Evidential Softmax for Sparse Multimodal Distributions in Deep Generative Models

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Deep Generative Models with Discrete Probability Spaces

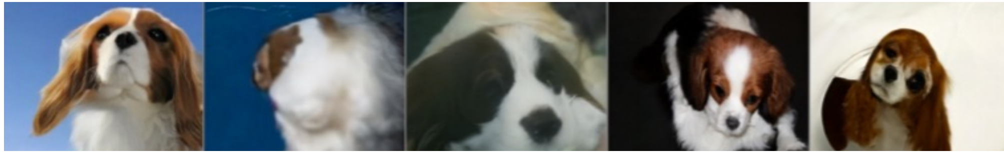
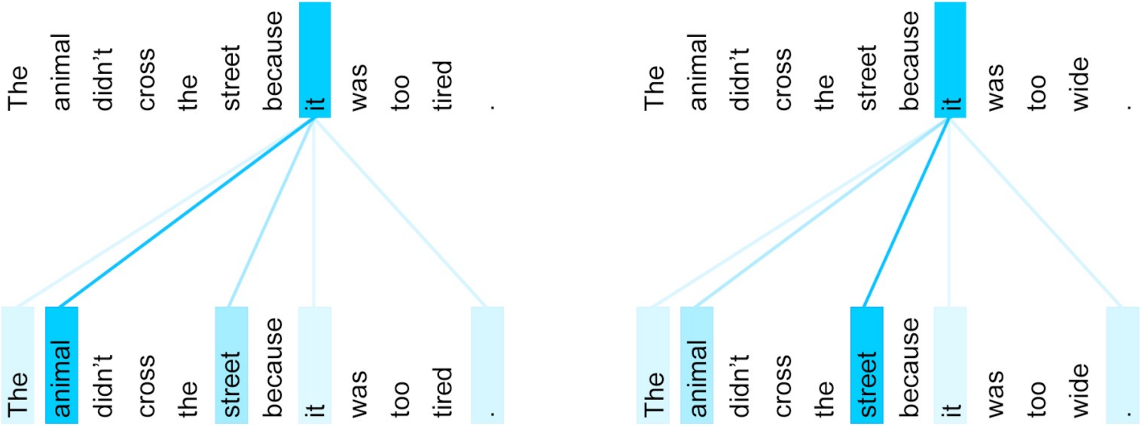


Image generation (VQ-VAE) [van den Oord et al. , NeurIPS, 2017]



Language Modeling [Vaswani et al., NeurIPS, 2017]

Deep Generative Models with Discrete Probability Spaces

Problem: Discrete probability spaces need to be **sufficiently large** to capture the complexities of real-world data, rendering downstream tasks **computationally challenging** [Kaiser et al., ICML, 2018].

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Problem: Discrete probability spaces need to be **sufficiently large** to capture the complexities of real-world data, rendering downstream tasks **computationally challenging** [Kaiser et al., ICML, 2018].

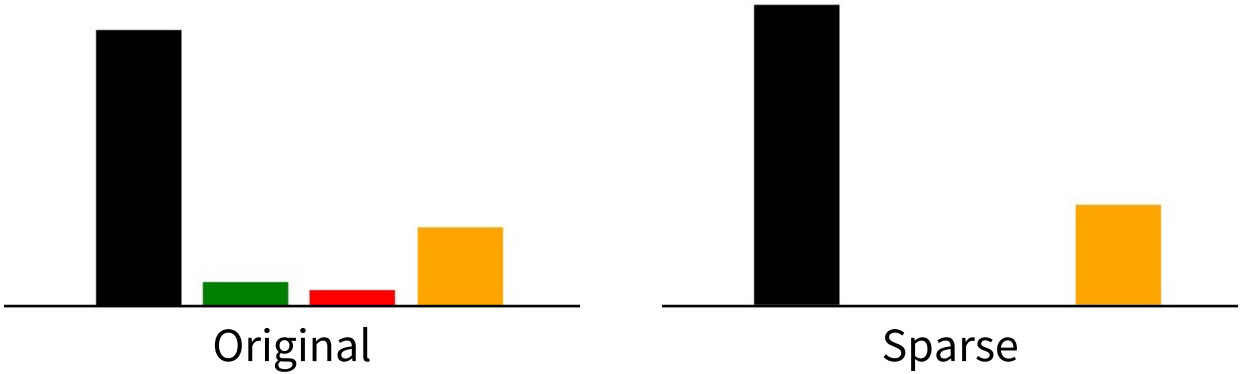
Solutions:

- Sample stochastically (e.g., score function estimator [Glynn et al., ACM, 1990])
- Generate sparse distribution (e.g., sparsemax [Martins et al., ICML, 2016])

VQ-VAE for Image Generation [van den Oord et al., NeurIPS, 2017]

Challenges with Sparse Normalization Functions

- Sparsifying distributions may collapse valid modes [Itkina et al., NeurIPS, 2020].
- Traditional loss functions, such as NLL and KL divergence, are undefined for zero probabilities.



Can we train ***discrete generative models*** *to predict* ***sparse and multimodal*** *probability distributions?*

Evidential Sparsification

Itkina et al. [NeurIPS, 2020] introduce a normalization function which is a post-hoc procedure to sparsify the latent space of conditional variational autoencoders (CVAEs) at test time ***without sacrificing multimodality***.

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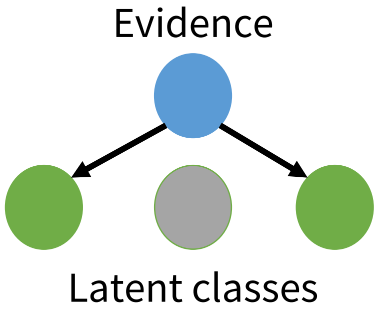
Evidential Conflict ↔ Multimodality

Lack of Evidence ↔ Sparsity



Contributions

1. We introduce **ev-softmax**, a strategy for training neural networks with sparse probability distributions that is compatible with NLL and KL divergence.

2. We derive **properties** of ev-softmax and its training-time approximation.

3. Our approach outperforms baselines in **distributional accuracy** across tasks in **image generation and machine translation**.

Ev-Softmax

We find a simple, equivalent closed form of the post hoc sparsification method [Itkina et al., NeurIPS, 2020].

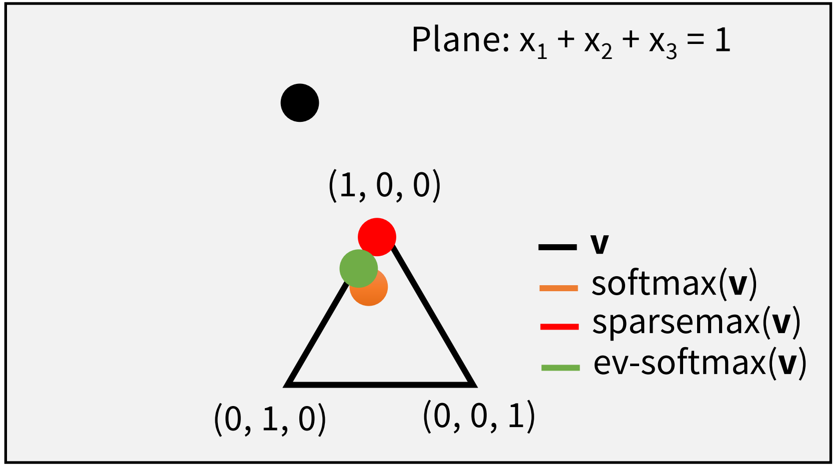
$$\textsc{Softmax}(\mathbf{v})_k \propto e^{v_k}$$

$$\textsc{EvSoftmax}(\mathbf{v})_k \propto \mathbb{1}\{v_k \geq \overline{v}\}e^{v_k}$$

where $\mathbf{v} = \hat{\beta}^T \phi \in \mathbb{R}^K$ and $\overline{v} = \frac{1}{K}\sum_{i=1}^{K} v_i$.

Ev-Softmax Examples

$\mathbf{v}$	Softmax($\mathbf{v}$)	Sparsemax($\mathbf{v}$)	**Ev-Softmax($\mathbf{v}$)**
$(1.3, 0.37, -0.67)$	$(0.65, 0.26, 0.09)$	$(0.97, 0.03, 0)$	$(0.72, 0.28, 0)$
$(0.4, 1.4, -0.8)$	$(0.25, 0.67, 0.07)$	$(0, 1, 0)$	$(0.27, 0.73, 0)$



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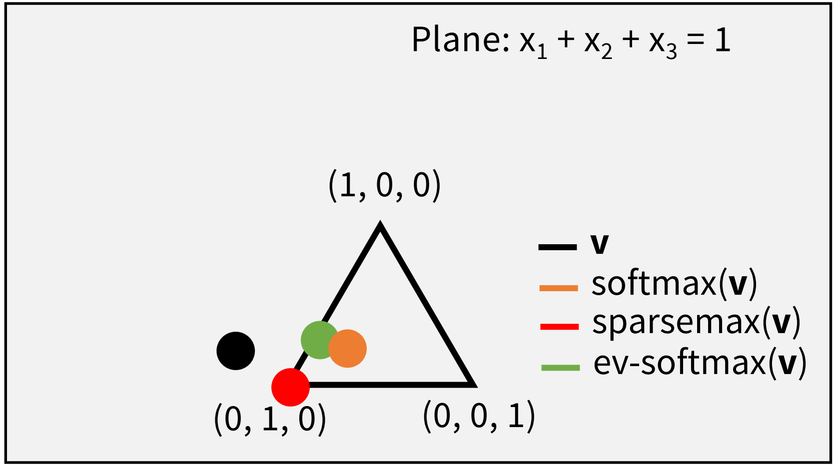


Ev-Softmax Jacobian

The Jacobians of softmax and ev-softmax are similar.

$$\frac{\partial \textsc{Softmax}(\mathbf{v})_i}{\partial v_j} = \textsc{Softmax}(\mathbf{v})_i(\delta_{ij} - \textsc{Softmax}(\mathbf{v})_j)$$

$$\frac{\partial \textsc{EvSoftmax}(\mathbf{v})_i}{\partial v_j} = \textsc{EvSoftmax}(\mathbf{v})_i(\delta_{ij} - \textsc{EvSoftmax}(\mathbf{v})_j)$$

Ev-Softmax Properties

Ev-softmax exhibits similar properties to softmax.

Property	Softmax	Sparsemax [8]	Sparsehourglass [17]	**Ev-Softmax (Ours)**
Idempotence		✓	✓	
Monotonic	✓	✓	✓	✓
Translation Invariance	✓	✓	✓*	✓
Scale Invariance			✓*	
Full Domain	✓	✓	✓	✓
Lipschitz	1	1	$1 + \frac{1}{Kq}$	1^*

Ev-Softmax Training

During training, we modify ev-softmax as follows.

$$\textsc{EvSoftmax}_{\text{train},\epsilon}(\mathbf{v})_i \propto (\mathbb{1}\{v_i \geq \overline{v}\} + \epsilon)e^{v_k}$$

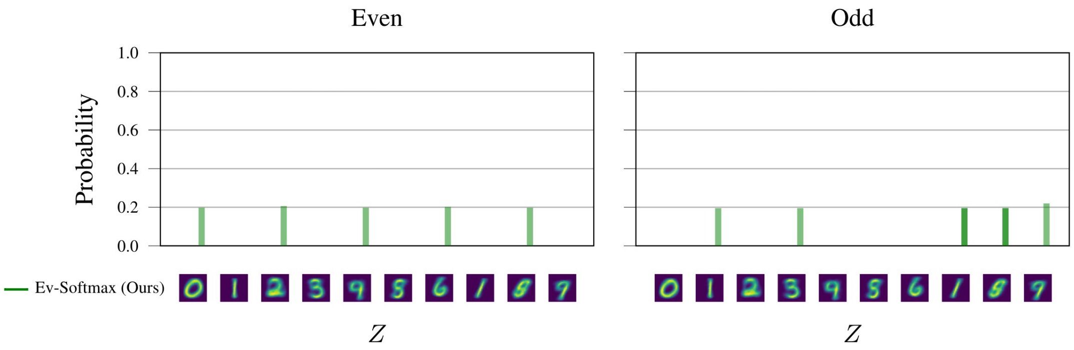
In the limit, the NLL loss term takes a similar form to softmax.

$$\nabla_{\mathbf{v}} \log\left[\textsc{Softmax}(\mathbf{v})_i\right] = \boldsymbol{\delta}_i - \textsc{Softmax}(\mathbf{v})$$
$$\lim_{\epsilon \to 0} \nabla_{\mathbf{v}} \log\left[\textsc{EvSoftmax}_{\text{train},\epsilon}(\mathbf{v})_i\right] = \boldsymbol{\delta}_i - \textsc{EvSoftmax}(\mathbf{v})$$

Experiments: Toy MNIST Example

Task: generate images of even and odd numbers.

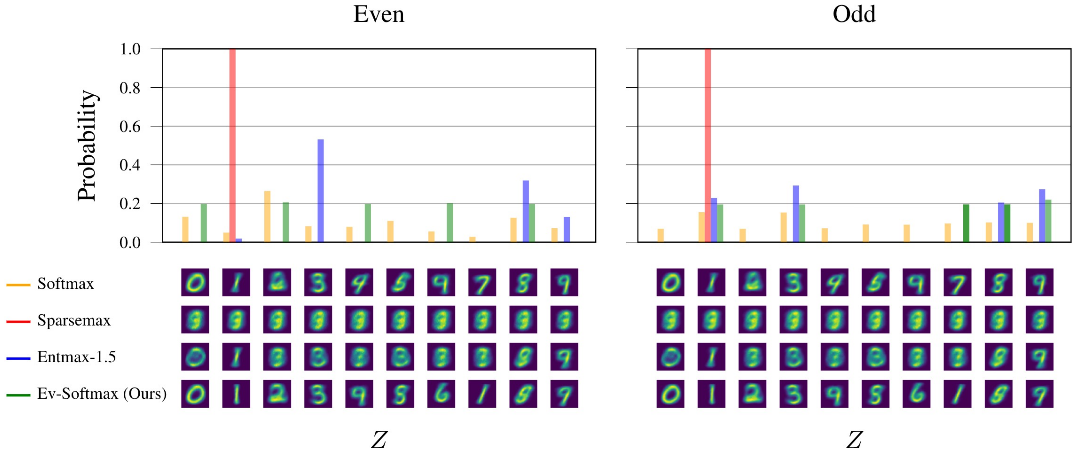
Results: Plot shows our ev-softmax (green) distribution.



Experiments: Toy MNIST Example

Task: generate images of even and odd numbers.

Results: Plot shows softmax (yellow), sparsemax (orange) [Martins et al., ICML, 2016], entmax-1.5 (blue) [Peters et al., ACL, 2019], and our ev-softmax (green) distributions.

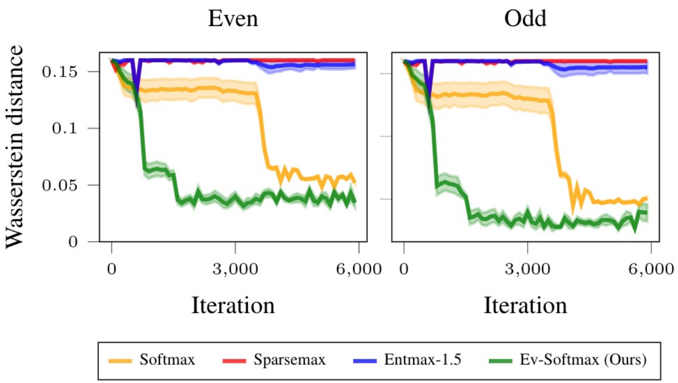


Note: Sparsemax and entmax-1.5 appear to collapse the latent space.

Experiments: Toy MNIST Example

Task: generate images of even and odd numbers.

Results: Plot shows the Wasserstein distance for the softmax (yellow), sparsemax (orange) [Martins et al., ICML, 2016], entmax-1.5 (blue) [Peters et al., ACL, 2019], and ev-softmax (green) distributions.



Note: Our method yields the lowest Wasserstein distance.

Experiments: Image Generation

Task: image generation on *tiny*ImageNet
Network Architecture: VQ-VAE [van den Oord et al., NeurIPS, 2017], 16x16 512-class latent space
Results: 85% reduction in the latent sample space

Method	Acc-5	Acc-10	K
Softmax	38.4	48.8	512
Sparsemax	40.0	52.0	46
Entmax-1.5	38.4	49.2	90
Ev-softmax	**43.6**	**55.6**	77

Note: Our method sparsifies the distribution at a level between sparsemax and entmax-1.5, but outperforms in accuracy.

Experiments: Machine Translation

Task: machine translation on IWSLT 2014 [Cettolo et al., IWSLT, 2017]
Network Architecture: OpenNMT transformer [Klein et al., AMTA, 2020]

Metric	Softmax	Post-hoc Evidential	Sparsemax	Entmax-1.5	Ev-softmax
BLEU	29.2 ± 0.06	29.2 ± 0.05	29.0 ± 0.05	29.2 ± 0.07	$\mathbf{29.4 \pm 0.05}$
ROUGE-1	59.31	59.09	58.47	58.94	**59.32**
ROUGE-2	35.62	35.42	34.76	35.20	**35.74**
ROUGE-L	56.09	55.93	55.39	55.75	**56.18**
METEOR	57.02	56.84	56.33	5.83	**57.20**
p-val (METEOR)	< 0.05	< 0.01	< 0.001	< 0.01	N/A
# attended	39.5 ± 11.5	3.8 ± 0.93	2.3 ± 0.54	4.1 ± 1.3	8.2 ± 1.3

Note: Our method attends to a larger number of words than sparsemax and entmax-1.5, and outperforms all methods in all computed metrics.

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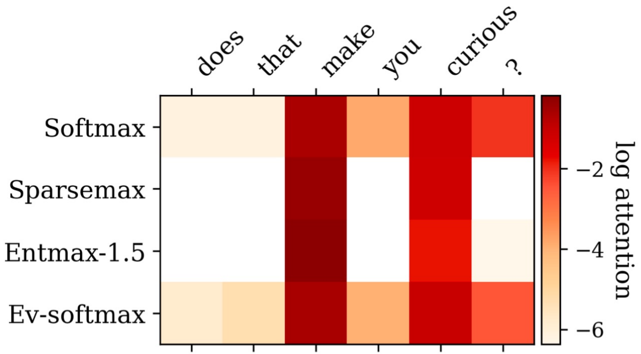

Note: Sparsemax and entmax-1.5 both attend over two words while ev-softmax and softmax attend over the entire source.

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- Ev-softmax outperforms softmax and sparse normalization functions across tasks in image generation and machine translation.
- Future work can involve training computer vision and machine translation models from scratch on a larger scale.
- Our code is available at https://github.com/sisl/EvSoftmax

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Thank you!

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