Efficient Marginalization of Discrete and Structured Latent Variables via Sparsity

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Latent Variable Models

Latent variable z can be

Latent Variable Models

Latent variable z can be continuous

Source: Bouges et al., 2013

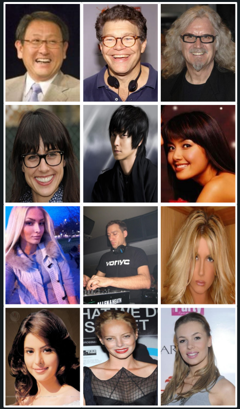
Latent Variable Models

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

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Training Discrete or Structured Latent Variable Models

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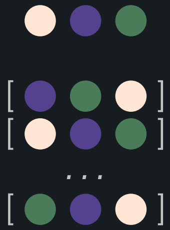
Training Discrete or Structured Latent Variable Models

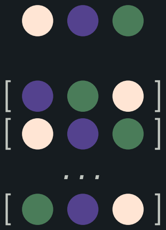
Latent variable z can be discrete or structured



Training Discrete or Structured Latent Variable Models

Latent variable z can be discrete or structured

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



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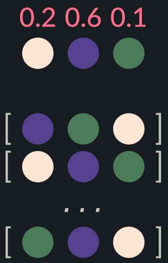

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If $\mathcal{Z}$ is large, this sum can get very expensive due to $\ell(x, z; \theta)$! 😱

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

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Does the expectation over possible z need to be expensive?

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

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\end{aligned}
$$

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

(Martins and Astudillo, 2016; Niculae, Martins, et al., 2018)

Sparse normalizers

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

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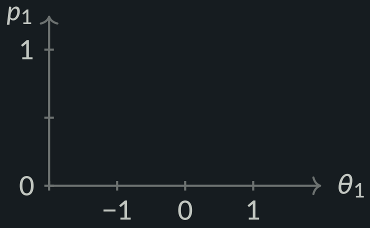
No need for computing $\ell(x,z;\theta)$ for all $z \in \mathcal{Z}$!

Discrete, unstructured case: sparsemax

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



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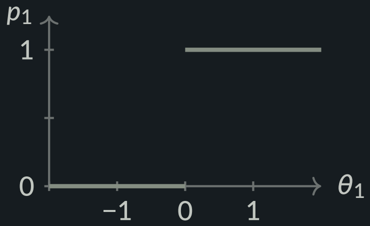

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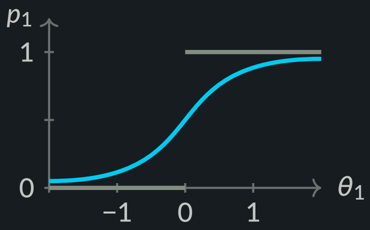

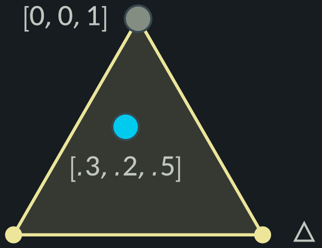

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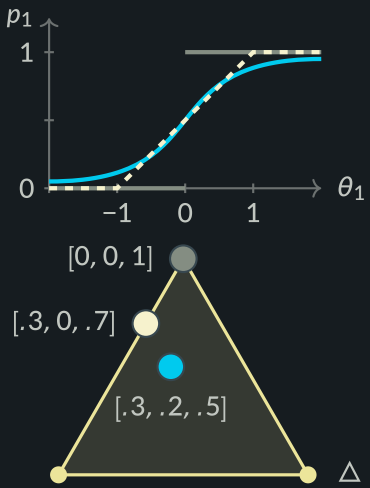
- sparsemax: $\Omega(\boldsymbol{p}) = 1/2 \|\boldsymbol{p}\|_2^2$



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Semi-Supervised VAE

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

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classification network

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

Semi-Supervised VAE

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

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Sparse	$96.87_{\pm .001}$	$1.01_{\pm 0.01}$

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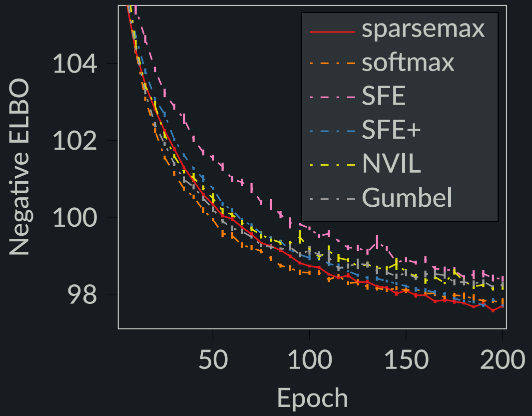

Emergent communication

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Emergent communication

sender

receiver

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$$= \mathbb{E}_{z \sim \pi(z|x)}\ \ell(x, z)$$

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

Emergent communication

sum over
all possible messages
in the vocabulary

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- images come from ImageNet

(Lazaridou et al., 2017; Correia et al., 2020)

Emergent Communication

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

Method	success (%)	Dec. calls
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SFE	33.05 $\pm$2.84	1
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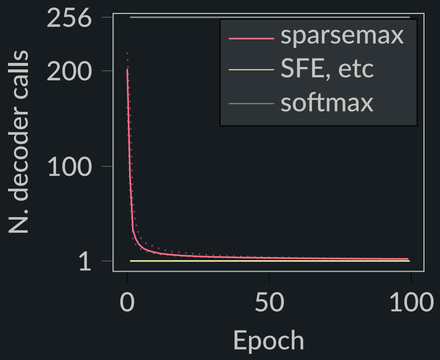

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One solution: top-k sparsemax

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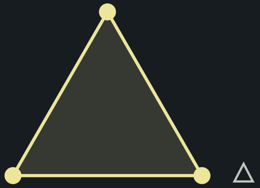
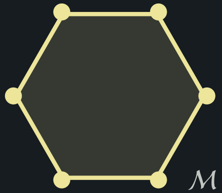
- Non-convex but easy: sparsemax over the k highest scores (Kyrillidis et al., 2013).
- Top-k oracle available for some structured problems.
- Certificate: if at least one of the top-k z gets $p(z) = 0$, **k-sparsemax = sparsemax**!
  thus, biased early on, but it goes away.


△


$\mathcal{M}$

$$
\begin{aligned}
\mathcal{M} := \operatorname{conv}\left\{\boldsymbol{a}_z : z \in \mathcal{Z}\right\} \\
= \left\{\boldsymbol{A}\boldsymbol{p} : \boldsymbol{p} \in \triangle\right\} \\
= \left\{\mathbb{E}_{Z\sim \boldsymbol{p}}\, \boldsymbol{a}_Z : \boldsymbol{p} \in \triangle\right\}
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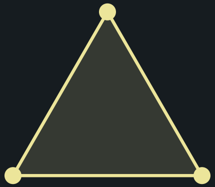

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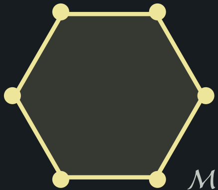

$\mathcal{M}$

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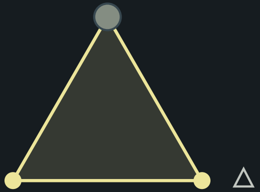
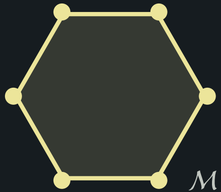
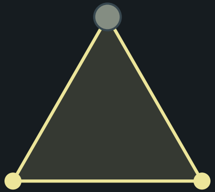




- **argmax** $\arg\max_{\boldsymbol{p} \in \triangle} \boldsymbol{p}^\top \boldsymbol{s}$
- **MAP** $\arg\max_{\boldsymbol{\mu} \in \mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{t}$



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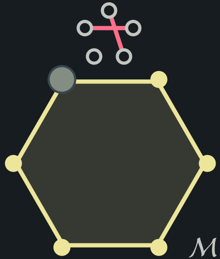

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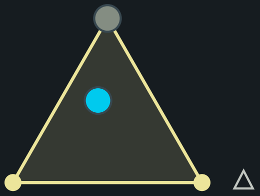
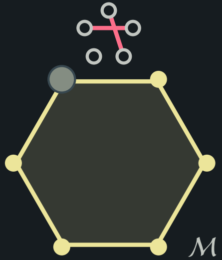
softmax $\arg\max_{\boldsymbol{p} \in \triangle} \boldsymbol{p}^\top \boldsymbol{s} + \mathrm{H}(\boldsymbol{p})$





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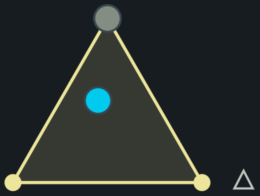

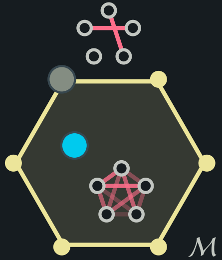

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- **softmax** $\arg\max_{\boldsymbol{p}\in\triangle} \boldsymbol{p}^\top \boldsymbol{s} + \mathrm{H}(\boldsymbol{p})$
- **sparsemax** $\arg\max_{\boldsymbol{p}\in\triangle} \boldsymbol{p}^\top \boldsymbol{s} - 1/2\|\boldsymbol{p}\|^2$

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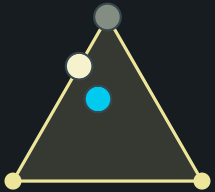

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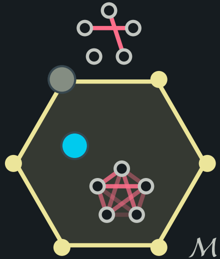

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(Niculae, Martins, Blondel, and Cardie, 2018)

argmax $\arg\max_{\boldsymbol{p}\in\triangle} \boldsymbol{p}^\top \boldsymbol{s}$

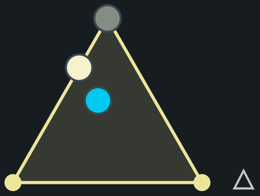
softmax $\arg\max_{\boldsymbol{p}\in\triangle} \boldsymbol{p}^\top \boldsymbol{s} + \mathrm{H}(\boldsymbol{p})$

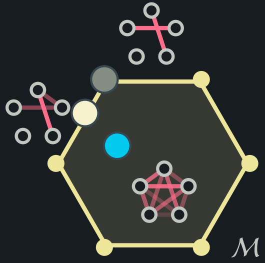
sparsemax $\arg\max_{\boldsymbol{p}\in\triangle} \boldsymbol{p}^\top \boldsymbol{s} - 1/2\|\boldsymbol{p}\|^2$

MAP $\arg\max_{\boldsymbol{\mu}\in\mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{t}$

marginals $\arg\max_{\boldsymbol{\mu}\in\mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{t} + \widetilde{\mathrm{H}}(\boldsymbol{\mu})$

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





Bit-vector VAE

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

Bit-vector VAE

generative network

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

inference network

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- VAE where z is a collection of D bits

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

Bit-vector VAE

sum over
an exponetially large
set of structures

generative network

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Bit-vector VAE

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

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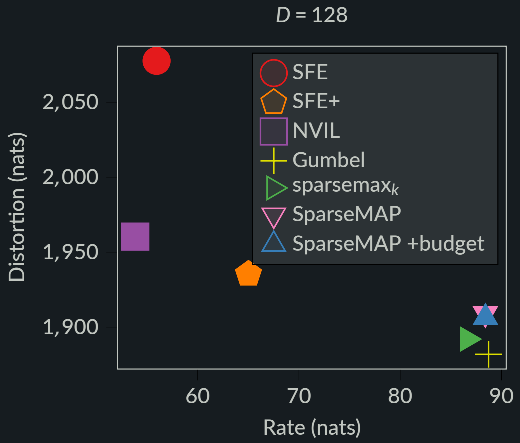

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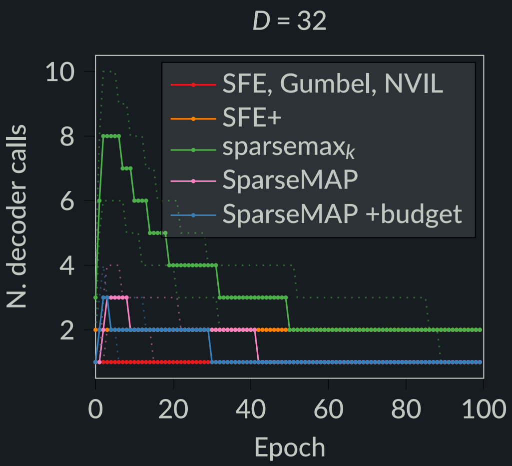

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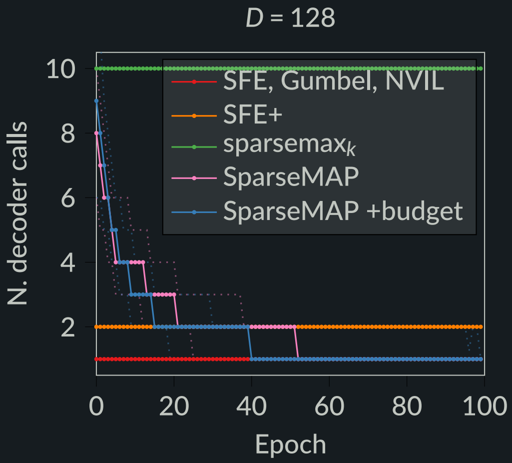

Key Takeaways

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to train latent variable models.

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discrete and structured

deterministic, yet efficient

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

Key Takeaways

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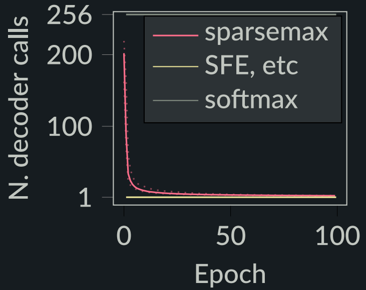
$$\begin{aligned}\mathcal{L}_x(\theta) = {} & \pi(z_1|x,\theta)\ \ell(x,z_1;\theta) \\ & + \underbrace{\pi(z_2|x,\theta)}_{=0}\ \cancel{\ell(x,z_2;\theta)} \\ & + \dots + \pi(z_i|x,\theta)\ \ell(x,z_i;\theta) \\ & + \dots + \underbrace{\pi(z_N|x,\theta)}_{=0}\ \cancel{\ell(x,z_N;\theta)}\end{aligned}$$

adaptive, as needed



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