# Is the Likelihood-based Deep Generative Modeling appropriate for Representation Learning?

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VU VRIJE UNIVERSITEIT AMSTERDAM

# Representation learning

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*"A **good representation** is (...) one that is **useful** **as input to a supervised predictor**."*



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$$q_\phi(\mathbf{z}|\mathbf{x})$$

**q**(**z**|**x**) is non-trivial (?), e.g., N(0, **1**)



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What makes a representation good (guidelines) [1]:

- smoothness: x ≈ y implies f(x) ≈ f(y)
- multiple explanatory factors
- a hierarchy of explanatory factors
- spatial/temporal coherence
- sparsity
- factors explain x and help to predict *y*
- geometrical properties (manifolds)
- generalizability (shared factors across tasks)
- simplicity of factor dependencies



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**What about compression?**



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**flexible parameterization of distributions**



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After [2]:

**Generative modeling**: formulating a model of the joint distribution, $p_\vartheta(\mathbf{x}, y)$

**Discriminative modeling**: formulating a model of the conditional, $p_\vartheta(y|\mathbf{x})$


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Why do we need **generative modeling**?


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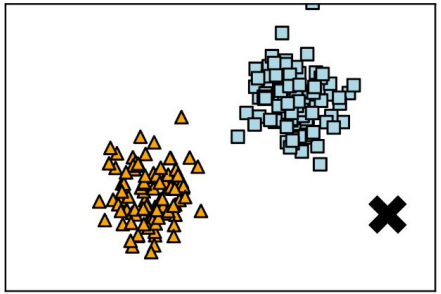

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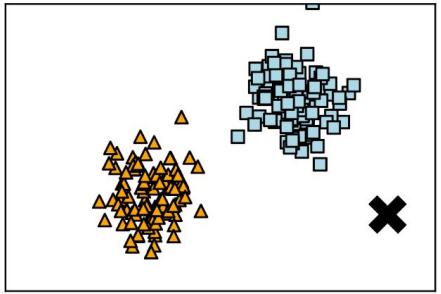

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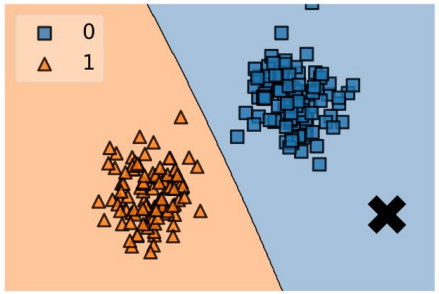


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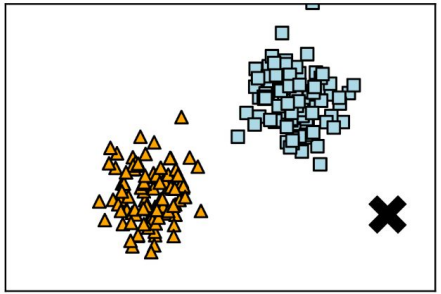

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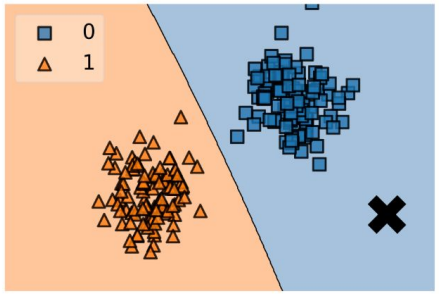


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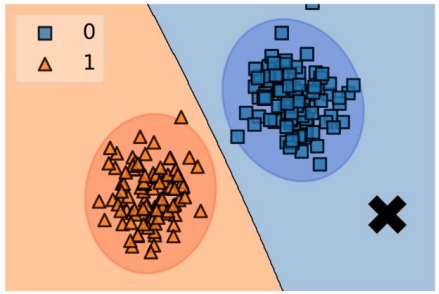


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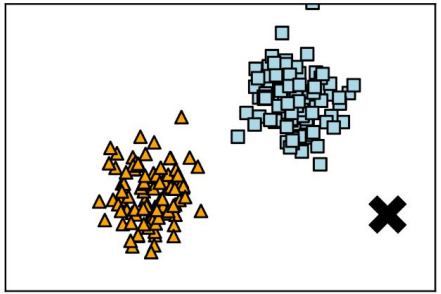

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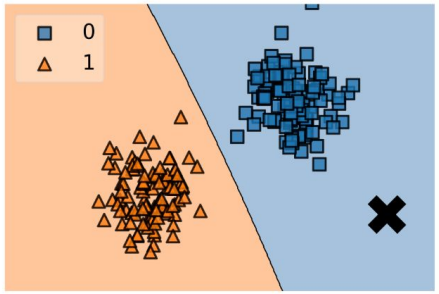


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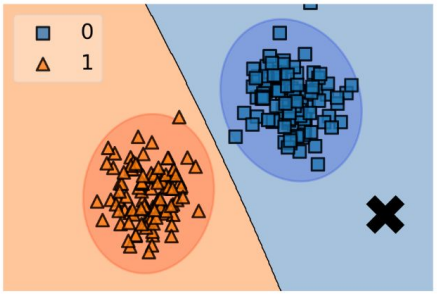


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**Considering the joint could be crucial for decision making!**

# Deep Generative Modeling

We consider the joint distribution factorized as follows:

$$p_\vartheta(\mathbf{x}, y) = p_\vartheta(y|\mathbf{x})\ p_\vartheta(\mathbf{x})$$

Then the log-**likelihood** function (assuming *iid*) takes the following form:

$$\ln p_\vartheta(\mathcal{D}) = \sum_n \ln p_\vartheta(y_n|\mathbf{x}_n) + \sum_n \ln p_\vartheta(\mathbf{x}_n)$$

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**Parameterized by deep neural nets**

**Various models:**
**→ Deep Latent Variable Models (e.g., VAEs, diffusion models)**
**→ Autoregressive Models (ARMs)**
**→ Energy-based Models (EBMs)**

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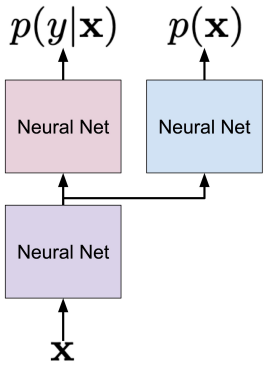
**We can use a shared parameterization.**



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**1. Are there any problems with this objective?**

**2. Is this objective appropriate for representation learning?**

# The likelihood function

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**infinite mixture model**

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→ If we take Gaussians, then we get an **unbounded likelihood** [3]!

**Solution: add a constant diagonal matrix to the decoder's covariance matrix.**


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$$
\begin{aligned}
KL[p_{data}(\mathbf{x})||p_\theta(\mathbf{x})] &= -\mathbb{H}[p_{data}(\mathbf{x})] + \mathbb{CE}[p_{data}(\mathbf{x})||p_\theta(\mathbf{x})] \\
&= const + \mathbb{CE}[p_{data}(\mathbf{x})||p_\theta(\mathbf{x})] \\
&= const - \int p_{data}(\mathbf{x}) \ln p_\theta(\mathbf{x}) \, \mathrm{d}\mathbf{x} \\
&= const - \frac{1}{N} \sum_{n=1}^{N} \ln p_\theta(\mathbf{x}_n)
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**The likelihood-based approach is equivalent to calculating a match between a model and the empirical distribution according to the KL-divergence.**

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**The likelihood function alone does <u>not</u> help representation learning *explicitly*.**



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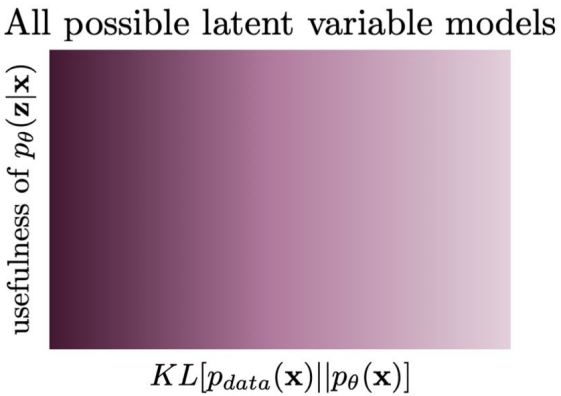
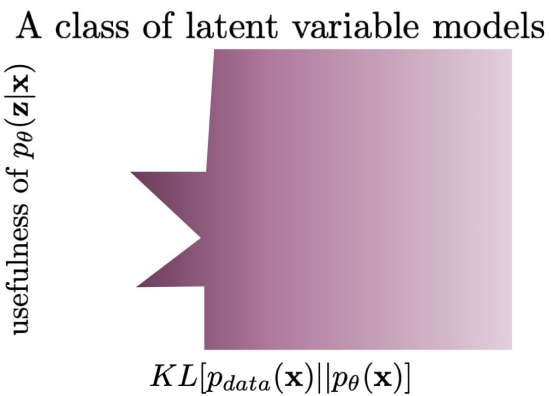
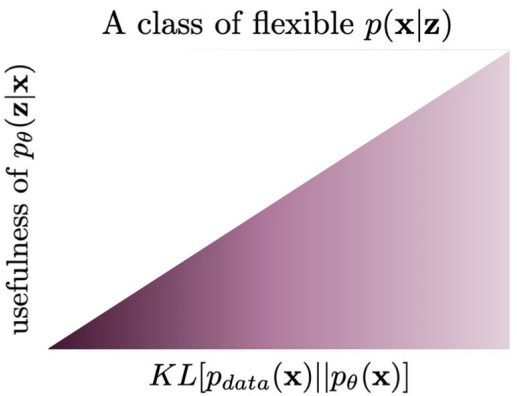
Three scenarios:





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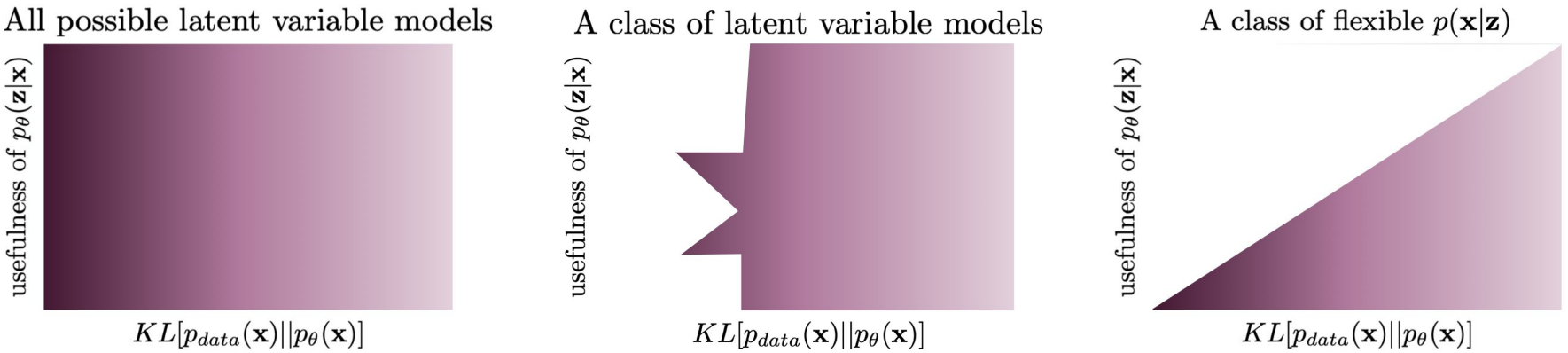


**The likelihood function has <u>no</u> incentive to learn *useful* representations.**


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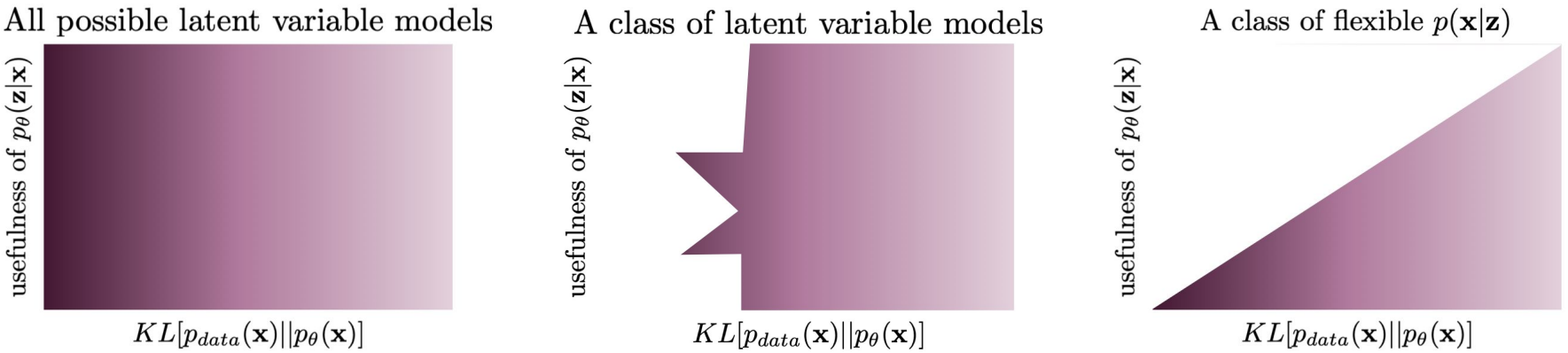


**The likelihood function has no incentive to learn *useful* representations.**

**But is it bad? Maybe we should focus on the parameterization instead!**


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**The likelihood function is a *general* objective and the parameterization is key?**

# How to model the marginal distribution? What parameterization?

# Classes of DGMs

Before we delve into the parameterizations, let us recap the DGMs:

- Latent Variables Models: $p(\mathbf{x}) = \int p(\mathbf{x}|\mathbf{z})\ p(\mathbf{z})\ \mathrm{d}\mathbf{z}$
- Flow-based models: $p(\mathbf{x}) = p\big(\mathbf{z} = f(\mathbf{x})\big)|\mathbf{J}_{f(\mathbf{x})}|$
- Autoregressive models: $p(\mathbf{x}) = p(x_0)\prod_{i=1}^{D} p(x_i|\mathbf{x}_{<i})$
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**Latent variables = representation**

**What is a *representation* here?**

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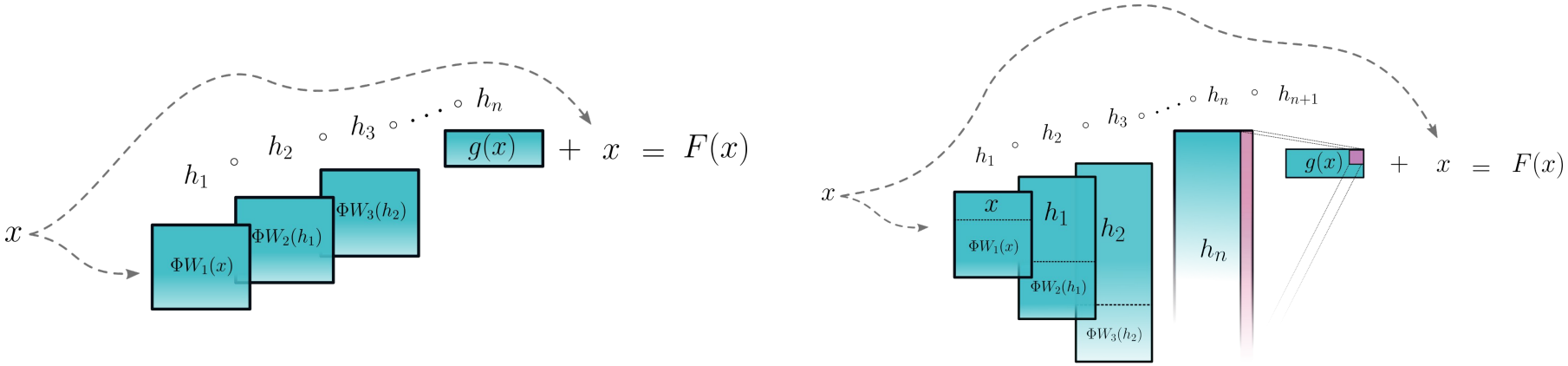



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[6] Perugachi-Diaz, Y., Tomczak, J. M., & Bhulai, S. (2021). Invertible densenets with concatenated lipswish. NeurIPS 2021

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or/and **invertible structure** with **easily computable Jacobian**, e.g.:

→ Householder flows [7], Sylvester flows [8]

→ Convolution Exponential + Sylvester flows [9]


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[6] Perugachi-Diaz, Y., Tomczak, J. M., & Bhulai, S. (2021). Invertible densenets with concatenated lipswish. NeurIPS 2021
[7] Tomczak, J. M., & Welling, M. (2016). Improving variational auto-encoders using householder flow. Bayesian Deep Learing @ NeurIPS 2016
[8] van den Berg, R., Hasenclever, L., Tomczak, J. M., & Welling, M. Sylvester Normalizing Flows for Variational Inference. UAI 2018
[9] Hoogeboom, E., Garcia Satorras, V., Tomczak, J., & Welling, M. (2020). The Convolution Exponential and Generalized Sylvester Flows. NeurIPS 2020

# Flows for joint modeling

We can use flows to formulate a joint distribution [10]:

- The marginal distribution is a flow-based model.
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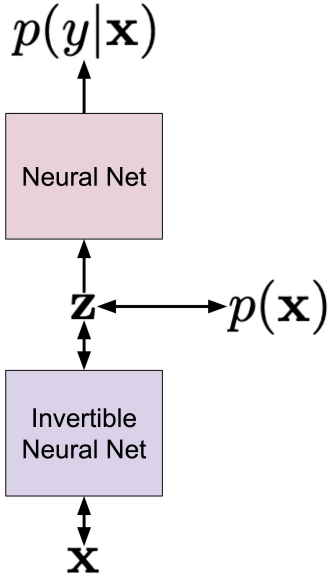



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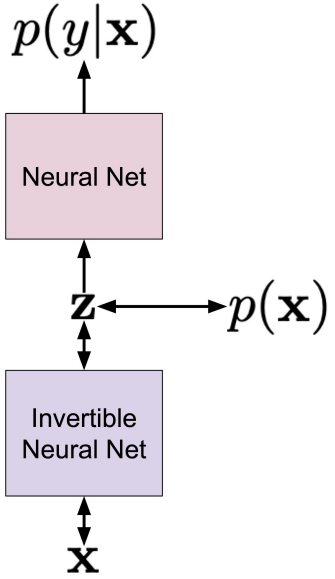


**The gradient flow is uneven from the conditional and the marginal.**


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# Flows for joint modeling

We see that $\lambda$ is crucial [6]:

| | $\lambda = 0$ | $\lambda = \frac{1}{D}$ | | $\lambda = 1$ | |
|---|---|---|---|---|---|
| Model \Evaluation | Acc ↑ | Acc ↑ | bpd ↓ | Acc ↑ | bpd ↓ |
| Coupling | 89.77% | 87.58% | 4.30 | 67.62% | 3.54 |
| + $1 \times 1$ conv | 90.82% | 87.96% | 4.09 | 67.38% | 3.47 |
| Residual Blocks (full) | 91.78% | 90.47% | 3.62 | 70.32% | 3.39 |
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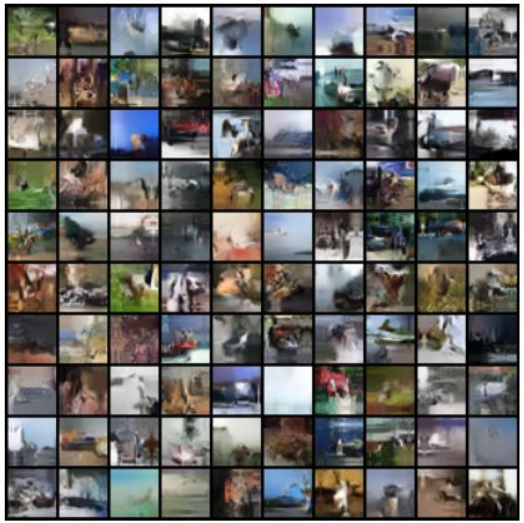
(a) Hybrid model trained with $\lambda = \frac{1}{D}$



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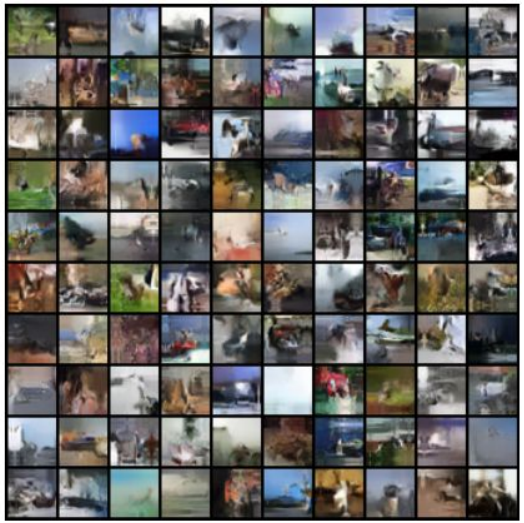

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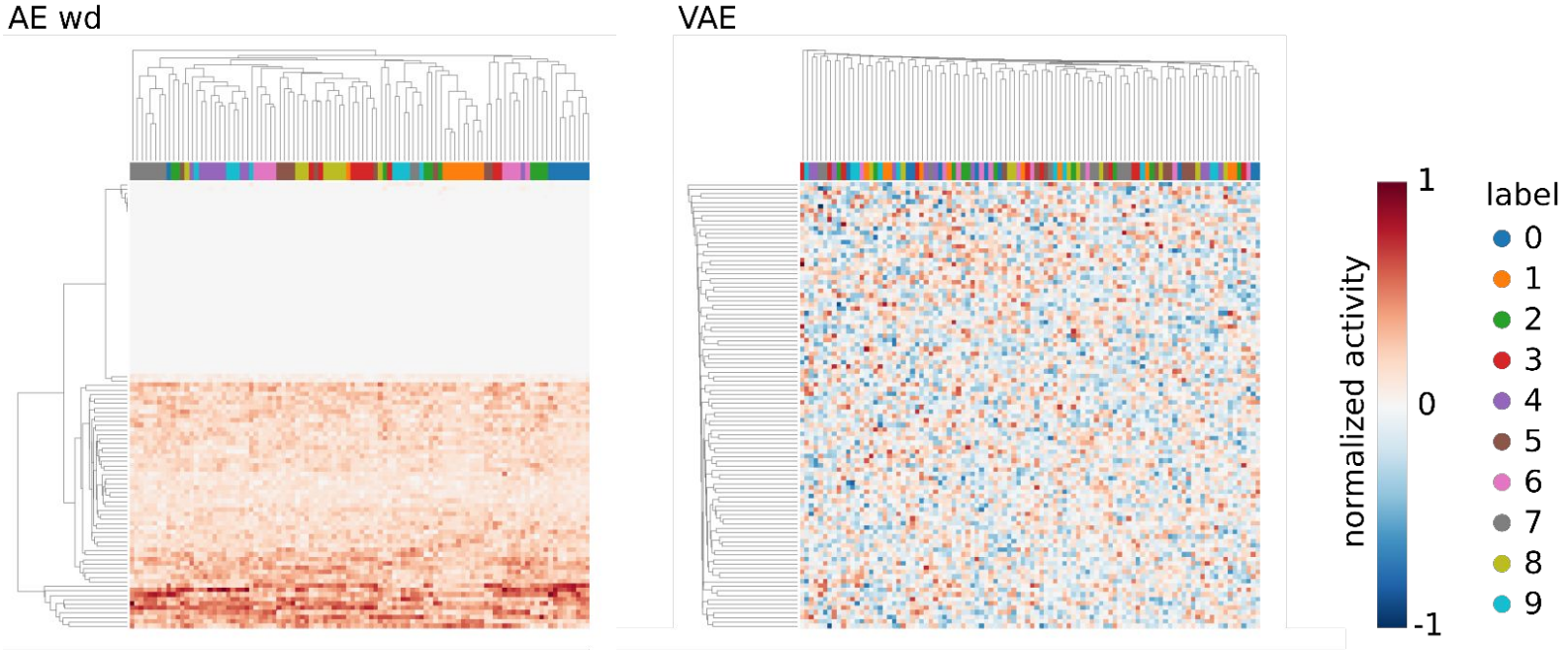


[11] Hübotter, J. F., Lanillos, P., & Tomczak, J. M. (2021). Training Deep Spiking Auto-encoders without Bursting or Dying Neurons through Regularization. arXiv preprint arXiv:2109.11045.

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- But they fail to learn a *representation* [11].
- It is possible to introduce geometrical perspective to VAEs:

→ Hyperspherical VAEs [12], Riemaniann manifolds [13], Lie groups [14]

- Hierarchical latent structure is crucial for learning powerful VAEs.

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[14] Falorsi, L., de Haan, P., Davidson, T. R., & Forré, P. (2019). Reparameterizing distributions on lie groups. AISTATS 2019

# Hierarchical VAEs

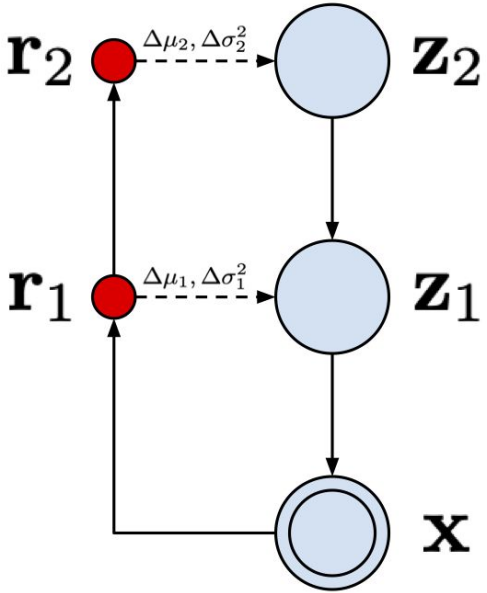
A proper **parameterization** of hierarchical VAEs is important to get SOTA.

So called top-down VAEs:

→ ResNet VAE [15], Ladder VAE [16], BIVA [17], NVAE [18], vdVAE [19]

$$p(\mathbf{x}|\mathbf{z}_1)p(\mathbf{z}_1|\mathbf{z}_2)p(\mathbf{z}_2)$$

$$q(\mathbf{z}_1|\mathbf{z}_2,\mathbf{x})q(\mathbf{z}_2|\mathbf{x})$$





[15] Kingma, D. P., Salimans, T., Jozefowicz, R., Chen, X., Sutskever, I., & Welling, M. (2016). Improved variational inference with inverse autoregressive flow. NeurIPS 2016

[16] Sønderby, C. K., Raiko, T., Maaløe, L., Sønderby, S. K., & Winther, O. (2016). Ladder variational autoencoders. NeurIPS 2016

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[19] Child, R. (2020). Very Deep VAEs Generalize Autoregressive Models and Can Outperform Them on Images. ICLR 2020




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# VAEs for joint modeling

However, still, using VAEs for modeling the marginal and sharing the encoder with the predictor requires applying a fudge factor.

The objective can take the following form [20, 21]:

$$\ell_\alpha(\mathbf{x}, y) = \alpha \mathbb{E}_{q(\mathbf{z}|\mathbf{x})} \left[\ln p(y|\mathbf{z})\right] + ELBO(\mathbf{x})$$

The encoder is shared with the classifier.

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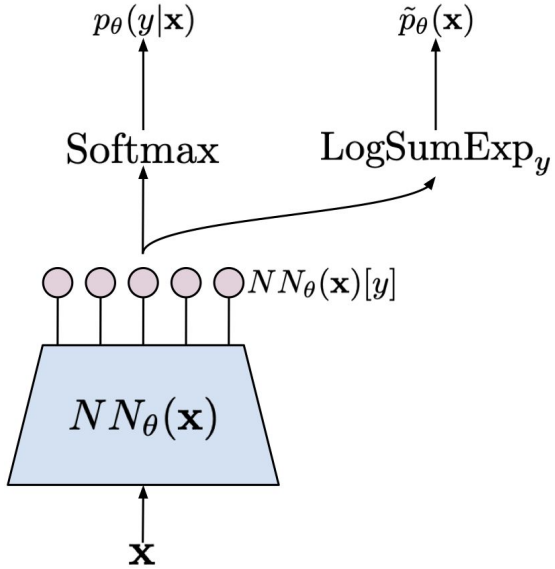




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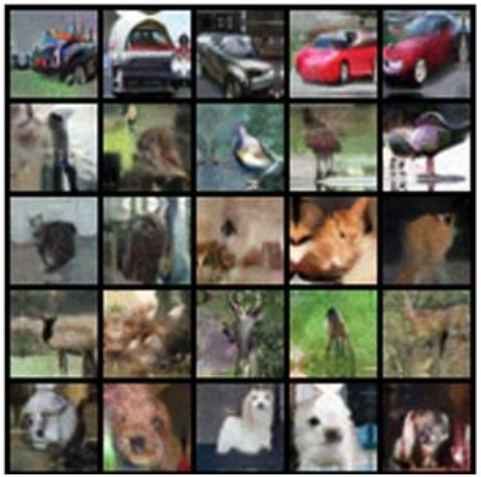
| Class | Model | Accuracy% ↑ | IS↑ | FID↓ |
|---|---|---|---|---|
| **Hybrid** | Residual Flow | 70.3 | 3.6 | 46.4 |
| | Glow | 67.6 | 3.92 | 48.9 |
| | IGEBM | 49.1 | 8.3 | **37.9** |
| | JEM $p(\mathbf{x}\|y)$ factored | 30.1 | 6.36 | 61.8 |
| | JEM (Ours) | **92.9** | **8.76** | 38.4 |
| **Disc.** | Wide-Resnet | 95.8 | N/A | N/A |
| **Gen.** | SNGAN | N/A | 8.59 | 25.5 |
| | NCSN | N/A | 8.91 | 25.32 |





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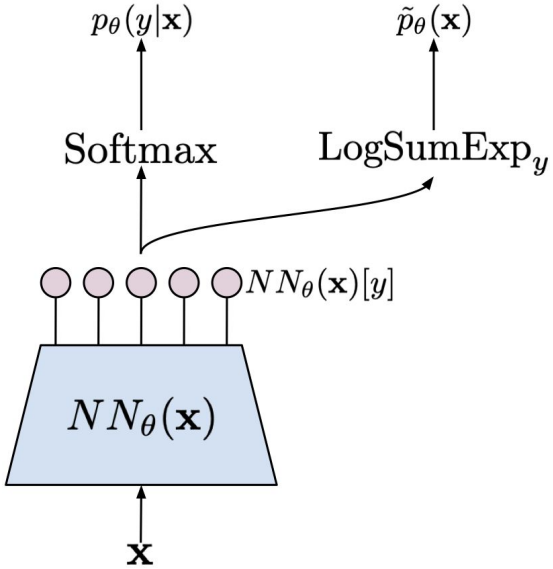


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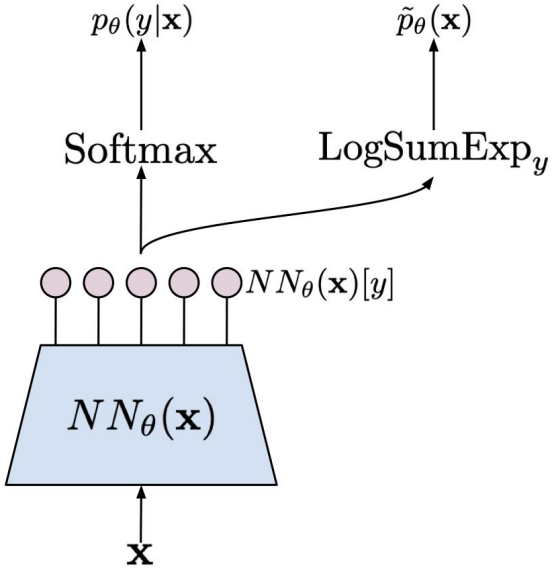


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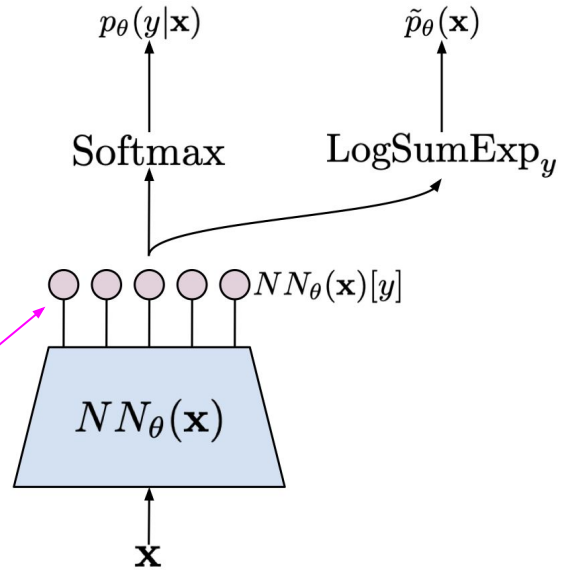


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**Do we really need one?**

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**Where is the problem?**



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# Do we need a notion of *representation learning*?

# What is a *representation*?

Learning a joint distribution raises questions:

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**So do we really need a *representation*?**

**Or maybe we misinterpret the *representation*?**



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In other words:

***Maximizing the model log-likelihood*** *is equivalent to* ***minimizing the expected number of bits required per message****, if the encoder is optimal.*

So we want to get $p_{real}(\mathbf{x}) \approx p_{\theta}(\mathbf{x})$.

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**But then, how to use compression in the context of prediction?**

# Questions

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3. Is the notion of *representation learning* even necessary? Is it a different label for compression?

# Thank you!

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