Malaviya, Ferreira & Martins, 2018, ACL):

- Allows placing a **budget** on how much attention a word can receive
- Useful to model fertility in NMT

Fusedmax (Niculae & Blondel, 2017, NeurIPS):

 Can promote structured sparsity (e.g. contiguous words more likely to be selected together)

SparseMAP (Niculae, Martins, Blondel & Cardie, 2018, ICML):

Extends sparsemax to sparse structured prediction

SparseMAP

(Niculae et al., 2018, ICML)

- Generalizes sparsemax to sparse structured prediction
- Works both as output layer and hidden layer
- As hidden layer, similar to structured attention networks (Kim et al., 2017), but sparse!
- Efficient forward/backprop requiring only an argmax (MAP) oracle!

Example: Latent Structured Alignments in SNLI



Example: Dependency Parsing

Suitable for capturing ambiguity in natural language!



LP-SparseMAP (Niculae & Martins, 2020, ICML)

Extension of SparseMAP for latent factor graphs!

Can handle latent logic variables and constraints.

Example: latent syntax with valency constraints.



```
fg = TorchFactorGraph()
u = fg.variable_from(arc_scores)
fg.add(DepTree(u))
for k in range(n):
    fg.add(Budget(u[:, k], budget=5))
fg.solve()
```

Dynamic Computation Graphs and Exact Expectations

(Niculae, Martins & Cardie, 2018, EMNLP)

(Correia, Niculae, Aziz & Martins, 2020, NeurIPS)

When combinatorial structures are used as latent variables in a neural network, it may become intractable to compute expectations:

Have to sum through exponentially many terms (one per structure)

SparseMAP offers a solution to this! Only a sparse subset of structure will have non-zero terms in the summation!

We do this for:

- Discriminative models with dynamic computation graphs (Niculae, Martins & Cardie, 2018, EMNLP)
- Generative models (combinatorial discrete VAEs) (Correia, Niculae, Aziz & Martins, 2020, NeurIPS)

Sparse and Continuous Attention

(Martins, Farinhas, Treviso, Niculae, Aguiar & Figueiredo, 2020, NeurIPS)

- So far: attention over a finite set (words, pixel regions, etc.)
- We generalize attention to *arbitrary sets*, possibly continuous.



Example: Visual Question Answering



(original image)

(discrete attention)

(continuous softmax)

(continuous sparsemax)

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Entmax Losses

- Entmax can also be used as a loss in the output layer (to replace logistic/cross-entropy loss)
- However, not expressed as a log-likelihood (which could lead to log(0) problems due to sparsity)
- Instead, we build a entmax loss inspired by Fenchel-Young losses.

Entmax Transformations and Losses

(Blondel, Martins & Niculae, 2020, JMLR)



- For $\alpha > 1$, losses have margins
- Interesting case: 1.5-entmax (specialized forward pass algorithm).

Pytorch code: https://github.com/deep-spin/entmax

Sparse Sequence-to-Sequence (Peters, Niculae & Martins, 2019, ACL)

Key idea:

- Replace all instances of softmax by sparsemax or α-entmax.
- We consider both sparsity in the attention mechanism and sparsity in the output layer

Two tasks:

- Machine translation (word-based)
- Morphological inflection (character-based).

Training and Inference

Training

Minimize token-level loss:

$$\mathcal{L}(\boldsymbol{\theta}) = \sum_{(x,y)\in\mathcal{D}} \sum_{t=1}^{|y|} L(y_t, \boldsymbol{z}_t)$$
$$= \sum_{(x,y)\in\mathcal{D}} \sum_{t=1}^{|y|} -\log[\operatorname{softmax}(\boldsymbol{z}_t)]_{y_t}$$

Inference

Approximate MAP decoding:

$$\hat{y} = \underset{y \in V^*}{\operatorname{argmax}} p_{\theta}(y \mid x)$$
$$= \underset{y \in V^*}{\operatorname{argmax}} \prod_{t=1}^{|y|} p_{\theta}(y_t \mid x, y_{< t})$$
$$= \underset{y \in V^*}{\operatorname{argmax}} \prod_{t=1}^{|y|} \operatorname{softmax}(z_t)_{y_t}$$

$$p_{\theta}(y \mid x) = \prod_{t=1}^{|y|} p_{\theta}(y_t \mid x, y_{< t}).$$

The chain rule favors short sequences!

$$p_{\theta}(y \mid x) = \prod_{t=1}^{|y|} p_{\theta}(y_t \mid x, y_{\leq t}).$$

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The chain rule favors short sequences!

- Softmax → all strings have positive probability
- Often the empty string is the most likely sequence (Stahlberg & Byrne, 2019)

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The chain rule favors short sequences!

- Softmax → all strings have positive probability
- Often the empty string is the most likely sequence (Stahlberg & Byrne, 2019)
- Beam search prunes it.









Can Entmax Save Us? (Peters, Niculae & Martins, 2019, ACL)



 $(\text{Same } \mathbf{z} = [1.0716, -1.1221, -0.3288, 0.3368, 0.0425])$

Cat Got Your Tongue? Maybe Not.



Cat Got Your Tongue? Maybe Not.



Example: Machine Translation

(Peters et al., 2019, ACL)



(Source: "Dies ist ein weiterer Blick auf den Baum des Lebens.")

- Only a few words get non-zero probability at each time step
- Auto-completion when several words in a row have probability 1
- Useful for predictive translation.

Sparsity in Attention and in Output Layer

(Peters et al., 2019, ACL)



- Sparsity in the output leads to higher accuracy
- Sparse attention leads to more interpretable alignments.



 1.5-entmax attains better performance faster.

Example: Morphological Inflection

$$d \rightarrow r \rightarrow a \rightarrow w \xrightarrow{66.4\%} d \rightarrow d \rightarrow$$

Only a few inflected words get nonzero probability.

Variants with double/gated attention: Peters & Martins (2019, SIGMORPHON).



Entmax and Label Smoothing (Peters & Martins, 2021, NAACL)

- Sparse functions do mitigate the cat-got-your-tongue problem for MT
- Fenchel-Young Label Smoothing: FY loss with smoothed target instead of a one-hot label

$$L_{\Omega,\epsilon}(\boldsymbol{z}, \boldsymbol{e}_{y_t}) := L_{\Omega}(\boldsymbol{z}, (1-\epsilon)\boldsymbol{e}_{y_t} + \epsilon \boldsymbol{u}).$$



Entmax Loss and Label Smoothing (Peters & Martins, 2021, NAACL)

Grapheme-to-Phoneme (SIGMORPHON 2020 Task 1):

		Sin	gle	Ensemble		
α	ϵ	$WER \downarrow$	$PER\downarrow$	$WER \downarrow$	$PER\downarrow$	
1	0	18.14	3.95	14.74	2.96	
	0.15	15.55	3.09	13.87	2.77	
1.5	0	15.25	3.05	13.79	2.77	
	0.04	14.18	2.86	13.47	2.69	

Machine Translation (BLEU scores; WMT14 is En-De):

α	ϵ	De-En	En-De	Ja-En	En-Ja	Ro-En	En-Ro	WMT14
1 1.5	0 > 0 0 > 0	27.05 27.72 28.12 28.11	23.36 24.24 24.03 24.36	20.52 20.99 21.23 21.34	26.94 27.28 27.58 27.58	29.41 30.03 30.27 30.37	22.84 23.15 23.74 23.47	25.10 25.21 25.46 25.45

Entmax Sampling (Martins, Marinho & Martins, 2020, EMNLP)

Use the entmax loss for training language models.

At test time, sample from this sparse distribution.

Better quality with less repetitions than other methods:



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Fine-tuned GPT-2; repetitions and off-topic text are *highlighted*.

Context: "Are they ready to go live?" Zuko asked. "Yup, in just a minute" Tomi replied as he leaned back in his reclining chair. This was a moment that the entire galaxy would see. After 10 years...

Fine-tuned GPT-2; repetitions and off-topic text are *highlighted*.

- **Context:** "Are they ready to go live?" Zuko asked. "Yup, in just a minute" Tomi replied as he leaned back in his reclining chair. This was a moment that the entire galaxy would see. After 10 years...
- **Greedy:** ... of study, the scientists had finally come to the conclusion that the universe was not a place for living. *The scientists* had been studying *the universe* for over a century. *They had been studying the universe for over a century.*

Fine-tuned GPT-2; repetitions and off-topic text are *highlighted*.

Context:	"Are they ready to go live?" Zuko asked. "Yup, in just a minute" Tomi
	replied as he leaned back in his reclining chair. This was a moment that
	the entire galaxy would see. After 10 years

Top-*k*: ... of studying this phenomenon, the team had finally come up with a plan to *study* what the aliens were doing. *The team* would be looking for a way to create a space station. "And what would you call it?" *"What would you call the space station?"*

Fine-tuned GPT-2; repetitions and off-topic text are *highlighted*.

Context: "Are they ready to go live?" Zuko asked. "Yup, in just a minute" Tomi replied as he leaned back in his reclining chair. This was a moment that the entire galaxy would see. After 10 years...

Nucleus: ... of diligent testing, *and some test run after that*, the results were well received. "they're waiting for you, because *there's no way they would*." *Stowedly at a local wedding place, the two archaeologists spoke together.*

Fine-tuned GPT-2; repetitions and off-topic text are *highlighted*.

- **Context:** "Are they ready to go live?" Zuko asked. "Yup, in just a minute" Tomi replied as he leaned back in his reclining chair. This was a moment that the entire galaxy would see. After 10 years...
- **Entmax:** ... of hibernation, Tomi was back. These last days had been a significant step forward in his mission. This time, Tomi was not alone. All the empires had aligned together and the world's leadership began to openly support his mission.
Human Evaluation of Story Completion

	Fluency	Coherence	Engagement
Greedy	2.5	2.3	2.3
top- <i>k</i>	3.3	2.9	2.9
Nucleus	3.5	3.1	3.2
Unlikelihood	3.3	3.0	3.2
Entmax	3.5	3.2	3.6

Human Evaluation of Dialogue Generation

We followed the ConvAl2 challenge: 12 volunteers had 30 conversations each with models using the different sampling methods.

The model's personas were randomly selected from the PersonaChat validation set.

	Fluency	Consistency	Engagement
Greedy	4.1	3.0	2.5
top- <i>k</i>	4.0	3.2	3.3
Nucleus	4.1	3.4	3.3
Entmax	4.1	3.6	3.9

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Conclusions

- Transformations from real numbers to distributions are ubiquitous
- We introduced new transformations that handle sparsity, constraints, and structure
- All are differentiable and their gradients are efficient to compute
- Can be used as hidden layers or as output layers
- The sparsity can be adaptive
- Encouraging results in NMT and other tasks
- Sparse communication potentially useful as a path for explainability.

Thank You!

DeepSPIN ("Deep Structured Prediction in NLP")

- ERC starting grant, started in 2018
- Topics: deep learning, structured prediction, NLP
- More details: https://deep-spin.github.io





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