Evidential Softmax for Sparse Multimodal Distributions in Deep Generative Models

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Abstract

Many applications of generative models rely on the marginalization of their high-dimensional output probability distributions. Normalization functions that yield sparse probability distributions can make exact marginalization more computationally tractable. However, sparse normalization functions usually require alternative loss functions for training since the log-likelihood is undefined for sparse probability distributions. Furthermore, many sparse normalization functions often collapse the multimodality of distributions. In this work, we present ev-softmax, a sparse normalization function that preserves the multimodality of probability distributions. We derive its properties, including its gradient in closed-form, and introduce a continuous family of approximations to ev-softmax that have full support and can be trained with probabilistic loss functions such as negative log likelihood and Kullback-Leibler divergence. We evaluate our method on a variety of generative models, including variational autoencoders and auto-regressive architectures. Our method outperforms existing dense and sparse normalization techniques in distributional accuracy. We demonstrate that ev-softmax successfully reduces the dimensionality of probability distributions while maintaining multimodality.

1 Introduction

Learning deep generative models over discrete probability spaces has enabled state-of-the-art performance across tasks in computer vision [1], natural language processing [2]–[4], and robotics [5]–[7]. The probability distributions of deep generative models are often obtained from a neural network using the softmax transformation. Since the softmax function has full support, the logarithm of the output probabilities is well-defined, which is important for common probabilistic loss functions such as the negative log likelihood, cross entropy, and Kullback-Leibler (KL) divergence.

Several applications highlight the importance of achieving sparsity in high dimensional dense distributions to make downstream tasks computationally feasible and perhaps even interpretable [8]–[11]. In discrete variational autoencoders (VAEs), for instance, calculating the posterior probabilities exactly requires marginalization over all possible latent variable assignments, which is intractable for large latent spaces [9], [10]. Stochastic approaches to circumvent exact marginalization include the score function estimator [12], [13], which suffers from high variance, and continuous relaxations of the discrete latent variable, such as Gumbel-Softmax [14], [15], which introduce bias.

Alternatively, high-dimensional latent spaces can be tractably marginalized using normalization functions that produce sparse probability distributions. Several sparse alternatives to softmax have been proposed, including sparsemax [8], α-entmax [16], and sparsehourglass [17]. However, such approaches often collapse the multimodality of distributions, resulting in unimodal probability distributions [10] (see Fig. 1). When marginalizing over discrete latent spaces, maintaining this multimodality is crucial for applications such as image generation, where the latent space is multimodal in nature [1], and machine translation, where multiple words can be valid translations and require...
The VAE estimates parameters $\phi$ to model a data generating distribution, we consider data
post-hoc sparsification procedure introduced by Itkina et al. 
$\nu$ yields a unimodal distribution, while $\nu$ yields a bimodal distribution which is close to that of $\nu$.
context to distinguish between the optimal word choice [9]. Furthermore, these approaches either
require the construction of alternative loss functions to the negative log-likelihood, which is undefined
for zero-valued output probabilities [8], [16]–[18], or they are applied as a post-hoc transformation
at test time [10]. For the latter case, the latent distributions obtained through these existing sparse
normalization functions and their resulting posteriors are not trained directly.

The post-hoc sparsification procedure introduced by Itkina et al. [10] provides a method for obtaining
sparse yet multimodal distributions at test time. We generalize this method to a sparse normalization
function termed evidential softmax (ev-softmax) which can be applied during both training and test
time. We define continuous approximations of this function that have full support and are thus
compatible with typical loss terms, such as negative log-likelihood and KL divergence. We use this
full-support approximation of ev-softmax to directly optimize discrete generative models for objective
functions with probabilistic interpretations. This approach is in contrast with post-hoc sparsification
methods that optimize a proxy model [10] and methods that use non-probabilistic objective functions,
such as sparsemax [8]. We evaluate these discrete generative models at test time with the ev-softmax
function to obtain sparse yet multimodal latent distributions.

Contributions: This paper proposes a strategy for training neural networks with sparse probability
distributions that is compatible with negative log-likelihood and KL-divergence computations. We
generalize the evidential sparsification procedure developed by Itkina et al. [10] to the ev-softmax
function. We prove properties of ev-softmax and its continuous approximation, which has full support.
Our approach outperforms existing dense and sparse normalization functions in distributional accuracy
across image generation and machine translation tasks.

2 Background

Notation: We denote scalars, vectors, matrices, and sets as $a$, $a$, $A$, and $A$, respectively. The
vectorized Kronecker delta $\delta$ is defined to be 1 at the $i$th index and 0 at all the other indices. The
$K$-dimensional simplex is written as $\Delta^K := \{ \xi \in \mathbb{R}^{K+1} : 1^T \xi = 1, \xi \geq 0 \}$. The KL divergence
of probability distribution $p$ from distribution $q$ is denoted as $\text{KL}(p \mid \mid q)$.

2.1 Discrete Variational Autoencoders

To model a data generating distribution, we consider data $x \in \mathbb{R}^d$, categorical input variable $y \in Y$,
categorical latent variable $z \in Z$, and parameters $\theta \in \mathbb{R}^\theta$. In the VAE model, $z$ is sampled from a
prior $p_0(z)$, and we generate $x$ conditioned on $z$ as $p_0(x \mid z)$. The conditional variational autoencoder
(CVAE) [19] extends this framework by allowing for the generative process to be controlled by input
$y$. The latent variable $z$ is thus conditioned on the input $y$ in the prior $p_0(z \mid y)$.

The VAE estimates parameters $\phi$ and an auxiliary distribution $q_\phi(z \mid x)$ to calculate the evidence
lower bound (ELBO) of the log-likelihood for the observed data [20]:

$$
\log p_\theta(x) \geq \mathbb{E}_{q_\phi(x \mid x)} \log p_\theta(x \mid z) - \text{KL}(q_\phi(z \mid x) \mid \mid p_\theta(z))
$$

(1)

The CVAE estimates parameters $\phi$ of an auxiliary distribution $q_\phi(z \mid x, y)$ to obtain the ELBO [19]:

$$
\log p_\theta(x \mid y) \geq \mathbb{E}_{q_\phi(x \mid x, y)} \log p_\theta(x \mid z) - \text{KL}(q_\phi(z \mid x, y) \mid \mid p_\theta(z \mid y)).
$$

(2)
The subsequent discussion focuses on VAEs, and analogous expressions for CVAEs may be obtained by replacing $p_0(x)$, $q_\phi(z \mid x)$, and $p_0(z)$ with $p_0(x \mid y)$, $q_\phi(z \mid x, y)$, and $p_0(z \mid y)$, respectively.

Maximizing the VAE ELBO using gradient-based methods involves computing the term $\nabla_\phi E_{q_\phi(z \mid x)} \log p_0(x \mid z)$ in Eq. (1), which requires marginalization over the auxiliary distribution $q_\phi(z \mid x)$. Many Monte Carlo approaches estimate this quantity without explicit marginalization over all possible latent classes $z \in Z$. The score function estimator (SFE) is an unbiased estimator which uses the identity $\nabla_\phi E_{q_\phi(z \mid x)} \log p_0(x \mid z) = E_{q_\phi(z \mid x)} p_0(x) \nabla_\phi \log q_\phi(z \mid x)$ to estimate the gradient through samples drawn from $q_\phi(z \mid x)$. However, the SFE is prone to high variance, and in practice, sampling-based approaches generally require variance reduction methods such as baselines, control variates, and Rao-Blackwellization techniques [21]. Alternatively, a low-variance gradient estimate can be obtained by the reparameterization trick, which separates the parameters of the distribution from the source of stochasticity [20]. The Gumbel-Softmax and Straight-Through reparameterization trick rely on a continuous relaxation of the discrete latent space [14], [15]. In contrast to these stochastic approaches, our method, like sparsemax [8], $\alpha$-entmax [16], and sparsehourglass [17], focuses on obtaining sparse auxiliary distributions $q_\phi(z \mid x)$ to enable exact marginalization over all latent classes $z \in Z$ for which the auxiliary distribution has nonzero probability mass.

### 2.2 Normalization Functions

A common normalization function that maps vectors $v \in \mathbb{R}^K$ to probability distributions in $\Delta^{K-1}$ is the softmax function:

$$\text{SOFTMAX}(v)_k \propto e^{v_k}. \quad (3)$$

One limitation of this function is the resulting probability distribution always has full support, i.e. $\text{SOFTMAX}(v)_k \neq 0$ for all $v$ and $k$. Thus, if the distributions $q_\phi$ in Eq. (1) and Eq. (2) are outputs of the softmax function, then calculating the expectations over $q_\phi$ exactly requires marginalizing over all one-hot vectors $z \in \mathbb{R}^K$, which can be computationally intractable when $K$ is large [9], [10].

Recent interest in sparse alternatives has led to the development of many new sparse normalization functions [8], [10], [16]–[18]. The sparsemax function projects inputs onto the simplex to achieve a sparse distribution [8]. The $\alpha$-entmax family of functions generalizes the softmax and sparsemax functions through a learnable parameter $\alpha$ which tunes the level of sparsity [16]. Sparsehourglass is another generalization of sparsemax with a controllable level of sparsity [17]. Despite the controls, we find that these methods achieve sparsity at the expense of collapsing valid modes.

### 2.3 Post-Hoc Evidential Sparsification

Of particular interest is a sparse normalization function that maintains multimodality in probability distributions. Balancing sparsity and multimodality has been shown to be beneficial for tasks such as image generation [10] or machine translation [16]. Itkina et al. [10] propose a post-hoc sparsification method for discrete latent spaces in CVAEs which preserves multimodality in distributions. The method calculates evidential weights as affine transformations of an input feature vector and interprets these weights as evidence either for a singleton latent class $\{z_k\}$ or its complement $\{\bar{z}_k\}$ depending on the sign of the weights. This interpretation, with origins in evidential theory [22], [23], allows for the distinction between conflicting evidence and lack of evidence, which is normally not possible with ordinary multinomial logistic regression. Conflicting evidence can be interpreted as multimodality whereas lack of evidence can correspond to sparsity [10].

For a given dataset and model, the resulting post-hoc sparsification is as follows. A CVAE is trained on a dataset using the softmax normalization and the ELBO in Eq. (2). At test time, for a given query $y$ from the dataset, the learned weights of the last layer of the encoder $\hat{\beta} \in \mathbb{R}^{(J+1) \times K}$, and the corresponding output of the last hidden layer $\phi(y) \in \mathbb{R}^J$, the evidential weights are:

$$w_k = \hat{\beta}_{0k} - \frac{1}{K} \sum_{\ell=1}^K \hat{\beta}_{0\ell} + \sum_{j=1}^J \phi_j \left( \hat{\beta}_{jk} - \frac{1}{K} \sum_{\ell=1}^K \hat{\beta}_{j\ell} \right) \quad (4)$$

for each $k \in \{1, \ldots, K\}$. Evidence in support of a latent class $z_k$ then corresponds to $w_k^+ = \max(0, w_k)$ and evidence against it as $w_k^- = \max(0, -w_k)$. The resulting sparse distribution is:

$$p(z_k \mid y) \propto \mathbb{I}\{m_k \neq 0\} e^{w_k}, \quad (5)$$
We briefly sketch the proof of Theorem 3.1 and refer the reader to Appendix B for the full derivation.

We propose a transformation, which we call ev-softmax, on inputs \( \mathbf{v} \in \mathbb{R}^K \). We claim that this transformation is equivalent to that of the post-hoc evidential sparsification procedure with the advantages of having a simple closed form and requiring only \( O(K) \) computations.

Let \( \tau = \frac{1}{K} \sum_{i=1}^{K} v_i \) be the arithmetic mean of the elements of \( \mathbf{v} \). We define our transformation as,

\[
\text{EVSOFTMAX}(\mathbf{v})_k \propto \mathbb{I}\{v_k \geq \tau\} e^{v_k}.
\]

Note that the post-hoc sparsification procedure in Section 2.3 takes input vectors \( \phi \in \mathbb{R}^J \) and the weights \( \beta \in \mathbb{R}^{(J+1) \times K} \) of the neural network’s last layer whereas the ev-softmax function takes as input \( \mathbf{v} = \beta^T \phi \in \mathbb{R}^K \). We formalize the equivalence of ev-softmax with the post-hoc sparsification procedure as follows:

**Theorem 3.1.** For any input vector \( \phi \in \mathbb{R}^J \), weight matrix \( \beta \in \mathbb{R}^{(J+1) \times K} \), define the score vector \( \mathbf{v} = \beta^T \phi \) and variables \( w_k, m_k \), and \( p(z_k) \) as in Section 2.3 for all \( k \in \{1, \ldots, K\} \). If the probability distribution of \( \mathbf{v} \) is non-atomic, then \( \text{EVSOFTMAX}(\mathbf{v})_k = p(z_k) \) for each \( k \).

The proof of this theorem uses the following two lemmas:

**Lemma 3.2.** Let \( \tau = \frac{1}{K} \sum_{i=1}^{K} v_i \). Then \( v_k - \tau = w_k \) for all \( k \in \{1, \ldots, K\} \).

**Proof.** The result follows from algebraic manipulation of Eq. \( \text{[4]} \). Full details are in Appendix B. \( \square \)

**Lemma 3.3.** For \( m_k \) as defined in Eq. \( \text{[6]} \), \( \mathbb{I}\{m_k \neq 0\} = \mathbb{I}\{v_k \geq \tau\} \) for all \( k \in \{1, \ldots, K\} \).

**Proof.** Observe that the condition \( \mathbb{I}\{m_k = 0\} = 1 - \mathbb{I}\{m_k \neq 0\} \) is equivalent to the conjunction of the following two conditions: 1) \( w_k \leq 0 \) and 2) there exists some \( \ell \neq k \) such that \( v_\ell \geq 0 \). From Lemma 3.2, these statements are equivalent to 1) \( v_k \leq \tau \) and 2) there exists some \( \ell \neq k \) such that \( v_\ell \geq \tau \). Note that if \( v_k \leq \tau \), then either \( v_\ell = \tau \) or there must exist some \( \ell \neq k \) such that \( v_\ell > \tau \). In both cases, there exists \( \ell \neq k \) such that \( v_\ell \geq \tau \). Thus, we see that \( v_k \leq \tau \) implies there exists some \( \ell \neq k \) such that \( v_\ell \geq \tau \). We conclude that \( \mathbb{I}\{m_k = 0\} = \mathbb{I}\{v_k \leq \tau\} \) and the result follows. \( \square \)

We briefly sketch the proof of Theorem 3.1 and refer the reader to Appendix B for the full derivation. Lemma 3.2 implies that \( e^{w_k} \propto e^{v_k} \). In addition, combining Lemma 3.3 with the non-atomicity of the distribution of \( \mathbf{v} \) yields that \( \mathbb{I}\{m_k \neq 0\} = \mathbb{I}\{v_k \geq \tau\} \) (Lemma B.3). Eq. \( \text{[7]} \) follows from these two results.

### 3.1 Properties

Table \( \text{[1]} \) gives a list of softmax alternatives, desirable properties of a normalization function, and which properties are satisfied by each function as inspired by the analysis of Laha et al. \( \text{[17]} \). Refer to Appendix C for proofs of these properties. These results show that ev-softmax satisfies the same properties as the softmax transformation. While idempotence can be useful, these normalizations are generally only applied once, and in this regime the idempotence does not provide any further guarantees. Likewise, scale invariance is less applicable in practice because the scale of the inputs to
normalization functions is often one of the learned features of data, and the scale generally provides a measure of confidence in the predictions.

The Jacobians of softmax and ev-softmax have analogous forms (see Appendix C):

\[
\frac{\partial \text{SOFTMAX}(v)_i}{\partial v_j} = \text{SOFTMAX}(v)_i (\delta_{ij} - \text{SOFTMAX}(v)_j) \tag{8}
\]

\[
\frac{\partial \text{EV-SOFTMAX}(v)_i}{\partial v_j} = \text{EV-SOFTMAX}(v)_i (\delta_{ij} - \text{EV-SOFTMAX}(v)_j). \tag{9}
\]

For the Jacobian of the proposed ev-softmax function, there are two cases to consider. First, when either or both of $\text{EV-SOFTMAX}(v)_i$ and $\text{EV-SOFTMAX}(v)_j$ are exactly 0, we have $\frac{\partial \text{EV-SOFTMAX}(v)_i}{\partial v_j} = 0$. Intuitively, this occurs because classes that have a probability of 0 do not contribute to the gradient and also remain 0 under small local changes in the input. Second, when both $\text{EV-SOFTMAX}(v)_i$ and $\text{EV-SOFTMAX}(v)_j$ are nonzero, the partial derivative is equivalent to that of softmax over the classes that have nonzero probabilities. Hence, optimizing models using the ev-softmax function should yield similar behaviors to those using the softmax function.

One notable connection between ev-softmax and sparsemax is that the supports of both functions can be expressed in terms of mean conditions of their inputs. For an input $v \in \mathbb{R}^K$, the $i$th class is given zero probability by ev-softmax if $v_i < \frac{1}{K} \sum_{k=1}^{K} v_k$. Analogously, denoting the size of the support of sparsemax on $v$ as $\ell$, the $i$th class is given zero probability by sparsemax if $v_i \leq -\frac{1}{\ell} + \frac{1}{\ell} \sum_{k=1}^{\ell} v_{(k)}$, where $v_{(k)}$ is the $k$th largest element in $v$ [8]. Thus, sparsemax considers the arithmetic mean after sparsification, whereas ev-softmax considers the arithmetic mean before sparsification.

Figure 1 presents a visualization of an input point in $\mathbb{R}^3$ and the results upon applying softmax, sparsemax, and ev-softmax to this point. Informally, the interior of the simplex is the set of trimodal distributions, the edges constitute the set of bimodal distributions, and the vertices are the unimodal distributions. Thus, this input provides an example of when sparsemax yields a unimodal distribution whereas ev-softmax does not. Note that $\mathbb{R}^3$ is the lowest-dimensional space for which the ev-softmax function is nontrivial. In $\mathbb{R}^2$, ev-softmax is equivalent to the argmax function, which is piece-wise constant and has zero gradients everywhere. However, the focus of ev-softmax is on balancing multimodality with sparsity for spaces with higher dimension than $\mathbb{R}^2$.

### 3.2 Training-time Modification

Since ev-softmax outputs a sparse probability distribution, the negative log-likelihood and KL divergence cannot be directly computed. To address this limitation, we modify ev-softmax during training time as follows:

\[
\text{EV-SOFTMAX}_{\text{train}}(v)_i \propto (\mathbb{1} \{ v_i \geq \bar{v} \} + \epsilon) e^{v_k} \tag{10}
\]

for some small $\epsilon$. In practice, we set $\epsilon$ to $10^{-6}$.

The KL divergence with the above training modification takes the same form as the $\epsilon$-KL used for overcoming sparsity in language modeling [24, 25]. As $\epsilon$ approaches 0, the gradient of the negative
Using the proposed normalization function \textit{ev-softmax} at training time yields a more accurate distribution on the MNIST dataset than \textit{softmax}, \textit{sparsemax}, \textit{entmax}-1.5, and \textit{post-hoc evidential} baselines. The horizontal axis shows the decoded image for each latent class and the vertical axis shows the probability mass. Note that the latent space for the \textit{post-hoc evidential} method is the same as that of \textit{softmax}, since the method is applied only at test time to the latent space distribution. Unlike \textit{ev-softmax}, the sparse distributions produced by \textit{sparsemax} and \textit{entmax}-1.5 collapse the latent space.

\begin{align*}
\nabla_v \log [\text{SOFTMAX}(v)]_i &= \delta_i - \text{SOFTMAX}(v), \quad (11) \\
\lim_{\epsilon \to 0} \nabla_v \log [\text{EVSOFTMAX}_{\text{train},\epsilon}(v)]_i &= \delta_i - \text{EVSOFTMAX}(v), \quad (12)
\end{align*}

for any finite-dimensional, real-valued vector \( v \). A derivation of Eq. (12) is given in Appendix D.

While the Gumbel-Softmax relaxation also enables gradient computations through discrete spaces, Eq. (12) establishes the convergence and closed-form solution of the gradient as the relaxation goes to 0, which applies uniquely to the \textit{ev-softmax} function. Note that the limit of the log-likelihood of a distribution generated by the training-time modification (i.e. \( \lim_{\epsilon \to 0} \log[\text{EVSOFTMAX}_{\text{train},\epsilon}(v)]_i \)) is undefined, but Eq. (12) shows that the limit of the gradient of the log-likelihood is defined.

4 Experiments

We demonstrate the applicability of our proposed strategies on the tasks of image generation and machine translation. \footnote{Code for the experiments is available at \url{https://github.com/sisl/EvSoftmax}} We compare our method to the \textit{softmax} function as well as sparse normalization functions \textit{sparsemax} \cite{8} and \textit{entmax}-1.5 \cite{16}. We also compare with the \textit{post-hoc evidential sparsification} procedure \cite{10}. \textit{Sparsehourglass} is not used as it is similar to \textit{\alpha-entmax}. Experiments indicate that \textit{ev-softmax} achieves higher distributional accuracy than \textit{softmax}, \textit{sparsemax}, \textit{entmax}-1.5, and \textit{post-hoc evidential sparsification} by better balancing the objectives of sparsity and multimodality.

4.1 Conditional Variational Autoencoder (CVAE)

To gain intuition for the \textit{ev-softmax} function, we consider the multimodal task of generating digit images for \textit{even} and \textit{odd} queries (\( y \in \{\text{even}, \text{odd}\} \)) on MNIST. We use a CVAE with \( |Z| = 10 \) latent classes. Since the true conditional prior distribution given \( y \in \{\text{even}, \text{odd}\} \) is uniform over 5 digits, this task benefits from both sparsity and multimodality of a normalization function.

\textbf{Model:} We follow the CVAE architecture and training procedure of Itkina \textit{et al.} \cite{10} for this task. For each of the four normalization functions we consider (\textit{ev-softmax}, \textit{sparsemax}, \textit{entmax}-1.5, and \textit{softmax}), we train an encoder, which consists of two multi-layer perceptrons (MLPs), and a decoder. The first MLP of the encoder receives an input query \( y \) and outputs a categorical prior distribution \( p_0(z \mid y) \) over the latent variable \( z \) generated by the normalization function. The second MLP takes as input a feature vector \( x \) in addition to the query \( y \), and outputs the probability distribution for the

\url{https://github.com/sisl/EvSoftmax}
We also train a model using softmax. In this regime, we expect that we also train a model using softmax. We compare softmax with ev-softmax. To evaluate our method in a semi-supervised setting, we consider the semi-supervised VAE of Kingma et al. [9]. We model the joint probability of an MNIST image \( x \in \mathbb{R}^d \), a continuous latent variable \( h \in \mathbb{R}^n \), and a discrete latent variable \( z \in \{ \delta_1, \ldots, \delta_v \} \) as \( p_\theta(x) = p_\theta(x | z, h)p(z)p(h) \). We assume \( h \) has an \( n \)-dimensional standard Gaussian prior and \( z \) a uniform prior.

We compare ev-softmax to other sparse normalization functions, including sparsemax and entmax-1.5. We also train a model using softmax and apply posthoc evidential sparsification at test time. Since we follow the procedure of Correia et al. [9], we additionally report the results they obtained for stochastic methods. Unbiased gradient estimators that they report include SFE with a moving average baseline; SFE with a self-critic baseline (SFE+) [27]; neural variational inference and learning (NVIL) with a...
learned baseline \cite{28}; and sum-and-sample, a Rao-Blackwellized version of SFE \cite{21}. They also evaluate biased gradient estimators including Gumbel-Softmax and straight-through Gumbel-Softmax (ST Gumbel) \cite{14, 15}. Each model was trained for 200 epochs.

**Results and discussion:** Table 2 shows that using ev-softmax yields the highest classification accuracy of models using either Monte Carlo methods or marginalization. Compared to sparsemax and entmax-1.5, ev-softmax maintains higher multimodality in the output distribution, reducing the latent space by 84% on average. In particular, both sparsemax and entmax-1.5 reduce the latent space by almost 90%, but at the cost of decreased accuracy. On the other hand, post-hoc evidential sparsification preserves more latent classes than ev-softmax but with a higher variance, and it also achieves a lower accuracy. This suggests that in this semi-supervised setting, training with sparsity and multimodality in the output distribution are both important for distributional accuracy, which benefits overall performance.

| Method                | Accuracy (%) | Decoder calls |
|-----------------------|--------------|---------------|
| **Monte Carlo**       |              |               |
| SFE                   | 94.75 ± 0.02 | 1             |
| SFE+                  | 96.53 ± 0.01 | 2             |
| NVIL                  | 96.01 ± 0.02 | 1             |
| Sum&Sample            | 96.73 ± 0.01 | 2             |
| Gumbel                | 95.46 ± 0.01 | 1             |
| ST Gumbel             | 86.35 ± 0.06 | 1             |
| **Marginalization**   |              |               |
| Softmax               | 96.93 ± 0.01 | 10            |
| Sparsemax             | 96.87 ± 0.01 | 1.01 ± 0.01   |
| Entmax-1.5            | 97.20 ± 0.01 | 1.01 ± 0.01   |
| Post-hoc evidential   | 96.90 ± 0.01 | 1.72 ± 0.05   |
| **Ev-softmax**        | 97.30 ± 0.01 | 1.64 ± 0.01   |

4.3 Vector-Quantized Variational Autoencoder (VQ-VAE)

We demonstrate the performance of our approach on a much larger latent space by training a Vector Quantized-Variational Autoencoder (VQ-VAE) model on tinyImageNet \cite{29} for image generation. The VQ-VAE learns discrete latent variables embedded in continuous vector spaces \cite{1}. We use the tinyImageNet dataset due to computational constraints.

**Model:** We train the VQ-VAE architecture in two stages. First the VQ-VAE model is trained assuming a uniform prior over the discrete latent space. For each normalization method, we train an autoregressive prior over the latent space from which we sample. We consider a latent space of \(16 \times 16\) discrete latent variables with \(K = 512\) classes each. We use the same PixelCNN \cite{30} as Itkina et al. \cite{10} for the autoregressive prior. For each normalization function, we train a PixelCNN prior using that function to generate the output probability over the latent space. To evaluate the accuracy of our VQ-VAE models, we train a Wide Residual Network classifier \cite{31} on tinyImageNet and calculate its classification accuracy on the images generated by the VQ-VAE models. Further experimental details are given in Appendix E.

**Results and discussion:** Table 3 shows that ev-softmax outperforms other sparse methods in accuracy and is able to generate images with the most resemblance to the ground truth. Our method reduces the number of latent classes by 85% on average, more than the 83% of entmax-1.5 but less than the 91% of sparsemax. With the exception of post-hoc evidential sparsification, the sparse methods all outperform softmax, suggesting that sparsity improves the model’s performance on the task of image generation by discarding irrelevant latent classes. The underperformance of the post-hoc evidential model is expected, as post-hoc evidential sparsification is applied only at test time to a model trained with the softmax function, which bounds its performance. Since the VQ-VAE samples directly from the output distribution of the PixelCNN prior, the probabilistic nature of this downstream task...
We use byte pair encoding (BPE) to encode rare and were pretrained on the EN-DE corpus from WMT 2016 [35]. We finetune for 40000 iterations.

Table 4: BLEU, ROUGE, and METEOR scores, and number of nonzero elements in the attention on the EN→DE corpus of IWSLT 2014. We report the mean and standard error for the BLEU score and number of nonzero elements over 5 random seeds. Our method outperforms all baselines in all metrics and maintains a higher number of nonzero attended elements than other sparse normalization functions. Higher is better for all metrics. The asterisk "*" denotes that ev-softmax outperformed the method with a significance level of 0.05, and "**" denotes a significance of 0.01.

| Metric     | Softmax | Sparsemax  | Entmax-1.5 | Post-hoc Evidential | Ev-softmax |
|------------|---------|------------|------------|---------------------|------------|
| BLEU       | 29.2 ± 0.06 | 29.0 ± 0.05 | 29.2 ± 0.07 | 29.2 ± 0.05         | 29.4 ± 0.05 |
| ROUGE-1    | 59.31   | 58.47**    | 58.94*     | 59.09*              | 59.32      |
| ROUGE-2    | 35.62   | 34.76**    | 35.20*     | 35.42*              | 35.74      |
| ROUGE-L    | 56.09   | 55.39**    | 55.75*     | 55.93*              | 56.18      |
| METEOR     | 57.02*  | 56.33**    | 5.83**     | 56.84**             | 57.20      |
| # attended | 39.5 ± 11.5 | 2.3 ± 0.54 | 4.1 ± 1.3   | 3.8 ± 0.93          | 8.2 ± 1.3  |

suggests that optimizing the prior for log-likelihood allows the model to learn a prior distribution that achieves better performance on the downstream task.

4.4 Machine Translation

We evaluate our method in the setting of machine translation. Attention-based translation models generally employ dense attention weights over the entire source sequence while traditional statistical machine translation systems are usually based on a lattice of sparse phrase hypotheses [9]. Thus, sparse attention offers the possibility of more interpretable attention distributions which avoid wasting probability mass on irrelevant source words. Furthermore, language modeling often requires the context of multiple words to correctly identify dependencies within an input sequence [2]. Hence, we investigate the impact of the multimodality of our proposed normalization function on the quality of translations.

Model: We train transformer models for each of the sparse normalization functions using the OpenNMT Neural Machine Translation Toolkit [32]. Each normalization function is used in the self-attention layers. We use byte pair encoding (BPE) to encode rare and unknown words and ensure an open vocabulary [33]. Due to computational constraints, we finetune transformer models on the English-German translation dataset from IWSLT 2014 [34]. These models were pretrained on the EN-DE corpus from WMT 2016 [35]. We finetune for 40000 iterations. Hyperparameters and further experimental details are given in Appendix E.

Results and discussion: As shown in Table 4, our method obtains the highest BLEU [36], METEOR [37], and ROUGE [38] scores of the considered normalization functions while reducing the average number of words attended to 8.2. In comparison with the other sparse normalization functions, ours maintains the highest number of attended source words. This supports the notion that attending over a subset of the source words benefits performance, but the performance of sparsemax and entmax-1.5 could be hurt by attending over too few words. For short sentences, ev-softmax maintains nonzero attention over the entire sentence, as Fig. 4 demonstrates. This allows for the model to identify relationships between words in the entire source sequence, such as tense and conjugation, enabling more accurate translation.

5 Related Work

Softmax Alternatives: There is considerable interest in alternatives to the softmax function that provide greater representational capacity [39, 40] and improved discrimination of features [41]. Sparse-
We apply our method in the domains of image generation and machine translation. Our work has
introduced sparse normalization functions and corresponding loss functions. While the \( \alpha \)-entmax family of functions contains a parameter \( \alpha \) to control the level of sparsity, the functions are all sparse for \( \alpha > 1 \) with no known continuous approximation with full support. Therefore, these methods are all trained with alternative loss functions that do not directly represent the likelihood of the data. Another controllable sparse alternative to softmax is sparsehourglass [17]. We baseline against only sparsemax and entmax-1.5 as more research has been conducted on these two methods and entmax-1.5 is semantically similar to sparsehourglass. In contrast, we develop a normalization function which has a continuous family of approximations that can be used during training time with the negative log-likelihood and KL divergence loss terms. This flexibility enables our method to substitute the softmax transformation in any context and model.

**Discrete Variational Autoencoders**: Recent advancements in VAEs with discrete latent spaces have introduced strategies for learning discrete latent spaces to tackle a wide-ranging set of tasks including image generation [1], video prediction [44], and speech processing [45]. For discrete VAEs, the gradient of the ELBO usually cannot be calculated directly [14]. While the SFE [12], [13] enables Monte Carlo-based approaches to estimate the stochastic gradient of the ELBO, it suffers from high variance and is consequently slow to converge. Continuous relaxation via the Gumbel-Sparsemax distribution allows for an efficient and convenient gradient calculation through discrete latent spaces [14], [15], but the gradient estimation is biased and requires sampling during training. Our work, in contrast, enables direct marginalization over a categorical space without sampling. Similar to our work, Correia et al. [9] apply sparsemax to marginalize discrete VAEs efficiently. While we also generate a sparse distribution over the latent space as in Correia et al. [9], we better balance sparsity with the multimodality of the distribution. Prior work on evidential sparsification focused on a post-hoc method for discrete CVAEs [10]. We extend this method to more classes of generative models and develop a modification to apply the method at training time.

**Sparse Attention**: In machine translation, sparse attention reflects the intuition that only a few source words are expected to be relevant for each translated word. The global attention model considers all words on the source side for each target word, which is potentially prohibitively expensive for translating longer sequences [46]. The softmax transformation has been replaced with sparse normalization functions, such as the sparsemax operation [11] and its generalization, \( \alpha \)-entmax [47]. Like our work, both sparsemax and \( \alpha \)-entmax can substitute softmax in the attention layers of machine translation models. Prior work on sparse normalization functions for attention layers has focused on global attention layers in recurrent neural network models. In contrast, we study the effect of incorporating these sparse normalization functions in transformers, where they are used in self-attention layers.

6 Conclusion

We present ev-softmax, a novel method to train deep generative models with sparse probability distributions. We show that our method satisfies many of the same theoretical properties as softmax and other sparse alternatives to softmax. By balancing the goals of multimodality and sparsity, our method yields better distributional accuracy and classification performance than baseline methods. Future work can involve training large computer vision and machine translation models from scratch with our method and examining its efficacy at a larger scale on more complex downstream tasks.

7 Broader Impact

Our work focuses on a method to train generative models that output sparse probability distributions. We apply our method in the domains of image generation and machine translation. Our work has the potential to improve the explainability and introspection of generative models. Furthermore, our work aims to reduce the computational cost of training generative models, which are used in unsupervised and semi-supervised approaches to learning. Although our empirical validation shows that our method can improve the accuracy of generated distributions, the use of sparse probability distributions can also amplify any inherent bias present in the data or modeling assumptions. One limitation of our work is that we do not provide explicit theoretical guarantees on the conditions for yielding an output probability of zero for a class. We hope that our work motivates further research into improving the accuracy of generative modeling and reducing bias of both models and data.
References

[1] A. van den Oord, O. Vinyals, and K. Kavukcuoglu, “Neural discrete representation learning,” in Advances in Neural Information Processing Systems (NeurIPS), 2017, pp. 6306–6315.

[2] A. Vaswani, N. Shazeer, N. Parmar, J. Uszkoreit, L. Jones, A. N. Gomez, L. Kaiser, and I. Polosukhin, “Attention is all you need,” in Advances in Neural Information Processing Systems (NeurIPS), 2017.

[3] A. Radford, K. Narasimhan, T. Salimans, and I. Sutskever, “Improving language understanding by generative pre-training,” 2018.

[4] Z. Yang, W. Chen, F. Wang, and B. Xu, “Improving neural machine translation with conditional sequence generative adversarial nets,” arXiv, 2017.

[5] T. Salzmann, B. Ivanovic, P. Chakravary, and M. Pavone, “Trajectron++: Dynamically-feasible trajectory forecasting with heterogeneous data,” in European Conference on Computer Vision (ECCV), 2020.

[6] J. Co- Reyes, Y. Liu, A. Gupta, B. Eysenbach, P. Abbeel, and S. Levine, “Self-consistent trajectory autoencoder: Hierarchical reinforcement learning with trajectory embeddings,” in International Conference on Machine Learning (ICML), PMLR, 2018, pp. 1009–1018.

[7] V. Fortuin, M. Hüs er, F. Locatello, H. Strathmann, and G. Rätsch, “SOM-VAE: Interpretable discrete representation learning on time series,” in International Conference on Learning Representations (ICLR), 2019.

[8] A. Martins and R. Astudillo, “From softmax to sparsemax: A sparse model of attention and multi-label classification,” in International Conference on Machine Learning (ICML), 2016, pp. 1614–1623.

[9] G. Correia, V. Niculae, W. Aziz, and A. Martins, “Efficient marginalization of discrete and structured latent variables via sparsity,” Advances in Neural Information Processing Systems (NeurIPS), vol. 33, 2020.

[10] M. Itkina, B. Ivanovic, R. Senanayake, M. J. Kochenderfer, and M. Pavone, “Evidential sparsification of multimodal latent spaces in conditional variational autoencoders,” Advances in Neural Information Processing Systems (NeurIPS), vol. 33, 2020.

[11] C. Malaviya, P. Ferreira, and A. F. Martins, “Sparse and constrained attention for neural machine translation,” in Annual Meeting of the Association for Computational Linguistics (ACL), 2018, pp. 370–376.

[12] R. J. Williams, “Simple statistical gradient-following algorithms for connectionist reinforcement learning,” Machine Learning, vol. 8, no. 3-4, pp. 229–256, 1992.

[13] P. W. Glynn, “Likelihood ratio gradient estimation for stochastic systems,” Communications of the ACM, vol. 33, no. 10, pp. 75–84, 1990.

[14] E. Jang, S. Gu, and B. Poole, “Categorical reparameterization with Gumbel-Softmax,” in International Conference on Learning Representations (ICLR), 2017.

[15] C. J. Maddison, A. Mnih, and Y. W. Teh, “The Concrete distribution: A continuous relaxation of discrete random variables,” in International Conference on Learning Representations (ICLR), 2017.

[16] B. Peters, V. Niculae, and A. F. Martins, “Sparse sequence-to-sequence models,” in Annual Meeting of the Association for Computational Linguistics (ACL), 2019, pp. 1504–1519.

[17] A. Laha, S. A. Chemmengath, P. Agrawal, M. Khapra, K. Sankaranarayanan, and H. G. Ramaswamy, “On controllable sparse alternatives to softmax,” in Advances in Neural Information Processing Systems (NeurIPS), 2018, pp. 6422–6432.

[18] V. Niculae, A. Martins, M. Blondel, and C. Cardie, “SparseMAP: Differentiable sparse structured inference,” in International Conference on Machine Learning (ICML), PMLR, 2018, pp. 3799–3808.

[19] K. Sohn, H. Lee, and X. Yan, “Learning structured output representation using deep conditional generative models,” in Advances in Neural Information Processing Systems (NeurIPS), 2015, pp. 3483–3491.

[20] D. P. Kingma and M. Welling, “Auto-encoding variational Bayes,” in International Conference on Learning Representations (ICLR), 2014.

[21] R. Liu, J. Regier, N. Tripuraneni, M. Jordan, and J. Mcauliffe, “Rao-Blackwellized stochastic gradients for discrete distributions,” in International Conference on Machine Learning (ICML), PMLR, 2019, pp. 4023–4031.

[22] A. P. Dempster, “A generalization of Bayesian inference,” Classic works of the Dempster-Shafer Theory of Belief Functions, pp. 73–104, 2008.

[23] T. Denoeux, “Logistic regression, neural networks and Dempster–Shafer theory: A new perspective,” Knowledge-Based Systems, vol. 176, pp. 54–67, 2019.

[24] B. Bigi, “Using Kullback-Leibler distance for text categorization,” in European Conference on Information Retrieval (ECIR), Springer, 2003, pp. 305–319.

[25] J. Hullman, N. Diakopoulos, and E. Adar, “Contextifier: Automatic generation of annotated stock visualizations,” in SIGCHI Conference on Human Factors in Computing Systems, ACM, 2013, pp. 2707–2716.
[26] D. P. Kingma, D. J. Rezende, S. Mohamed, and M. Welling, “Semi-supervised learning with deep generative models,” in *Advances in Neural Information Processing Systems (NeurIPS)*, 2014, pp. 3581–3589.

[27] S. J. Rennie, E. Marcheret, Y. Mroueh, J. Ross, and V. Goel, “Self-critical sequence training for image captioning,” in *IEEE Conference on Computer Vision and Pattern Recognition (CVPR)*, 2017, pp. 7008–7024.

[28] A. Mnih and K. Gregor, “Neural variational inference and learning in belief networks,” in *International Conference on Machine Learning (ICML)*, PMLR, 2014, pp. 1791–1799.

[29] Y. Le and X. Yang, “Tiny ImageNet visual recognition challenge,” *CS231N: Convolutional Neural Networks for Visual Recognition (Stanford University)*, 2015.

[30] A. van den Oord and B. Schrauwen, “Factoring variations in natural images with deep Gaussian mixture models,” in *Advances in Neural Information Processing Systems (NeurIPS)*, 2014.

[31] S. Zagoruyko and N. Komodakis, “Wide residual networks,” in *Proceedings of the British Machine Vision Conference (BMVC)*, 2015.

[32] G. Klein, F. Hernandez, V. Nguyen, and J. Senellart, “The OpenNMT neural machine translation toolkit: 2020 edition,” in *Conference of the Association for Machine Translation in the Americas (AMTA)*, 2020, pp. 102–109.

[33] R. Sennrich, B. Haddow, and A. Birch, “Neural machine translation of rare words with subword units,” in *Annual Meeting of the Association for Computational Linguistics (ACL)*, 2016, pp. 1715–1725.

[34] M. Cettolo, M. Federico, L. Bentivogli, N. Jan, S. Sebastian, S. Katsitho, Y. Koichiro, and F. Christian, “Overview of the IWSLT 2017 evaluation campaign,” in *International Workshop on Spoken Language Translation (IWSLT)*, 2017, pp. 2–14.

[35] O. Bojar, R. Chatterjee, C. Federmann, Y. Graham, B. Haddow, M. Huck, A. J. Yepes, P. Koehn, V. Logacheva, C. Monz, et al., “Findings of the 2016 Conference on Machine Translation,” in *Conference on Machine Translation (WMT)*, 2016, pp. 131–198.

[36] K. Papineni, S. Roukos, T. Ward, and W.-J. Zhu, “BLEU: A method for automatic evaluation of machine translation,” in *Annual Meeting of the Association for Computational Linguistics (ACL)*, 2002, pp. 311–318.

[37] M. Denkowski and A. Lavie, “METEOR 1.3: Automatic metric for reliable optimization and evaluation of machine translation systems,” in *Sixth Workshop on Statistical Machine Translation*, Association for Computational Linguistics, 2011, pp. 85–91.

[38] C.-Y. Lin, “ROUGE: A package for automatic evaluation of summaries,” in *Text Summarization Branches Out*, Association for Computational Linguistics, 2004, pp. 74–81.

[39] S. Kanai, Y. Yamanaka, Y. Fujiwara, and S. Adachi, “Sigmoidmax: Reanalysis of the softmax bottleneck,” in *Advances in Neural Information Processing Systems (NeurIPS)*, vol. 2018, 2018, pp. 286–296.

[40] R. Memisevic, C. Zach, M. Pollefeys, and G. E. Hinton, “Gated softmax classification,” in *Advances in Neural Information Processing Systems (NeurIPS)*, vol. 23, 2010, pp. 1603–1611.

[41] W. Liu, Y. Wen, Z. Yu, and M. Yang, “Large-margin softmax loss for convolutional neural networks,” in *International Conference on Machine Learning (ICML)*, PMLR, vol. 2, 2016, p. 7.

[42] V. Niculae and M. Blondel, “A regularized framework for sparse and structured neural attention,” in *Advances in Neural Information Processing Systems (NeurIPS)*, 2017, pp. 3340–3350.

[43] A. Razavi, A. van den Oord, and O. Vinyals, “Generating diverse high-fidelity images with VQ-VAE-2,” in *Advances in Neural Information Processing Systems (NeurIPS)*, 2019, pp. 14 837–14 847.

[44] J. Walker, A. Razavi, and A. v. d. Oord, “Predicting video with VQVAE,” *arXiv*, 2021.

[45] C. Gârbacea, A. van den Oord, Y. Li, F. S. Lim, A. Luebs, O. Vinyals, and T. C. Walters, “Low bit-rate speech coding with vq-vae and a wavenet decoder,” in *IEEE International Conference on Acoustics, Speech, and Signal Processing (ICASSP)*, 2019, pp. 735–739.

[46] M.-T. Luong, H. Pham, and C. D. Manning, “Effective approaches to attention-based neural machine translation,” in *Conference on Empirical Methods in Natural Language Processing (EMNLP)*, 2015, pp. 1412–1421.

[47] B. Peters, V. Niculae, and A. F. Martins, “Sparse sequence-to-sequence models,” in *Annual Meeting of the Association for Computational Linguistics (ACL)*, 2019, pp. 1504–1519.

[48] D. P. Kingma and J. Ba, “Adam: A method for stochastic optimization,” in *International Conference on Learning Representations (ICLR)*, 2014.