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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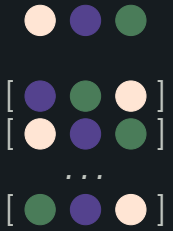
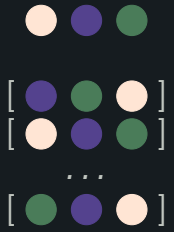
Latent variable z can be discrete or structured



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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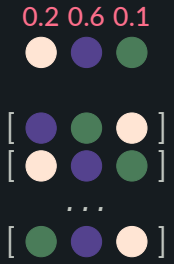

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If $\mathcal{Z}$ is large, this sum can get very expensive due to $\ell(x, z; \theta)$! 😱

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

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

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

(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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$$+ \pi(z_i|x, \theta)\, \ell(x, z_i; \theta) + \ldots + \underbrace{\pi(z_N|x, \theta)}_{=0}\, \ell(x, z_N; \theta)$$

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

(Niculae and Blondel, 2017)

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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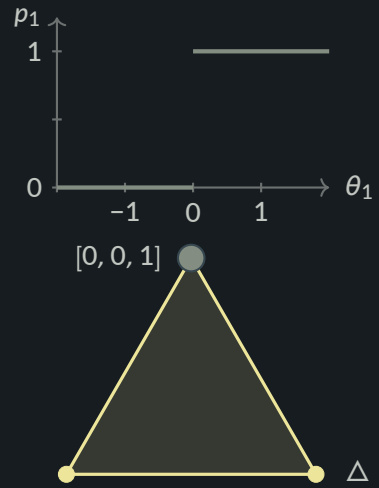

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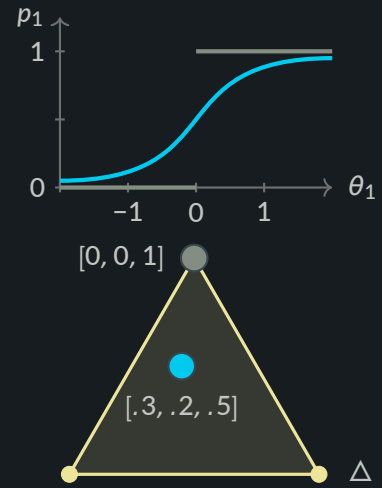

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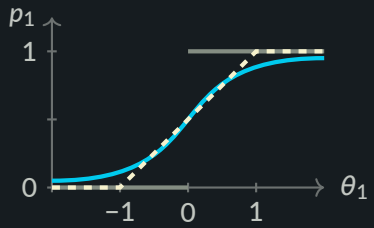

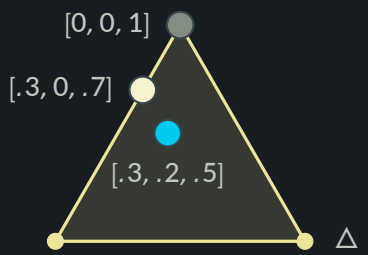

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Semi-Supervised VAE

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

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Semi-Supervised VAE

Gaussian VAE

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discrete inference network

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- Semi-Supervised VAE on MNIST: z is a possible digit

(Correia, Niculae, Aziz, and Martins, 2020)

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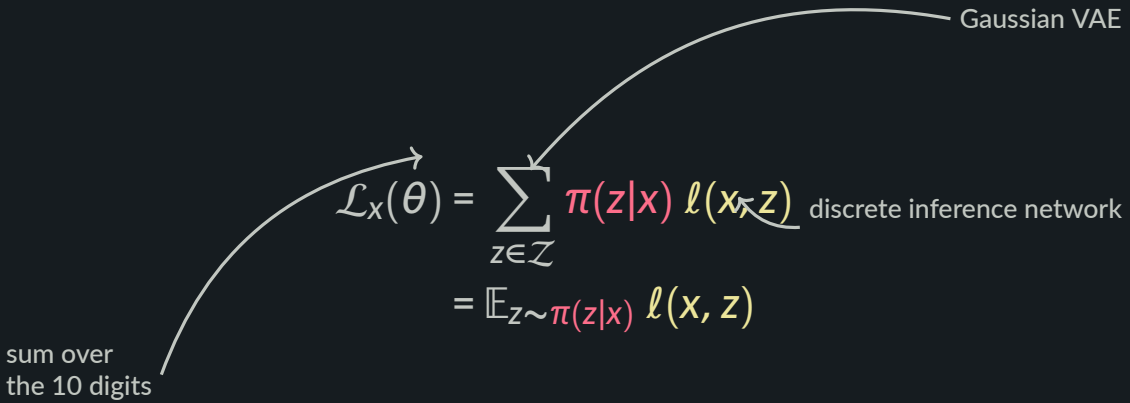

- Semi-Supervised VAE on MNIST: z is a possible digit
- Train this with 10% labeled data

Semi-Supervised VAE

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SFE	94.75±.002	1
SFE+	96.53±.001	2
NVIL	96.01±.002	1
Gumbel	95.46±.001	1
Marginalization		
Dense	96.93±.001	10
Sparse (proposed)	96.87±.001	1.01±0.01

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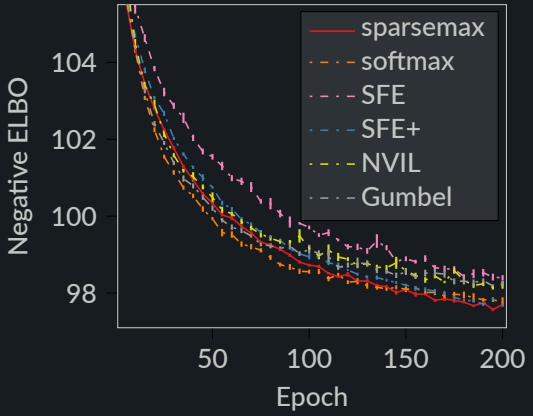

Emergent communication

$$p(y \mid x) = \sum_{h \in \mathcal{H}} p_{\boldsymbol{\phi}}(y \mid h, x)\, p_{\boldsymbol{\pi}}(h \mid x)$$
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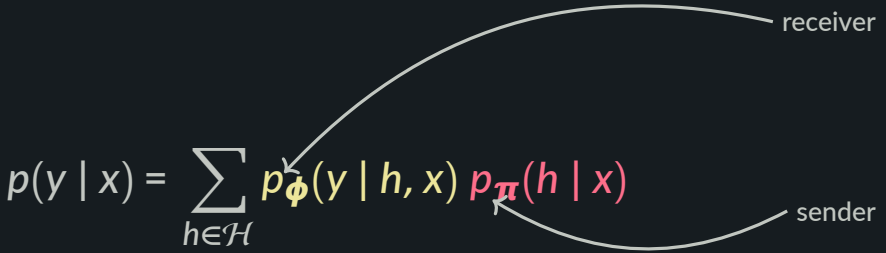

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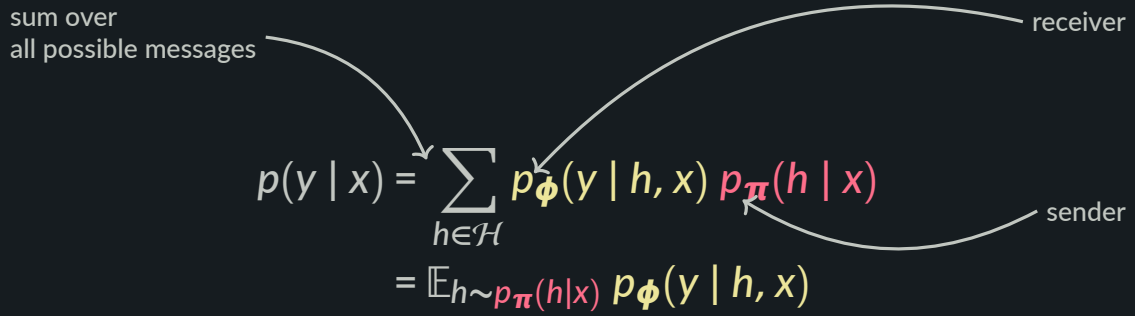

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(Lazaridou et al., 2017; Correia et al., 2020)

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

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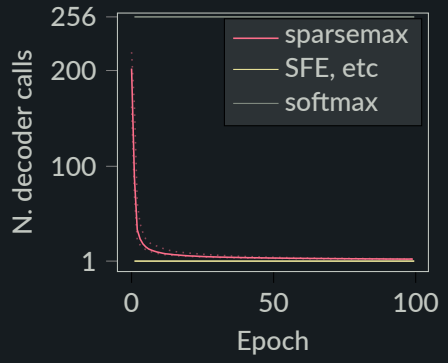

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Limitations

- Mostly (and eventually) very sparse.
  But fully dense worst case.
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One solution: top-k sparsemax

$$k\text{-sparsemax}(s) = \operatorname*{arg\,min}_{\boldsymbol{p}\in\triangle, \|\boldsymbol{p}\|_0 \le k} \|\boldsymbol{p} - s\|_2^2$$

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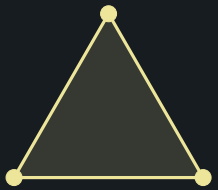
- Non-convex but easy: sparsemax over the k highest scores (Kyrillidis et al., 2013).
- Top-k oracle available for some structured problems.
- Certificate: if at least one of the top-k h gets $p(h) = 0$, **k-sparsemax = sparsemax**!
  thus, for latent variables: biased early on, but it goes away.



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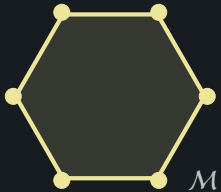

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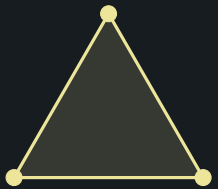
$$\mathcal{M} := \operatorname{conv}\left\{ \boldsymbol{a}_h : h \in \mathcal{H} \right\}$$



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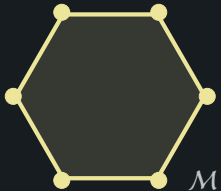

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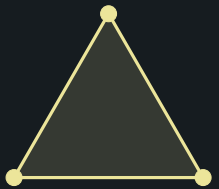

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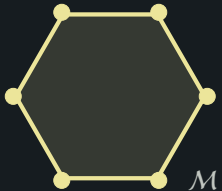

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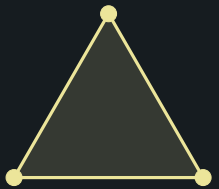

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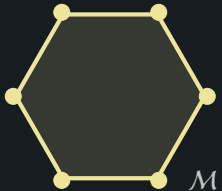

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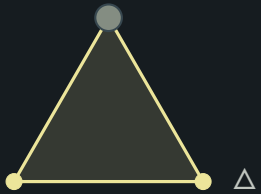
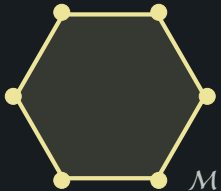
- **argmax** $\arg\max_{\boldsymbol{p} \in \triangle} \boldsymbol{p}^\top s$



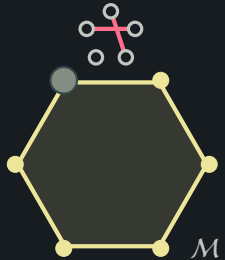
$\triangle$



$\mathcal{M}$

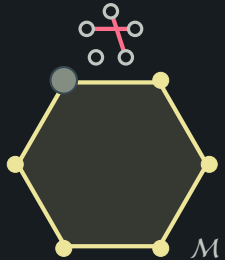
argmax $\arg\max_{\boldsymbol{p} \in \triangle} \boldsymbol{p}^\top s$

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

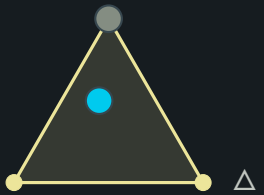


argmax $\arg\max_{\boldsymbol{p} \in \triangle} \boldsymbol{p}^\top s$

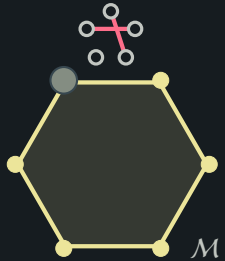
MAP $\arg\max_{\boldsymbol{\mu} \in \mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{\eta}$



- **argmax** $\arg\max_{\boldsymbol{p} \in \Delta} \boldsymbol{p}^\top s$
- **softmax** $\arg\max_{\boldsymbol{p} \in \Delta} \boldsymbol{p}^\top s + \mathrm{H}(\boldsymbol{p})$

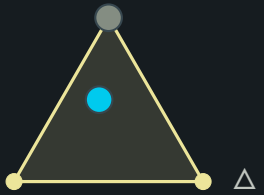


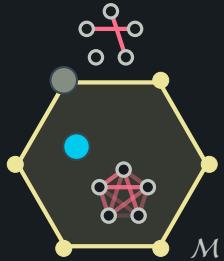
- **MAP** $\arg\max_{\boldsymbol{\mu} \in \mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{\eta}$



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

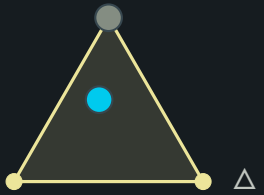
- **MAP** $\arg\max_{\boldsymbol{\mu} \in \mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{\eta}$
- **marginals** $\arg\max_{\boldsymbol{\mu} \in \mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{\eta} + \tilde{\mathrm{H}}(\boldsymbol{\mu})$

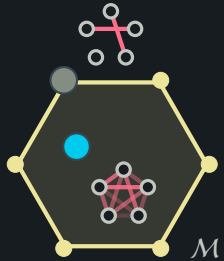




- **argmax** $\arg\max_{\boldsymbol{p} \in \triangle} \boldsymbol{p}^\top s$
- **softmax** $\arg\max_{\boldsymbol{p} \in \triangle} \boldsymbol{p}^\top s + \mathrm{H}(\boldsymbol{p})$

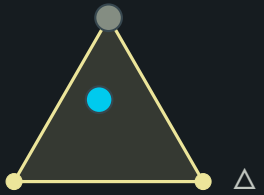
- **MAP** $\arg\max_{\boldsymbol{\mu} \in \mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{\eta}$
- **marginals** $\arg\max_{\boldsymbol{\mu} \in \mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{\eta} + \tilde{\mathrm{H}}(\boldsymbol{\mu})$

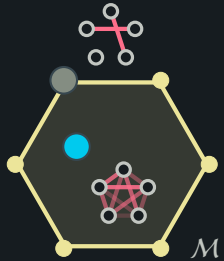




- **argmax** $\arg\max_{\boldsymbol{p} \in \triangle} \boldsymbol{p}^\top s$
- **softmax** $\arg\max_{\boldsymbol{p} \in \triangle} \boldsymbol{p}^\top s + \mathrm{H}(\boldsymbol{p})$

- **MAP** $\arg\max_{\boldsymbol{\mu} \in \mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{\eta}$
- **marginals** $\arg\max_{\boldsymbol{\mu} \in \mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{\eta} + \tilde{\mathrm{H}}(\boldsymbol{\mu})$





- **argmax** $\arg\max_{\boldsymbol{p} \in \triangle} \boldsymbol{p}^\top s$
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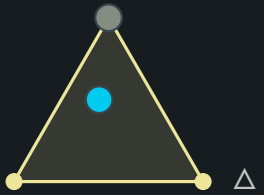
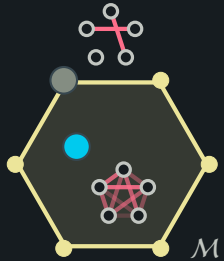
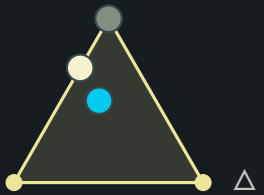
- **MAP** $\arg\max_{\boldsymbol{\mu} \in \mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{\eta}$
- **marginals** $\arg\max_{\boldsymbol{\mu} \in \mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{\eta} + \tilde{\mathrm{H}}(\boldsymbol{\mu})$

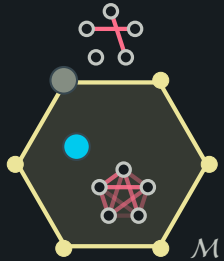




- **argmax** $\arg\max_{\boldsymbol{p} \in \triangle} \boldsymbol{p}^\top s$
- **softmax** $\arg\max_{\boldsymbol{p} \in \triangle} \boldsymbol{p}^\top s + \mathrm{H}(\boldsymbol{p})$
- **sparsemax** $\arg\max_{\boldsymbol{p} \in \triangle} \boldsymbol{p}^\top s - 1/2 \|\boldsymbol{p}\|^2$

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

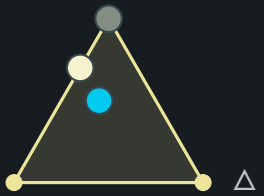


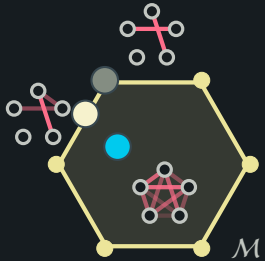


(Niculae, Martins, Blondel, and Cardie, 2018)

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

- **MAP** $\arg\max_{\boldsymbol{\mu} \in \mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{\eta}$
- **marginals** $\arg\max_{\boldsymbol{\mu} \in \mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{\eta} + \widetilde{\mathrm{H}}(\boldsymbol{\mu})$
- **SparseMAP** $\arg\max_{\boldsymbol{\mu} \in \mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{\eta} - \frac{1}{2}\|\boldsymbol{\mu}\|^2$





Bit-vector VAE

Key takeaways

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