

Efficient Marginalization of Discrete and Structured Latent Variables via Sparsity

Gonçalo Correia Instituto de Telecomunicações, Lisbon

Vlad Niculae Ivl, University of Amsterdam

Wilker Aziz ILLC, University of Amsterdam

André Martins Instituto de Telecomunicações & LUMLIS & Unbabel

Latent Variable Models

Latent variable z can be

Latent Variable Models

Latent variable z can be continuous



Source: Bouges et al., 2013

Latent Variable Models

Latent variable z can be **continuous**, **discrete**



Source: valleyeyecareaz.com

Latent Variable Models

Latent variable z can be continuous, discrete, or structured



Source: Liu et al., 2015

Training Discrete or Structured Latent Variable Models

Latent variable z can be

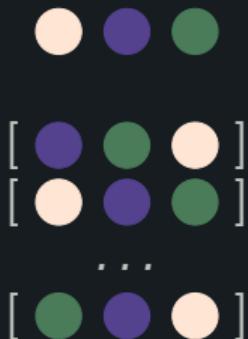
Training Discrete or Structured Latent Variable Models

Latent variable z can be discrete



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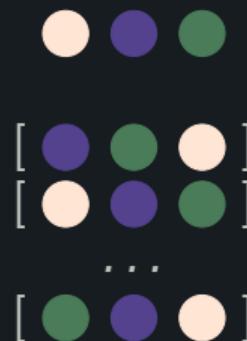
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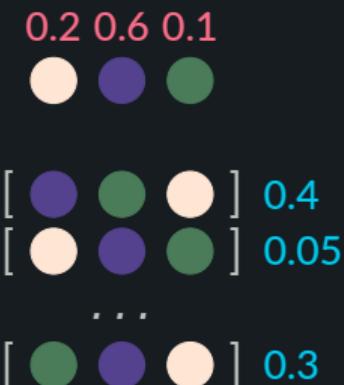


Training Discrete or Structured Latent Variable Models

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



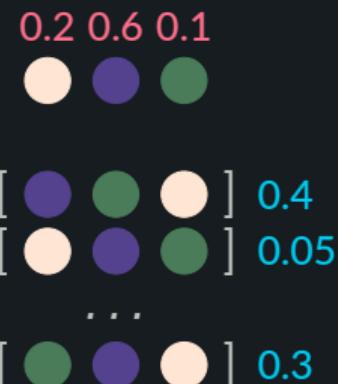
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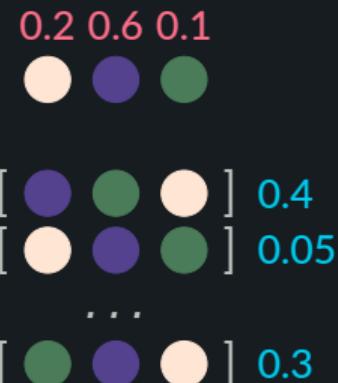
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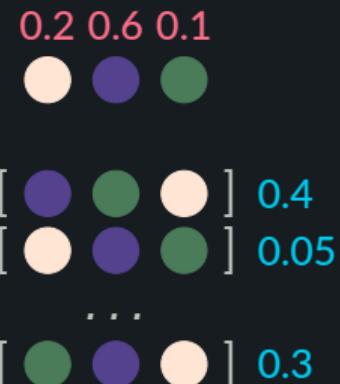


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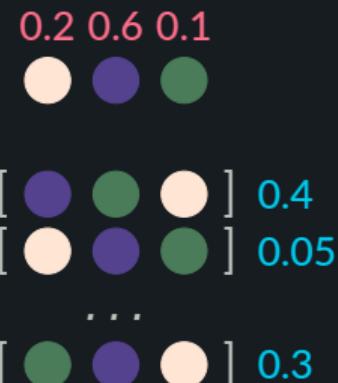
If \mathcal{Z} is **large**, this sum can get very expensive due to $\ell(x, z; \theta)$! 🍺

Training Discrete or Structured Latent Variable Models

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



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Taking a step back...

Does the expectation over possible z need to be expensive?

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

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

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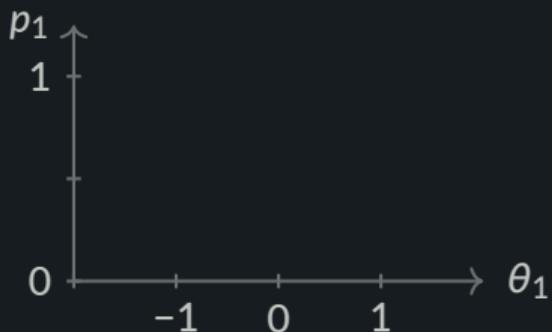
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 &\quad + \pi(z_i|x, \theta) \ell(x, z_i; \theta) + \dots + \underbrace{\pi(z_N|x, \theta) \ell(x, z_N; \theta)}_{=0}
 \end{aligned}$$

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

Discrete, unstructured case: sparsemax

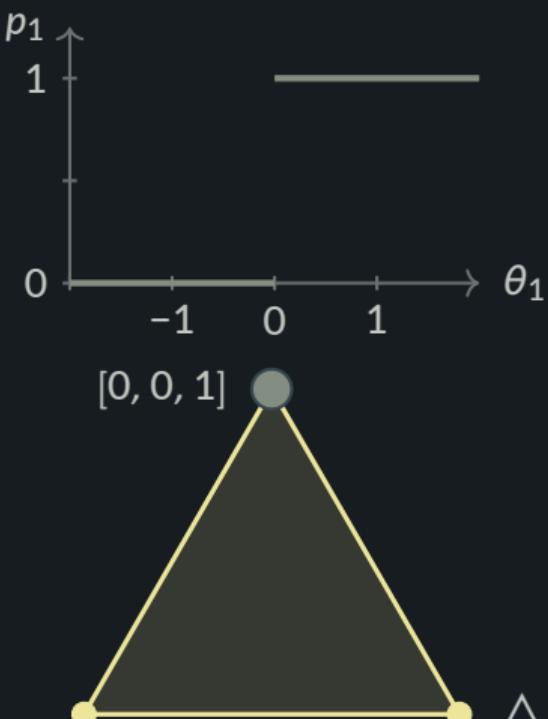
$$\boldsymbol{\pi}_\Omega(\mathbf{s}) = \arg \max_{\mathbf{p} \in \Delta} \mathbf{p}^\top \mathbf{s} - \Omega(\mathbf{p})$$



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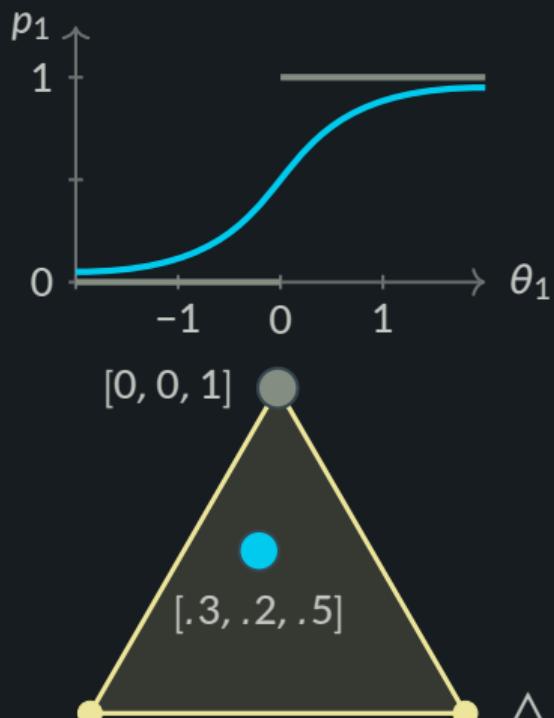
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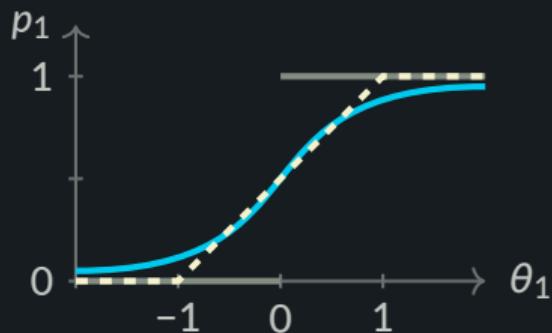
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- argmax: $\Omega(\mathbf{p}) = 0$ (*no smoothing*)
- softmax: $\Omega(\mathbf{p}) = \sum_j p_j \log p_j$
- sparsemax: $\Omega(\mathbf{p}) = 1/2 \|\mathbf{p}\|_2^2$



Semi-Supervised VAE

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

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

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Gaussian VAE

classification network

```
graph TD; A["\mathcal{L}_x(\theta) = \sum_{z \in \mathcal{Z}} \pi(z|x) \ell(x, z)"] --> B["\mathbb{E}_{z \sim \pi(z|x)} \ell(x, z)"]; A --> C["Gaussian VAE"]; B --> D["classification network"]
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sum over the 10 digits

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The diagram illustrates the loss function for a semi-supervised VAE. It shows two components: a Gaussian VAE loss, represented by the term "sum over the 10 digits" with an arrow pointing to the summation part of the equation, and a classification network loss, represented by the term "classification network" with an arrow pointing to the expectation term. The final equation is the sum of these two components.

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graph LR; A[sum over the 10 digits] --> B["\sum_{z \in \mathcal{Z}} \pi(z|x) \ell(x, z)"]; C[Gaussian VAE] --> D["\mathbb{E}_{z \sim \pi(z|x)} \ell(x, z)"]
```

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

Semi-Supervised VAE

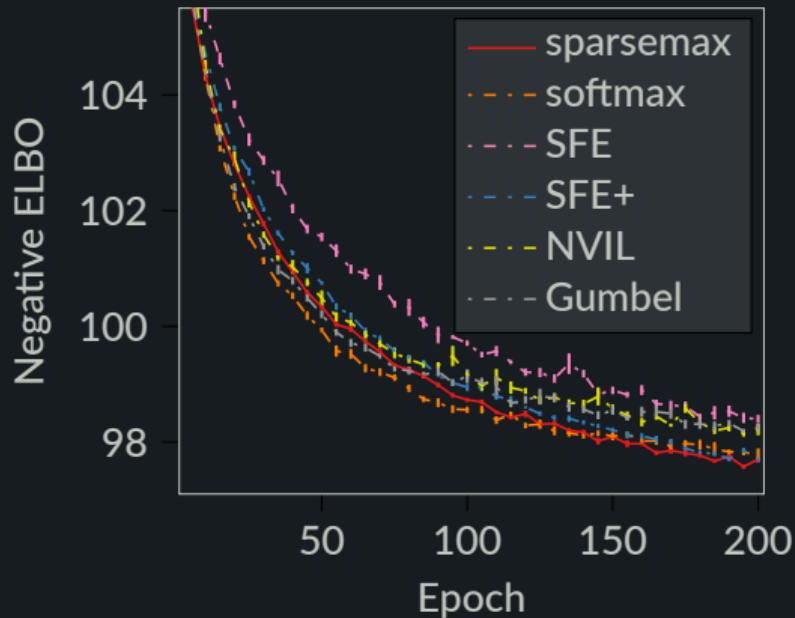
Method	Accuracy (%)	Dec. calls
<i>Monte Carlo</i>		
SFE	$94.75 \pm .002$	1
SFE+	$96.53 \pm .001$	2
NVIL	$96.01 \pm .002$	1
Gumbel	$95.46 \pm .001$	1
<i>Marginalization</i>		
Dense	$96.93 \pm .001$	10

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Emergent communication

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

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The diagram consists of two curved arrows. One arrow originates from the word "sender" at the top right and points to the term $\pi(z|x)$ in the first equation. Another arrow originates from the word "receiver" at the bottom right and points to the term $\ell(x, z)$ in the second equation.

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

Emergent communication

The diagram shows the loss function $\mathcal{L}_x(\theta)$ as a sum over all possible messages $z \in \mathcal{Z}$. The term $\pi(z|x)$ is highlighted in red. The equation is split into two parts: the first part shows the sum over z , and the second part shows the expectation $\mathbb{E}_{z \sim \pi(z|x)} \ell(x, z)$. Curved arrows point from the text "sum over all possible messages in the vocabulary" to the $\sum_{z \in \mathcal{Z}}$ term, and from "sender" and "receiver" to the $\pi(z|x)$ term.

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

- receiver picks image from a set \mathcal{V} based on message
- images come from ImageNet

Emergent Communication

... but make it harder: $|\mathcal{Z}| = 256$, $|\mathcal{V}| = 16$

Method	success (%)	Dec. calls
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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
<i>Marginalization</i>		

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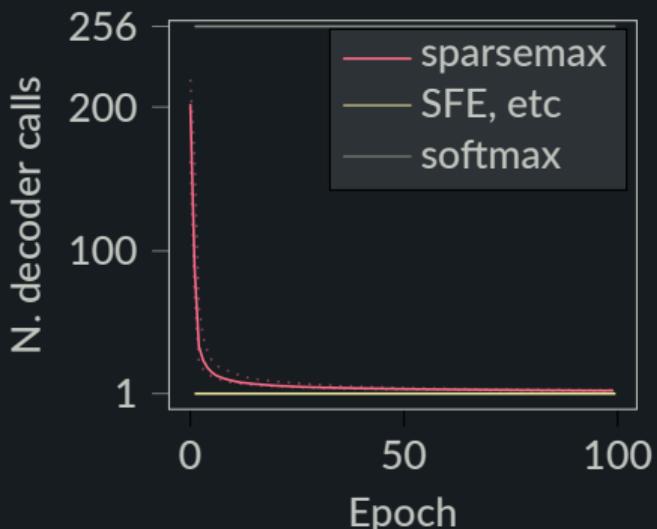
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But fully dense worst case.
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$$k\text{-sparsemax}(s) = \arg \min_{\mathbf{p} \in \Delta, \|\mathbf{p}\|_0 \leq k} \|\mathbf{p} - s\|_2^2$$

- 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.

 Δ  \mathcal{M}

$$\begin{aligned}\mathcal{M} &:= \text{conv} \left\{ \mathbf{a}_z : z \in \mathcal{Z} \right\} \\ &= \left\{ \mathbf{A}p : p \in \Delta \right\} \\ &= \left\{ \mathbb{E}_{Z \sim p} \mathbf{a}_Z : p \in \Delta \right\}\end{aligned}$$



Δ



\mathcal{M}

- $\text{argmax}_{p \in \Delta} p^T s$



-

$$\text{argmax}_{p \in \Delta} p^T s$$

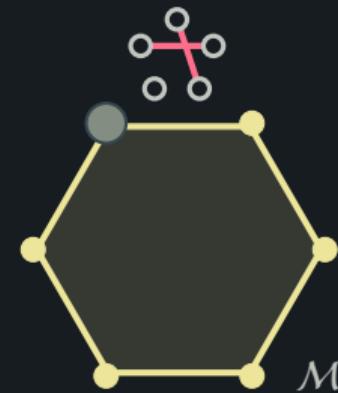


$$\text{MAP}_{\mu \in \mathcal{M}} \arg \max \mu^T t$$

-



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- **MAP** $\arg \max_{\boldsymbol{\mu} \in \mathcal{M}} \boldsymbol{\mu}^T \boldsymbol{t}$
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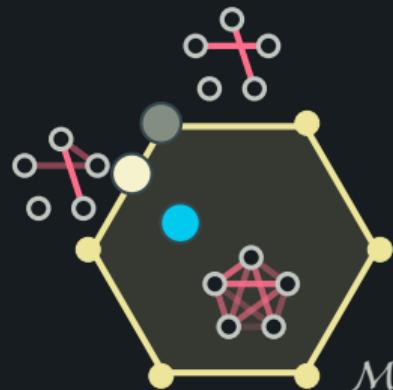
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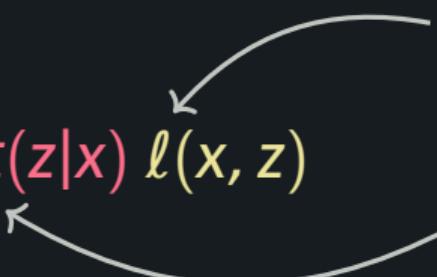
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- **SparseMAP** $\arg \max_{\boldsymbol{\mu} \in \mathcal{M}} \boldsymbol{\mu}^T \boldsymbol{t} - 1/2 \|\boldsymbol{\mu}\|^2$



Bit-vector VAE

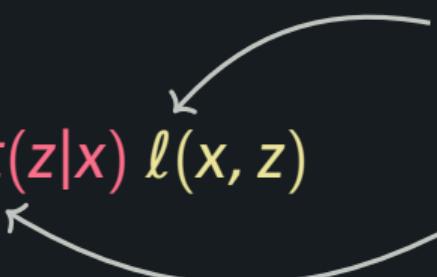
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- Minimize the negative ELBO

Bit-vector VAE

sum over
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generative network

inference network

The diagram illustrates the Bit-vector VAE loss function. It starts with the expression $\mathcal{L}_x(\theta)$ on the left, which is annotated with a curved arrow pointing to it from the text "sum over an exponentially large set of structures". This expression is then shown to be equivalent to a sum over all possible latent variable configurations $z \in \mathcal{Z}$, where each term is the product of the probability density $\pi(z|x)$ and the reconstruction loss $\ell(x, z)$. This sum is further simplified to an expectation $\mathbb{E}_{z \sim \pi(z|x)} \ell(x, z)$. The right side of the equation is annotated with two curved arrows: one pointing to the expectation term labeled "generative network", and another pointing to the $\pi(z|x)$ term labeled "inference network".

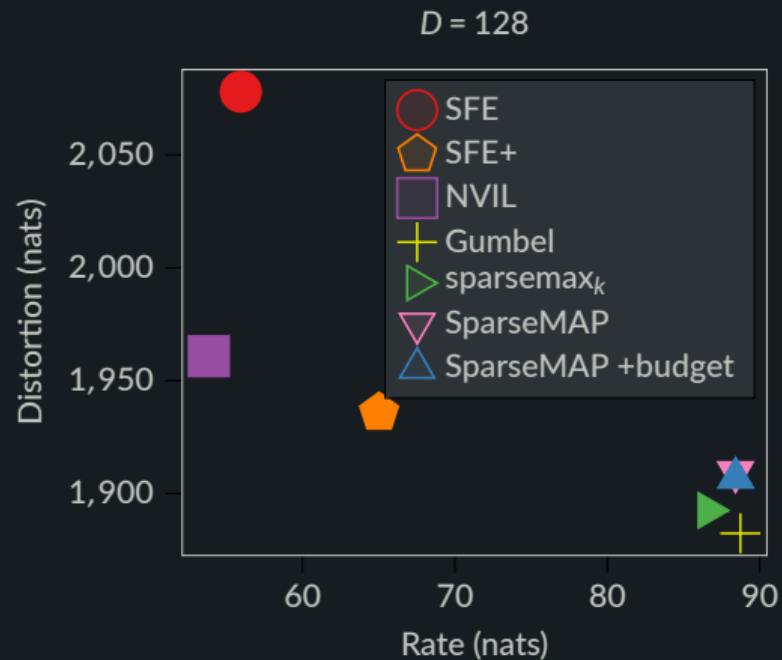
- VAE where z is a collection of D bits
- Minimize the negative ELBO

Bit-vector VAE

Method	$D = 32$	$D = 128$
<i>Monte Carlo</i>		
SFE	3.74	3.77
SFE+	3.61	3.59
NVIL	3.65	3.60
Gumbel	3.57	3.49
<i>Marginalization</i>		
Top- k sparsemax	3.62	3.61
SparseMAP	3.72	3.67
SparseMAP (w/ budget)	3.64	3.66

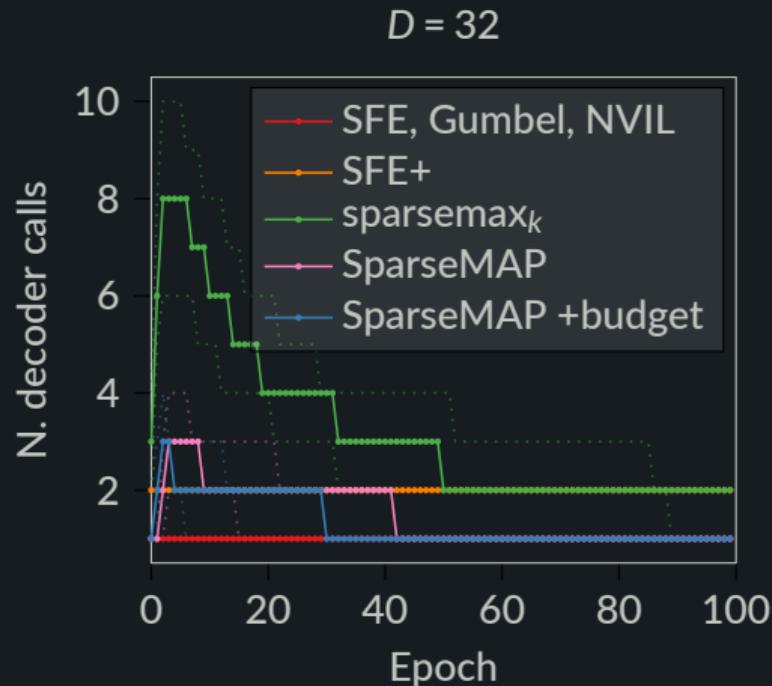
Bit-vector VAE

Method	$D = 32$	$D = 128$
<i>Monte Carlo</i>		
SFE	3.74	3.77
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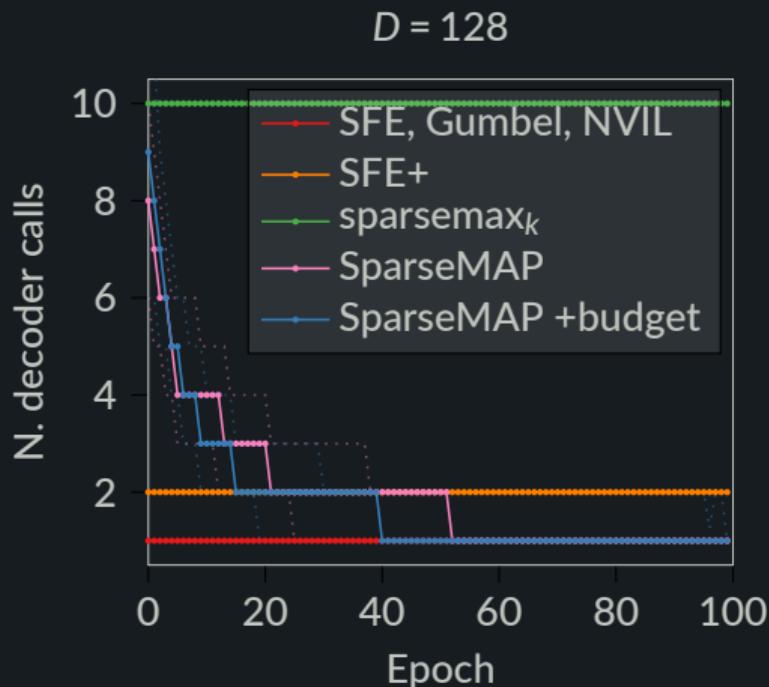
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Key Takeaways

We introduce a new method
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discrete and structured

0.2 0.6 0.1


[] 0.4
[] 0.05
...
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deterministic, yet efficient

$$\begin{aligned}\mathcal{L}_x(\theta) = & \pi(z_1|x, \theta) \ell(x, z_1; \theta) \\ & + \underbrace{\pi(z_2|x, \theta) \ell(x, z_2; \theta)}_{=0} \\ & + \dots + \pi(z_i|x, \theta) \ell(x, z_i; \theta) \\ & + \dots + \underbrace{\pi(z_N|x, \theta) \ell(x, z_N; \theta)}_{=0}\end{aligned}$$

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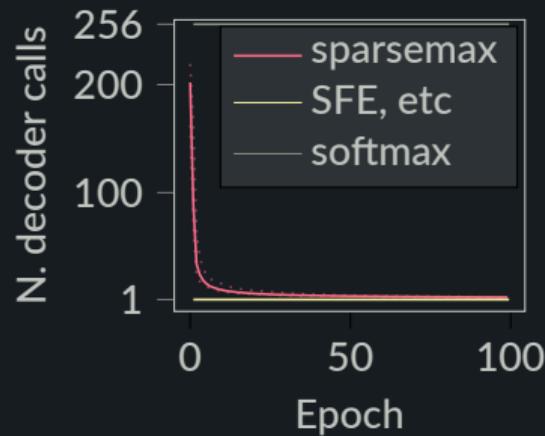
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adaptive, as needed



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