WHY DO WE NEED DEEP GENERATIVE MODELING?

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ML in PL Conference

VU VRIJE UNIVERSITEIT AMSTERDAM

Introduction

IS GENERATIVE MODELING IMPORTANT?

We learn a neural network to classify images:

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...

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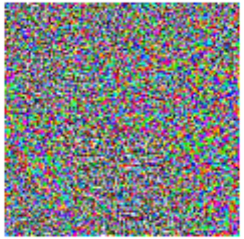
+



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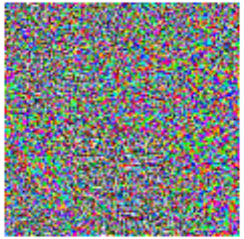

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IS GENERATIVE MODELING IMPORTANT?

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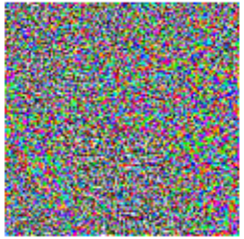

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...
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There is no semantic understanding of images.

IS GENERATIVE MODELING IMPORTANT?

This simple example shows that:

- A discriminative model is (probably) **not enough**.
- We need a notion of **uncertainty**.
- We need to **understand** the reality.

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A possible solution is **generative modeling**.

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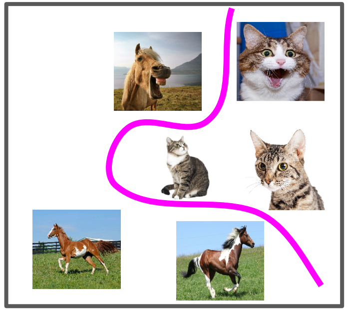

$$p_\theta(y|x)$$

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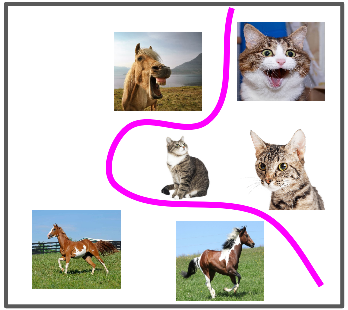

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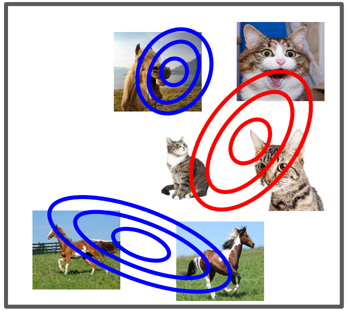

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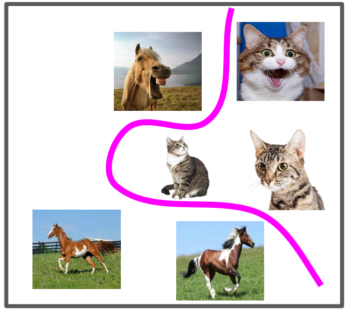

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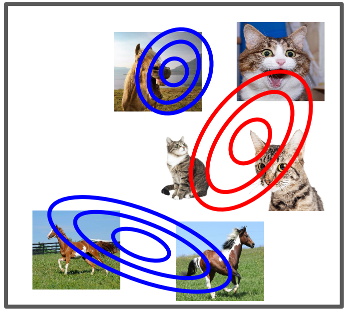

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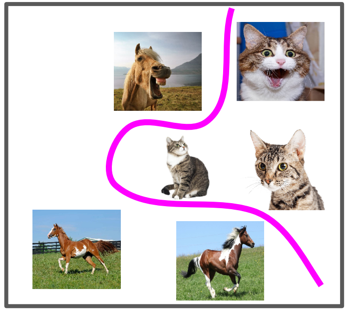
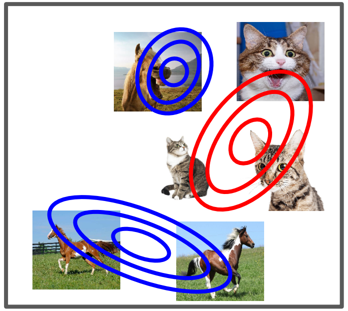


$$p_\theta(y|x)$$

High probability
of a **horse.**
=
Highly probable
decision!



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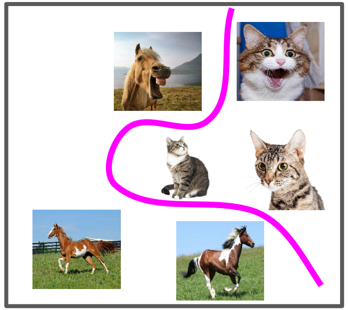

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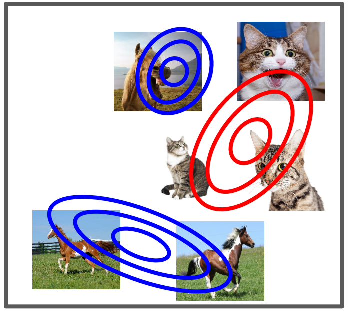

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High probability of a **horse.**

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Low probability of the **object**

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Uncertain decision!

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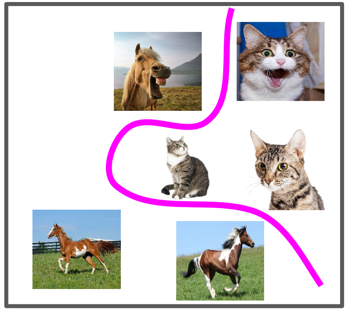

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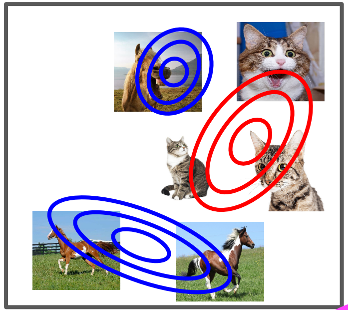

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High probability of a **horse.**

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Uncertain decision!

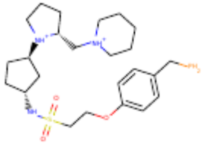
WHERE DO WE USE DEEP GENERATIVE MODELING?

" i want to talk to you . "
"i want to be with you . "
"i do n't want to be with you . "
i do n't want to be with you .
she did n't want to be with him .

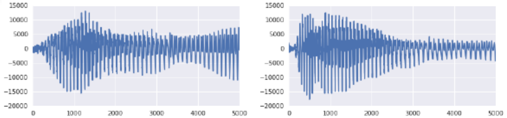
he was silent for a long moment .
he was silent for a moment .
it was quiet for a moment .
it was dark and cold .
there was a pause .
it was my turn .

Text analysis

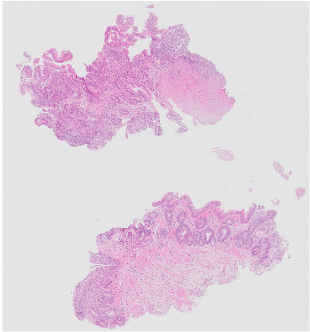
Image analysis



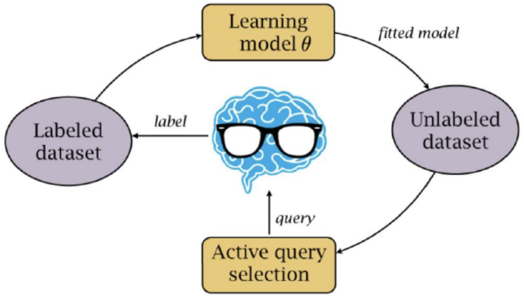
Graph analysis



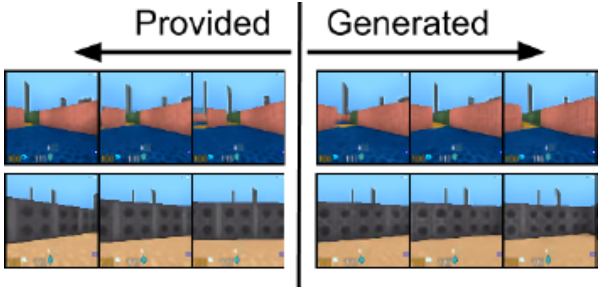
Audio analysis



Medical data



Active Learning



Reinforcement Learning

and more...

HOW TO FORMULATE GENERATIVE MODELS?

Generative model

Autoregressive (*e.g.*, PixelCNN)

Flow-based (e.g., RealNVP, GLOW)

Latent variable models

Implicit models (*e.g.*, GANs)

Prescribed models (*e.g.*, VAE)

HOW TO FORMULATE GENERATIVE MODELS?

	Training	Likelihood	Sampling	Compression
Autoregressive models (e.g., PixelCNN)	Stable	Exact	Slow	No
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flow-based models

latent variable models

Deep latent variable models

GENERATIVE MODELING

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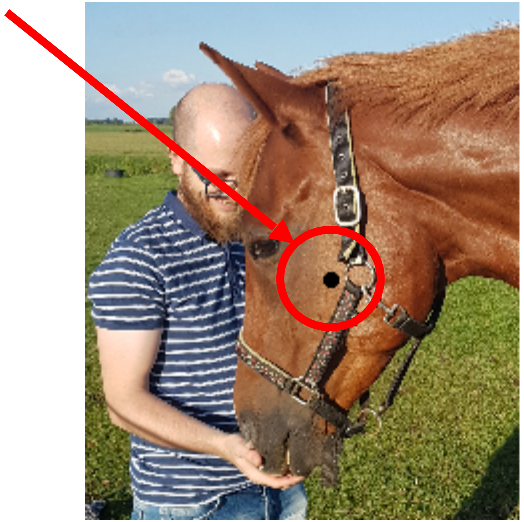

GENERATIVE MODELING

Modeling in high-dimensional spaces is difficult.

Modeling **all dependencies** among pixels:

$$p(\mathbf{x}) = \frac{1}{Z} \prod_{c=1}^{C} \psi_c(\mathbf{x}_c)$$

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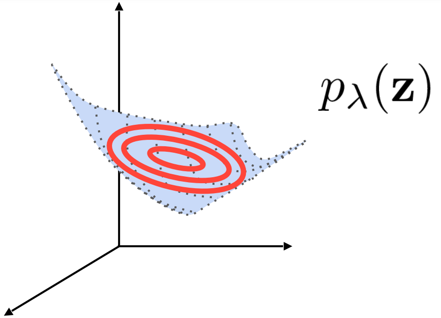
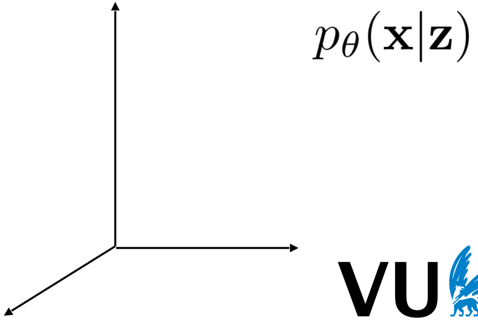
A possible **solution**: **Latent Variable Models**!

GENERATIVE MODELING WITH LATENT VARIABLES

Generative process:

1. $\mathbf{z} \sim p_\lambda(\mathbf{z})$
2. $\mathbf{x} \sim p_\theta(\mathbf{x}|\mathbf{z})$





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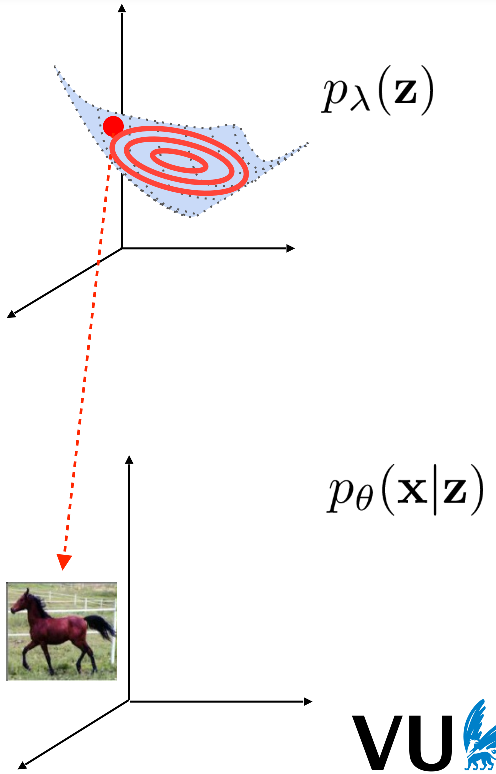

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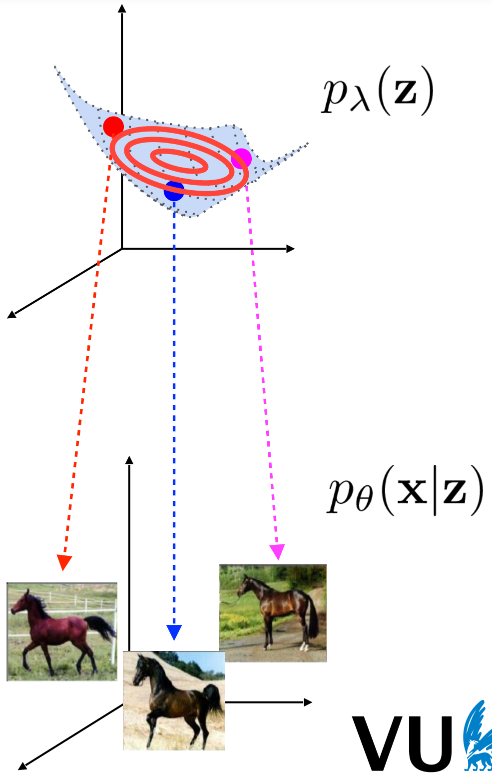

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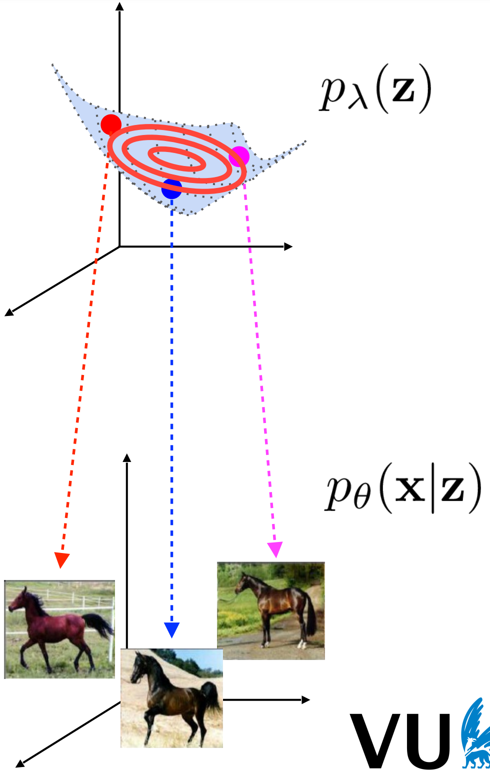

Log of marginal distribution:

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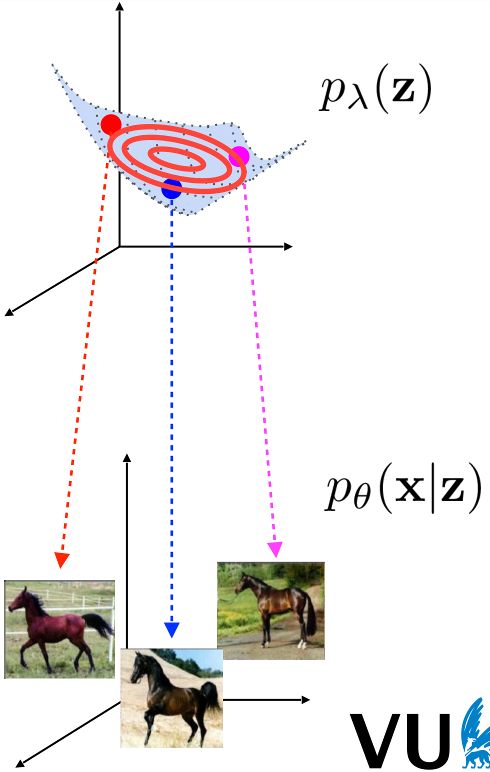

Log of marginal distribution:

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How to train such model efficiently?

VARIATIONAL INFERENCE FOR LATENT VARIABLE MODELS

$$\begin{aligned}
\log p_{\vartheta}(\mathbf{x}) &= \log \int p_{\theta}(\mathbf{x}|\mathbf{z})\ p_{\lambda}(\mathbf{z})\mathrm{d}\mathbf{z} \\
&= \log \int \frac{q_{\phi}(\mathbf{z}|\mathbf{x})}{q_{\phi}(\mathbf{z}|\mathbf{x})} p_{\theta}(\mathbf{x}|\mathbf{z})\ p_{\lambda}(\mathbf{z})\mathrm{d}\mathbf{z} \\
&\geq \int q_{\phi}(\mathbf{z}|\mathbf{x}) \log \frac{p_{\theta}(\mathbf{x}|\mathbf{z})\ p_{\lambda}(\mathbf{z})}{q_{\phi}(\mathbf{z}|\mathbf{x})} \mathrm{d}\mathbf{z} \\
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\end{aligned}$$

VARIATIONAL INFERENCE FOR LATENT VARIABLE MODELS

Variational posterior

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\end{aligned}
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Jensen's inequality

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&= \underbrace{\mathbb{E}_{\mathbf{z}\sim q_{\phi}(\mathbf{z}|\mathbf{x})}\Big[\log p_{\theta}(\mathbf{x}|\mathbf{z})\Big]}_{\text{Reconstruction error}} - \underbrace{\mathrm{KL}\Big(q_{\phi}(\mathbf{z}|\mathbf{x})||p_{\lambda}(\mathbf{z})\Big)}_{\text{Regularization}}
\end{aligned}
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decoder

encoder

marginal

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decoder

encoder

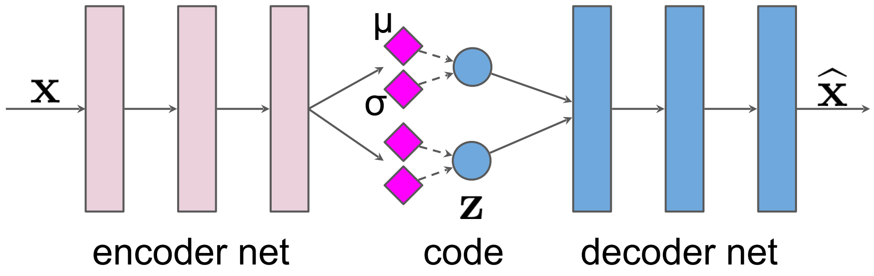
marginal

= Variational Auto-Encoder

VU

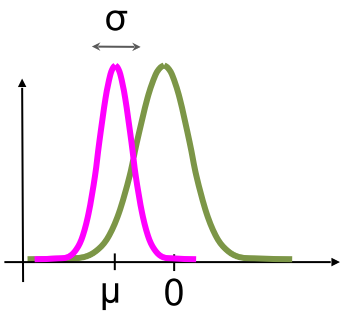
VARIATIONAL AUTO-ENCODERS

Variational posterior (**encoder**) and likelihood function (**decoder**) are parameterized by neural networks.



Reparameterization trick:
move the stochasticity to independent random variables

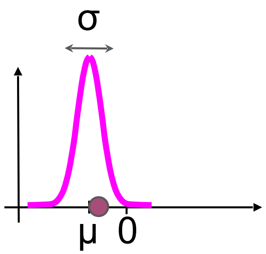
$$\mathbf{z} = f(\boldsymbol{\mu}, \boldsymbol{\sigma}; \boldsymbol{\varepsilon}), \text{ where } \boldsymbol{\varepsilon} \sim p(\boldsymbol{\varepsilon})$$

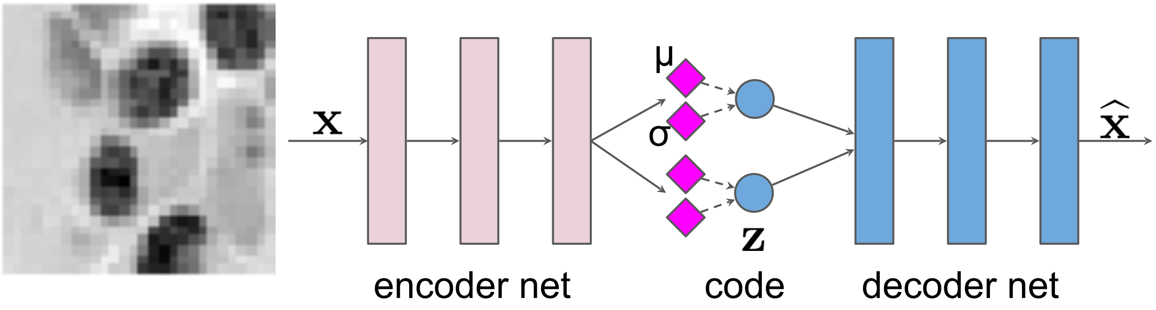


VARIATIONAL AUTO-ENCODERS

VAE copies input to output through a **bottleneck**.

VAE learns a **code** of the data.





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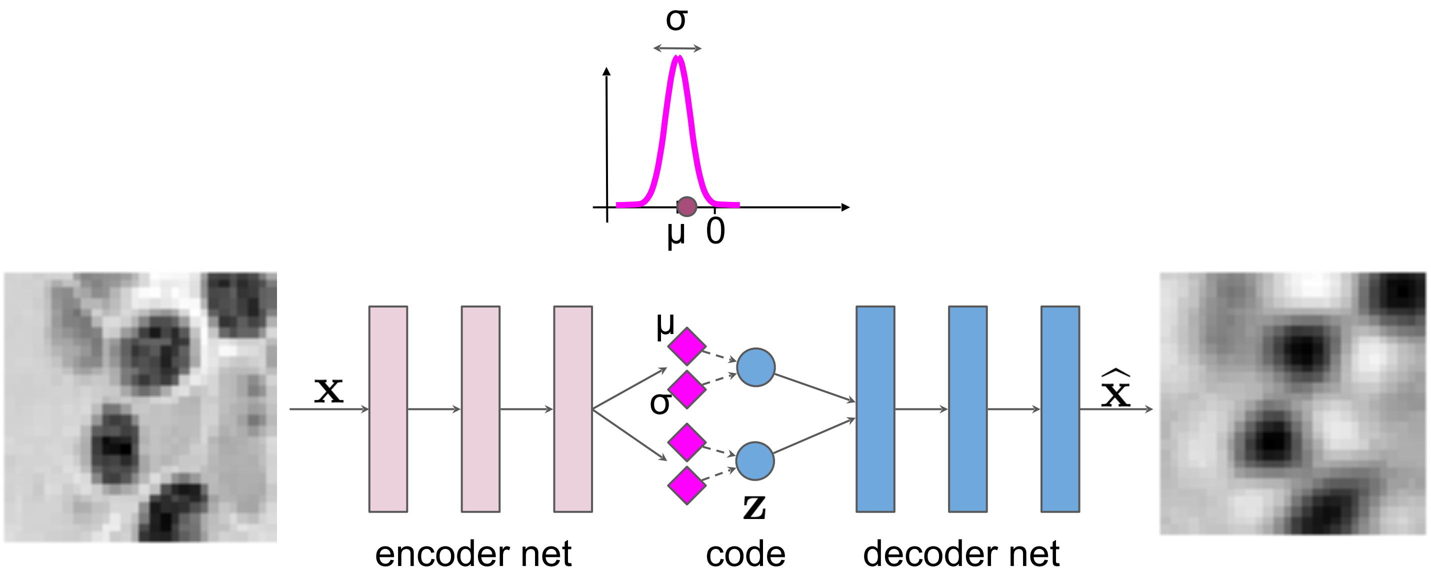

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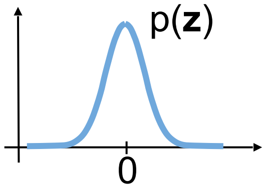
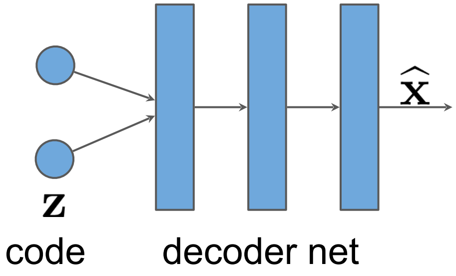
VAE has a **marginal** on the latent code.

VAE can **generate** new data.





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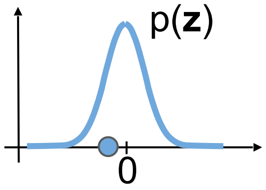

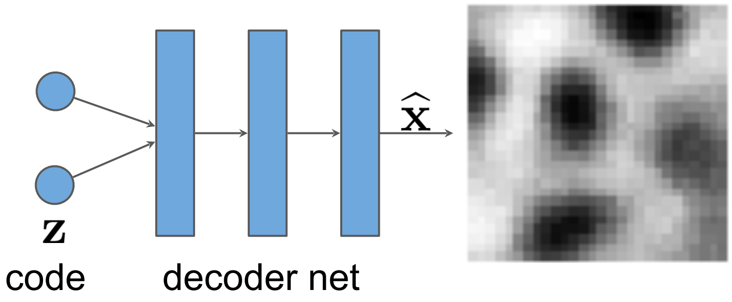

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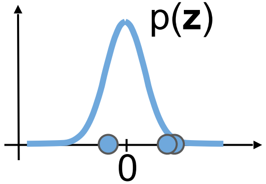

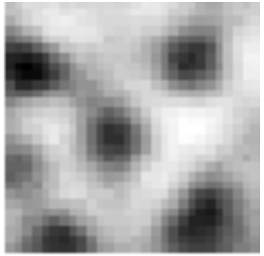

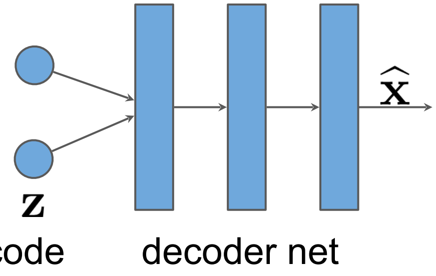

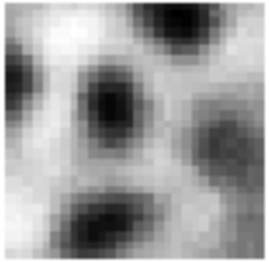

COMMON ISSUES WITH VAES

$$q_{\phi}(\mathbf{z}|\mathbf{x}) \propto p_{\theta}(\mathbf{x}|\mathbf{z})\ p_{\lambda}(\mathbf{z})$$

Weak decoders → bad generations/reconstructions

Weak encoders → bad latent representation

Weak marginals → bad generations

Variational posteriors → what family of distributions?

Others…

COMPONENTS OF VAES

$$q_{\phi}(\mathbf{z}|\mathbf{x}) \propto p_{\theta}(\mathbf{x}|\mathbf{z})\ p_{\lambda}(\mathbf{z})$$

Resnets
DRAW
Autoregressive models
Normalizing flows

Autoregressive models
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VampPrior
Implicit prior

COMPONENTS OF VAES

$$q_\phi(\mathbf{z}|\mathbf{x}) \propto p_\theta(\mathbf{x}|\mathbf{z})\; p_\lambda(\mathbf{z})$$

Normalizing flows
Discrete encoders
Hyperspherical dist.
Hyperbolic-normal dist.
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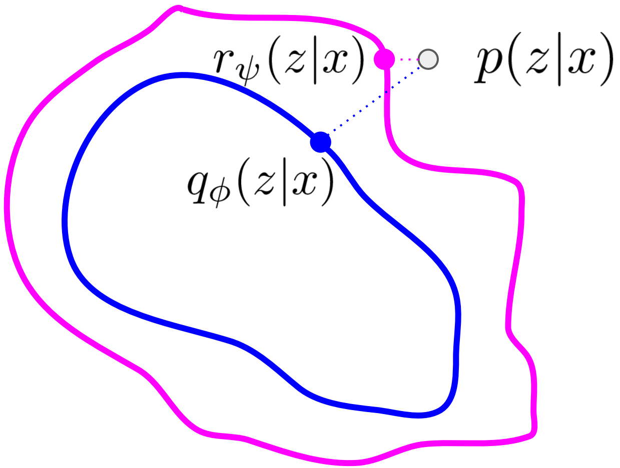
VARIATIONAL POSTERIOR IN VAES

Question: How to minimize the KL(q||p)?

$$\mathrm{ELBO}(\mathbf{x};\theta,\phi,\lambda) = \log p_{\vartheta}(\mathbf{x}) - \mathrm{KL}\Big(q_{\phi}(\mathbf{z}|\mathbf{x})||p(\mathbf{z}|\mathbf{x})\Big)$$

In other words: *How to formulate a more flexible family of approximate (variational) posteriors?*



Using Gaussian is not sufficiently **flexible**.

We need a **computationally efficient tool**.

Arvanitidis, G., Hansen, L. K., & Hauberg, S. (2017). Latent space oddity: on the curvature of deep generative models. *arXiv preprint arXiv:1710.11379*.

VARIATIONAL INFERENCE WITH NORMALIZING FLOWS

Sample from a “simple” distribution: $\mathbf{z}_0 \sim q_0(\mathbf{z}|\mathbf{x}) = \mathcal{N}\left(\mathbf{z}|\mu(\mathbf{x}), \mathrm{diag}(\sigma^2(\mathbf{x}))\right)$

Rezende, D. J., & Mohamed, S. (2015). Variational inference with normalizing flows. ICML 2015

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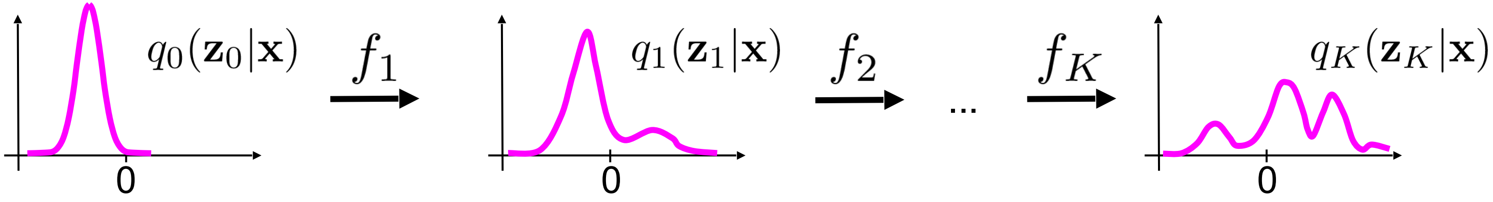

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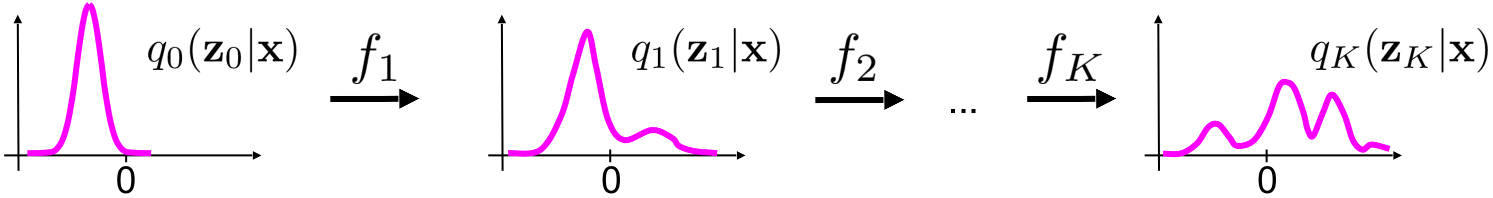

and the change of variables yields:

$$q_K(\mathbf{z}_K|\mathbf{x}) = q_0(\mathbf{z}_0|\mathbf{x}) \prod_{k=1}^{K} \left| \det \frac{\partial f_k(\mathbf{z}_{k-1})}{\partial \mathbf{z}_{k-1}} \right|^{-1}$$

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VARIATIONAL INFERENCE WITH NORMALIZING FLOWS

The learning objective (ELBO) with normalizing flows becomes:

$$\mathrm{ELBO}(\mathbf{x};\theta,\phi,\lambda) = \mathbb{E}_{\mathbf{z}_0\sim q_0(\mathbf{z}_0|\mathbf{x})}\Big[\log p_\theta(\mathbf{x}|\mathbf{z}_K)\Big] - \mathrm{KL}\Big(q_0(\mathbf{z}_0|\mathbf{x})||p_\lambda(\mathbf{z}_K)\Big)+$$

$$+\mathbb{E}_{\mathbf{z}_0\sim q_0(\mathbf{z}_0|\mathbf{x})}\Big[\sum_{k=1}^{K}\log\Big|\det\frac{\partial f_k(\mathbf{z}_{k-1})}{\partial \mathbf{z}_{k-1}}\Big|\Big]$$

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The difficulty lies in calculating the Jacobian determinant:

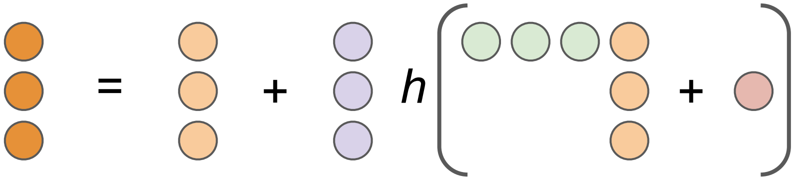
Volume-preserving flows: $\left|\det \frac{\partial f_k(\mathbf{z}_{k-1})}{\partial \mathbf{z}_{k-1}}\right| = 1$

General normalizing flows: $\left|\det \frac{\partial f_k(\mathbf{z}_{k-1})}{\partial \mathbf{z}_{k-1}}\right|$ is "easy" to compute.

Rezende, D. J., & Mohamed, S. (2015). Variational inference with normalizing flows. ICML 2015

PLANAR FLOWS

First, let us take a look at **planar flows** (Rezende & Mohamed, 2015):



$$\mathbf{z}_k = \mathbf{z}_{k-1} + \mathbf{u}\, h(\mathbf{w}^\top \mathbf{z}_{k-1} + b)$$

This is equivalent to a residual layer with a **single** neuron.

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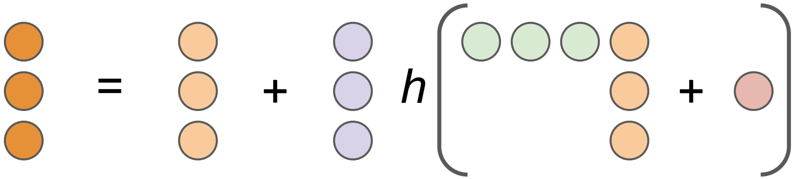

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Can we calculate the Jacobian determinant efficiently?

PLANAR FLOWS

We can use the **matrix determinant lemma** to get the Jacobian determinant:

$$\det \frac{\partial \mathbf{z}'}{\partial \mathbf{z}} = 1 + \mathbf{u}^\top h'(\mathbf{w}^\top \mathbf{z} + b)\mathbf{w}$$

which is **linear** wrt the number of $\mathbf{z}$'s.

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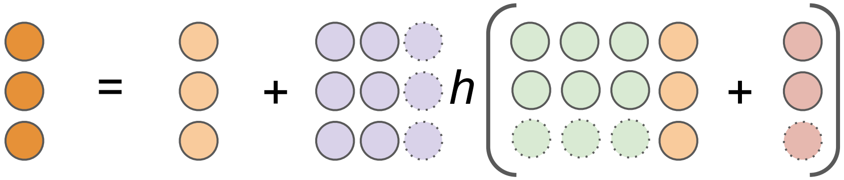
The bottleneck requires many steps, so how can we improve on that?

1. Can we **generalize** planar flows?

2. If yes, how can we compute the Jacobian determinant **efficiently**?

GENERALIZING PLANAR FLOWS: SYLVESTER FLOWS

We can control the bottleneck by generalizing **u** and **w** to **A** and **B**.



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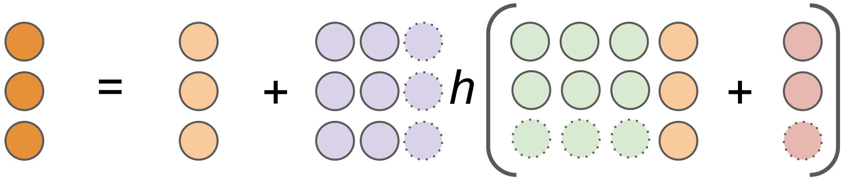

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How to calculate det of Jacobian? Use **Sylvester Determinant Identity**:

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v.d. Berg, R., Hasenclever, L., Tomczak, J.M., & Welling, M. (2018). Sylvester Normalizing Flows for Variational Inference. UAI 2018

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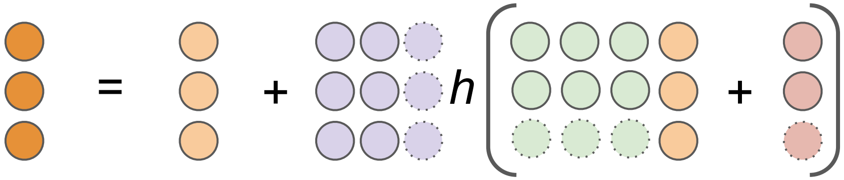

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OK, but it's very expensive! Can we simplify these calculations?

v.d. Berg, R., Hasenclever, L., Tomczak, J.M., & Welling, M. (2018). Sylvester Normalizing Flows for Variational Inference. UAI 2018

SYLVESTER FLOWS

Use of **Sylvester Determinant Identity** yields:

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Next, we can use **QR decomposition** to represent **A** and **B**:

$$\begin{aligned}\det \frac{\partial \mathbf{z}'}{\partial \mathbf{z}} &= \det\Big(\mathbf{I} + \mathrm{diag}\big(h'(\mathbf{R}_B\mathbf{Q}^\top\mathbf{z} + \mathbf{b})\mathbf{R}_B\mathbf{Q}^\top\mathbf{Q}\mathbf{R}_A\big) \\ &= \det\Big(\mathbf{I} + \mathrm{diag}\big(h'(\mathbf{R}_B\mathbf{Q}^\top\mathbf{z} + \mathbf{b})\mathbf{R}_B\mathbf{R}_A\big)\end{aligned}$$

$\mathbf{Q}$ columns are orthonormal vectors

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SYLVESTER FLOWS

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$\mathbf{Q}$ columns are orthonormal vectors **How to keep an orthogonal matrix?**

$\mathbf{R}_A,\ \mathbf{R}_B$ triangular matrices

SYLVESTER FLOWS: LEARNING ORTHOGONAL MATRIX

1.(**O-SNF**) Iterative orthogonalization procedure (e.g., Kovarik, 1970):

a. We can **backpropagate** through this procedure.

$$\mathbf{Q} := \mathbf{Q}\Big(\mathbf{I} + \frac{1}{2}(\mathbf{I} - \mathbf{Q}^\top\mathbf{Q})\Big)$$

b. We can control the bottleneck by changing the number of columns.

2.(**H-SNF**) Use Householder transformations to represent **Q**.

a. H-SNF is a non-linear **extension** of the Householder flow.

$$\mathbf{Q} = \mathbf{I} - 2\frac{\mathbf{v}\mathbf{v}^\top}{\mathbf{v}^\top\mathbf{v}}$$

b. No bottleneck!

3.(**T-SNF**) Alternate between identity matrix and a fixed permutation matrix.

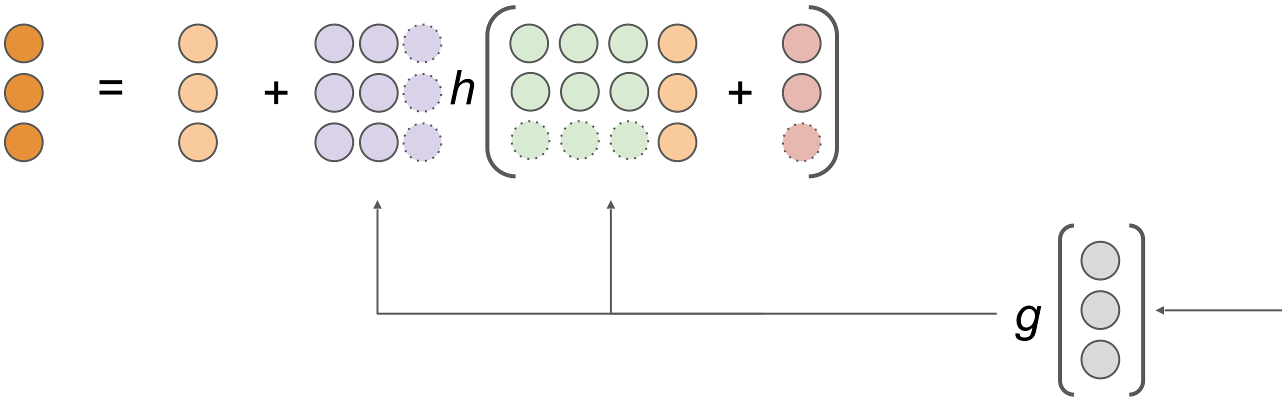
a. Used also in RealNVP and IAF.

SYLVESTER NORMALIZING FLOWS

A single step: $\mathbf{z}_k = \mathbf{z}_{k-1} + \mathbf{Q}\mathbf{R}_A\ h(\mathbf{R}_B\mathbf{Q}^\top \mathbf{z}_{k-1} + \mathbf{b})$

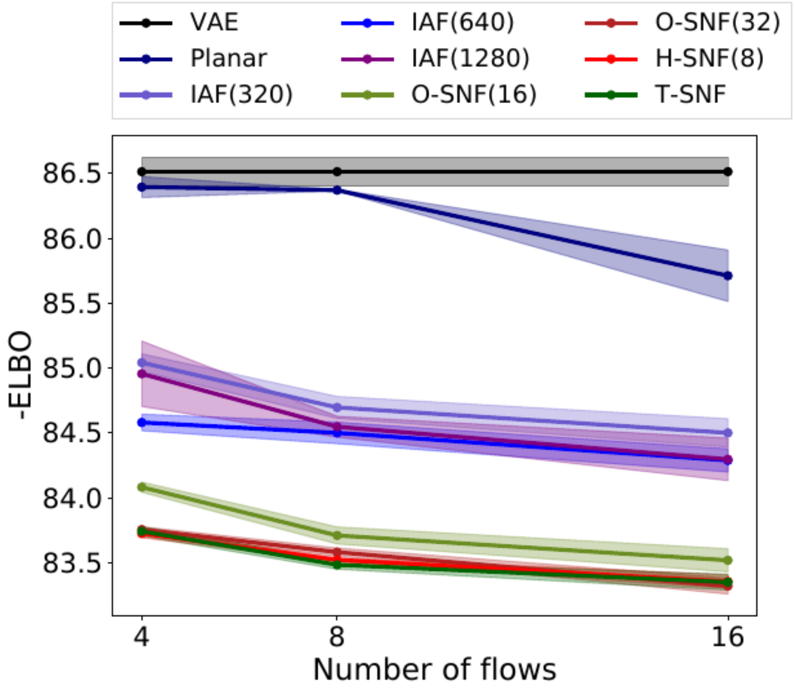
Keep **Q** **orthogonal**: (i) bottleneck: O-SNF, (ii) w/o: H-SNF, T-SNF.

Use **hypernets** to calculate **Q** and **R**'s:



VU

SYLVESTER FLOWS: RESULTS ON MNIST



Model	-ELBO	NLL
VAE	86.55 ± 0.06	82.14 ± 0.07
Planar	86.06 ± 0.31	81.91 ± 0.22
IAF	84.20 ± 0.17	80.79 ± 0.12
O-SNF	$\mathbf{83.32 \pm 0.06}$	$\mathbf{80.22 \pm 0.03}$
H-SNF	83.40 ± 0.01	80.29 ± 0.02
T-SNF	83.40 ± 0.10	80.28 ± 0.06

SYLVESTER FLOWS: RESULTS ON OTHER DATA

Model	Freyfaces		Omniglot		Caltech 101	
	-ELBO	NLL	-ELBO	NLL	-ELBO	NLL
VAE	4.53 ± 0.02	4.40 ± 0.03	104.28 ± 0.39	97.25 ± 0.23	110.80 ± 0.46	99.62 ± 0.74
Planar	$\mathbf{4.40 \pm 0.06}$	$\mathbf{4.31 \pm 0.06}$	102.65 ± 0.42	96.04 ± 0.28	109.66 ± 0.42	98.53 ± 0.68
IAF	4.47 ± 0.05	4.38 ± 0.04	102.41 ± 0.04	96.08 ± 0.16	111.58 ± 0.38	99.92 ± 0.30
O-SNF	4.51 ± 0.04	4.39 ± 0.05	99.00 ± 0.29	93.82 ± 0.21	106.08 ± 0.39	94.61 ± 0.83
H-SNF	4.46 ± 0.05	4.35 ± 0.05	$\mathbf{99.00 \pm 0.04}$	$\mathbf{93.77 \pm 0.03}$	$\mathbf{104.62 \pm 0.29}$	$\mathbf{93.82 \pm 0.62}$
T-SNF	4.45 ± 0.04	4.35 ± 0.04	99.33 ± 0.23	93.97 ± 0.13	105.29 ± 0.64	94.92 ± 0.73

No. of flows: 16
IAF: 1280 wide MADE, **no hypernets**
Bottleneck in O-SNF: 32
No. of Householder transformations in H-SNF: 8

COMPONENTS OF VAES

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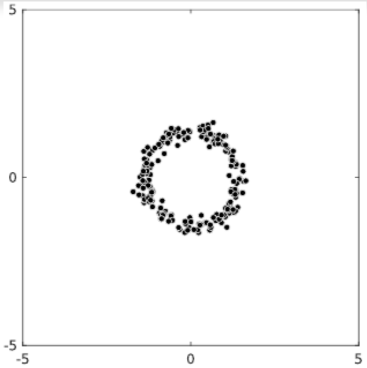
GEOMETRIC PERSPECTIVE ON VAES

Question: Is it possible to recover the true Riemannian structure of the latent space?

In other words:

Will geodesics follow data manifold?



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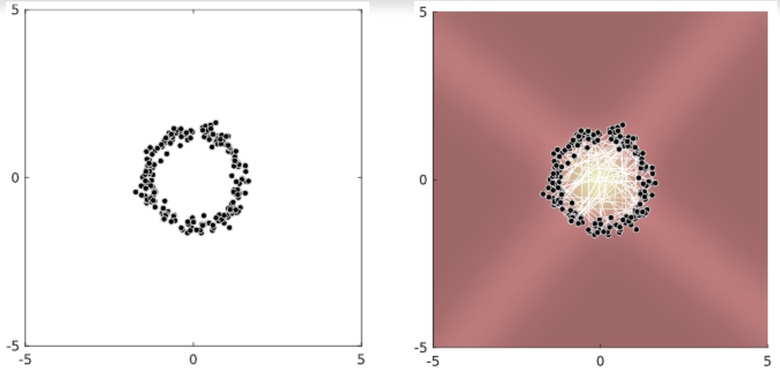

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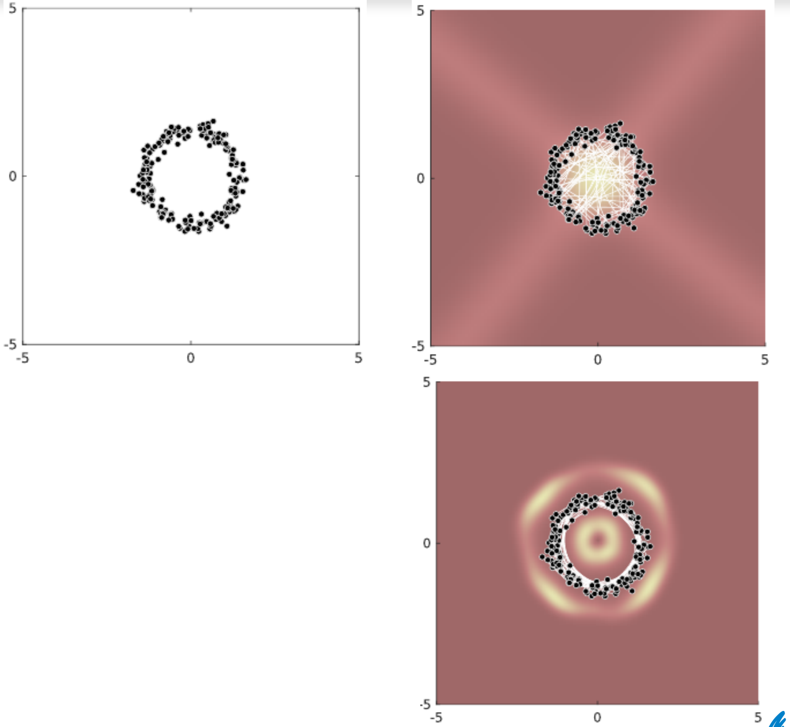

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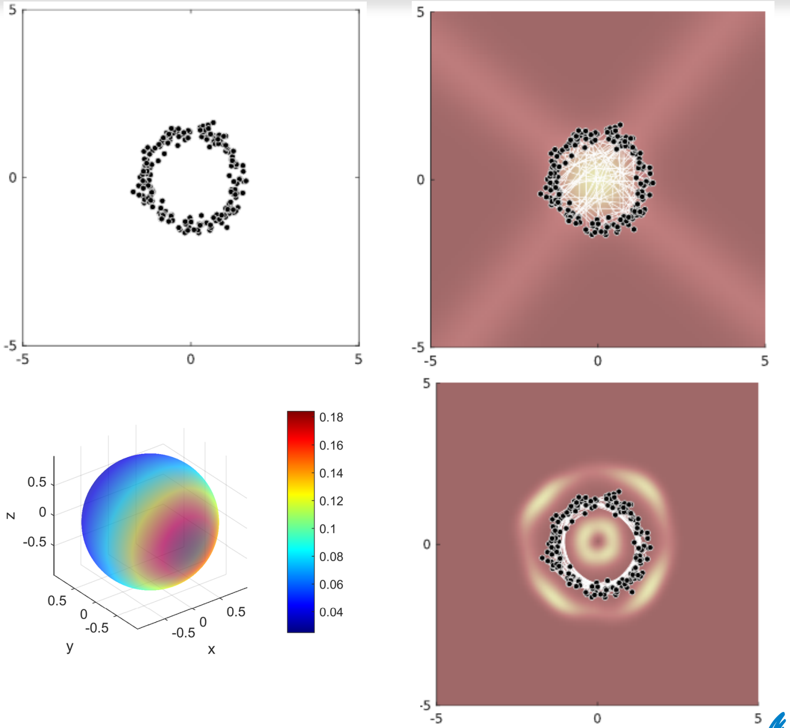

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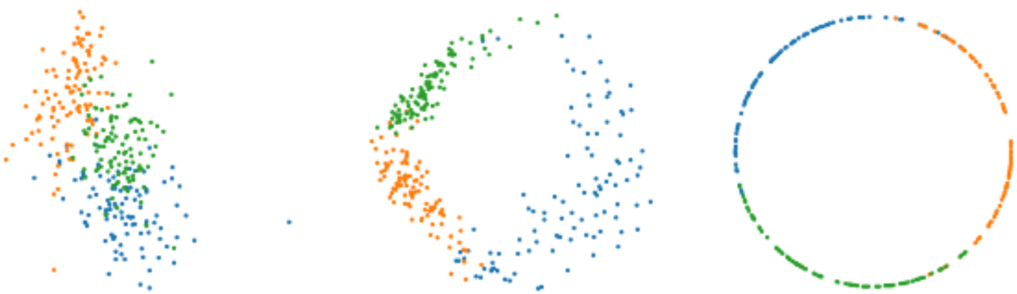

(a) Original (b) Autoencoder (c) $\mathcal{N}$-VAE (d) $\mathcal{N}$-VAE, $\beta = 0.1$ (e) $\mathcal{S}$-VAE

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In high-dim, Gaussians concentrate on a hypersphere $\longrightarrow$ ℓ_2 norm **fails**.

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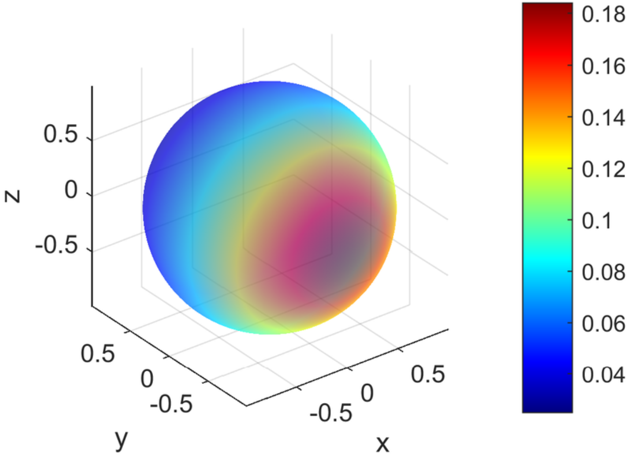
A HYPERSPHERICAL LATENT SPACE

Since in high-dim the Gaussian distribution concentrates on a **hypersphere**, we propose to use **von-Mises-Fisher** distribution defined on the hypersphere $\mathcal{S}^{m-1} \subset \mathbb{R}^m$

$$q(\mathbf{z}|\mu,\kappa) = \mathcal{C}_m(\kappa)\exp(\kappa\mu^\top\mathbf{z})$$

$$\mathcal{C}_m(\kappa) = \frac{\kappa^{m/2-1}}{(2\pi)^{m/2}\mathcal{I}_{m/2-1}(\kappa)}$$



where $||\mu||^2 = 1,\ \mathcal{I}_v$ is the modified Bessel function of the first kind of order *v*.

Davidson, T. R., Falorsi, L., De Cao, N., Kipf, T., & **Tomczak, J. M.** (2018). Hyperspherical Variational Auto-Encoders. *UAI 2018*

HYPERSPHERICAL VAES

The variational dist. is the **von-Mises-Fisher**, and the marginal is **uniform**, *i.e.*, von-Mises-Fisher with $\kappa = 0$. Then the **KL term** is as follows:

$$\mathrm{KL}(\mathrm{vMF}(\mu, \kappa) || \mathrm{U}(\mathcal{S}^{m-1})) = \kappa \frac{\mathcal{I}_{m/2}}{\mathcal{I}_{m/2-1}(\kappa)} + \log \mathcal{C}_m(\kappa) - \log \left(\frac{2\pi^{m/2}}{\Gamma(m/2)} \right)^{-1}$$

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There exist an efficient **sampling procedure** using Householder transformation (Ulrich, 1984).

HYPERSPHERICAL VAES

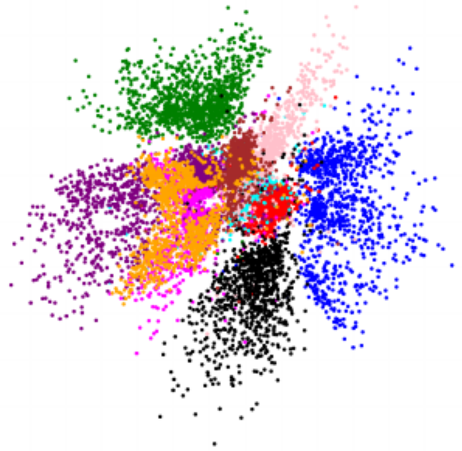
The variational dist. is the **von-Mises-Fisher**, and the marginal is **uniform**, *i.e.*, von-Mises-Fisher with $\kappa = 0$. Then the **KL term** is as follows:

$$\mathrm{KL}(\mathrm{vMF}(\mu,\kappa)||\mathrm{U}(\mathcal{S}^{m-1})) = \kappa \frac{\mathcal{I}_{m/2}}{\mathcal{I}_{m/2-1}(\kappa)} + \log \mathcal{C}_m(\kappa) - \log \left(\frac{2\pi^{m/2}}{\Gamma(m/2)} \right)^{-1}$$

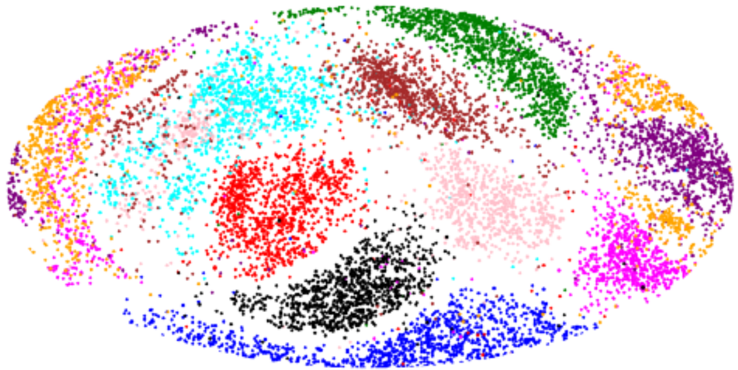
There exist an efficient **sampling procedure** using Householder transformation (Ulrich, 1984).

The reparameterization trick could be achieved by using the **rejection sampling** (Naesseth et al., 2017).

HYPERSPHERICAL VAE: RESULTS ON MNIST



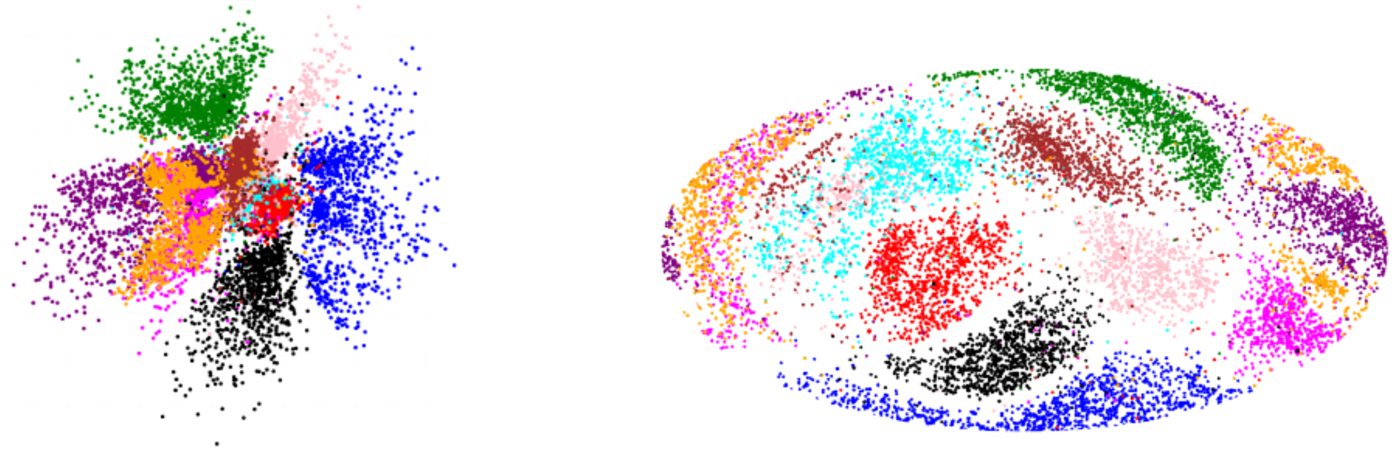
(a) $\mathbb{R}^2$ latent space of the $\mathcal{N}$-VAE.



(b) Hammer projection of $\mathcal{S}^2$ latent space of the $\mathcal{S}$-VAE.

Method	$\mathcal{N}$-VAE				$\mathcal{S}$-VAE			
	LL	$\mathcal{L}[q]$	RE	KL	LL	$\mathcal{L}[q]$	RE	KL
$d=2$	-135.73$\pm$.83	-137.08$\pm$.83	-129.84$\pm$.91	7.24$\pm$.11	**-132.50**$\pm$.73	-133.72$\pm$.85	-126.43$\pm$.91	7.28$\pm$.14
$d=5$	-110.21$\pm$.21	-112.98$\pm$.21	-100.16$\pm$.22	12.82$\pm$.11	**-108.43**$\pm$.09	-111.19$\pm$.08	-97.84$\pm$.13	13.35$\pm$.06
$d=10$	-93.84$\pm$.30	-98.36$\pm$.30	-78.93$\pm$.30	19.44$\pm$.14	**-93.16**$\pm$.31	-97.70$\pm$.32	-77.03$\pm$.39	20.67$\pm$.08
$d=20$	-88.90$\pm$.26	-94.79$\pm$.19	-71.29$\pm$.45	23.50$\pm$.31	-89.02$\pm$.31	-96.15$\pm$.32	-67.65$\pm$.43	28.50$\pm$.22
$d=40$	**-88.93**$\pm$.30	-94.91$\pm$.18	-71.14$\pm$.56	23.77$\pm$.49	-90.87$\pm$.34	-101.26$\pm$.33	-67.75$\pm$.70	33.50$\pm$.45

HYPERSPHERICAL VAE: RESULTS ON MNIST



(a) $\mathbb{R}^2$ latent space of the $\mathcal{N}$-VAE. (b) Hammer projection of $\mathcal{S}^2$ latent space of the $\mathcal{S}$-VAE.

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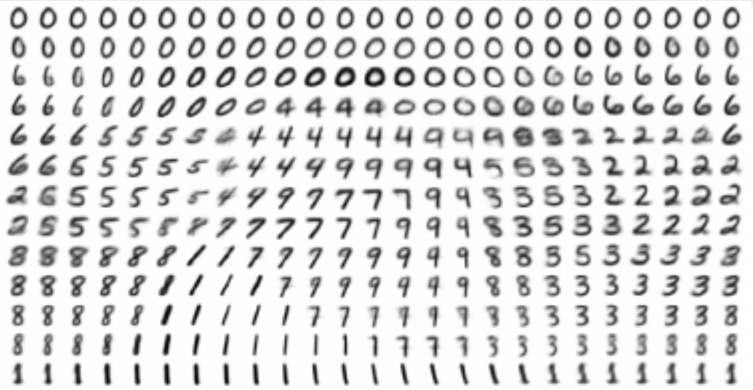
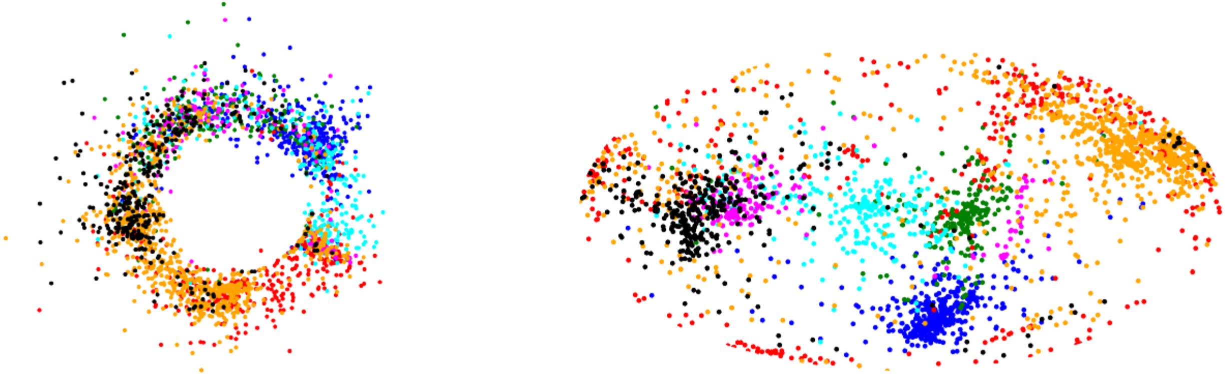
HYPERSPHERICAL VAE: RESULTS ON SEMI-SUPERVISED MNIST

Method		**100**		
dim $\mathbf{z}_1$	*dim* $\mathbf{z}_2$	$\mathcal{N}$+$\mathcal{N}$	$\mathcal{S}$+$\mathcal{S}$	$\mathcal{S}$+$\mathcal{N}$
5	5	90.0±.4	**94.0**±.1	93.8±.1
	10	90.7±.3	94.1±.1	**94.8**±.2
	50	90.7±.1	92.7±.2	**93.0**±.1
10	5	90.7±.3	91.7±.5	**94.0**±.4
	10	92.2±.1	**96.0**±.2	**95.9**±.3
	50	92.9±.4	95.1±.2	**95.7**±.1
50	5	92.0±.2	91.7±.4	**95.8**±.1
	10	93.0±.1	95.8±.1	**97.1**±.1
	50	93.2±.2	94.2±.1	**97.4**±.1



HYPERSPHERICAL GRAPHVAE: LINK PREDICTION



(a) $\mathbb{R}^2$ latent space of the $\mathcal{N}$-VGAE.

(b) Hammer projection of $\mathcal{S}^2$ latent space of the $\mathcal{S}$-VGAE.

Method		**$\mathcal{N}$-VGAE**	**$\mathcal{S}$-VGAE**
Cora	AUC	92.7$\pm$.2	**94.1**$\pm$.1
	AP	93.2$\pm$.4	**94.1**$\pm$.3
Citeseer	AUC	90.3$\pm$.5	**94.7**$\pm$.2
	AP	91.5$\pm$.5	**95.2**$\pm$.2
Pubmed	AUC	**97.1**$\pm$.0	96.0$\pm$.1
	AP	**97.1**$\pm$.0	96.0$\pm$.1

COMPONENTS OF VAES

$$q_\phi(\mathbf{z}|\mathbf{x}) \propto p_\theta(\mathbf{x}|\mathbf{z})\ p_\lambda(\mathbf{z})$$

Normalizing flows
Discrete encoders
Hyperspherical dist.
Hyperbolic-normal dist.
Group theory

Resnets
DRAW
Autoregressive models
Normalizing flows

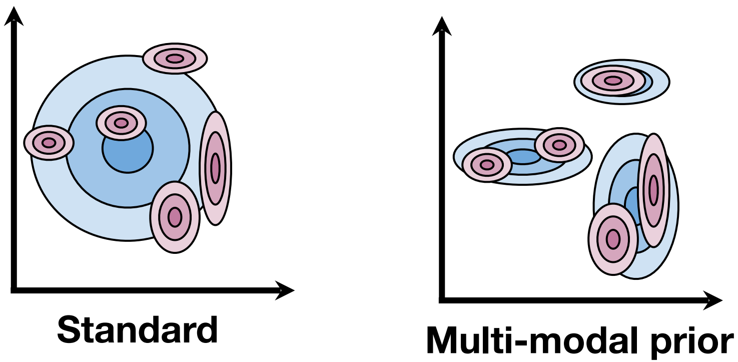
Autoregressive models
Normalizing flows
VampPrior
Implicit prior

$$\mathrm{ELBO}(\mathbf{x};\theta,\phi,\lambda)$$

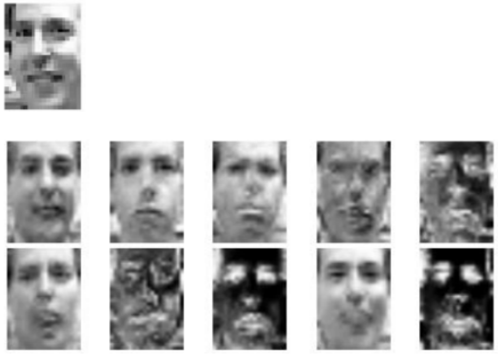
Adversarial learning
MMD
Wasserstein AE

PROBLEMS OF *HOLES* IN VAES

There is a discrepancy between posteriors and the Gaussian prior that results in regions that were never "seen" by the posterior (**holes**). → **multi-modal prior**



Sampling process could produce **unrealistic** samples.



Rezende, D.J. and Viola, F., 2018. Taming VAEs. *arXiv preprint arXiv:1810.00597*.

LOOKING FOR THE OPTIMAL PRIOR

Let's rewrite ELBO over the training data:

$$\mathbb{E}_{\mathbf{x}\sim p_{\mathcal{D}}(\mathbf{x})}\left[\log p_{\vartheta}(\mathbf{x})\right] \geq \mathbb{E}_{p_{\mathcal{D}}(\mathbf{x})q_{\phi}(\mathbf{z}|\mathbf{x})}\left[\log p_{\theta}(\mathbf{x}|\mathbf{z})\right] - \mathbb{I}_{\mathcal{D}}(\mathbf{x};\mathbf{z}) - \mathrm{KL}\left(q_{\phi,\mathcal{D}}(\mathbf{z})\|p_{\lambda}(\mathbf{z})\right)$$

Tomczak, J.M., Welling, M. (2018), VAE with a VampPrior, AISTATS 2018

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Summing over all training data is infeasible and since the sample is finite, it could cause some additional instabilities.

Tomczak, J.M., Welling, M. (2018), VAE with a VampPrior, AISTATS 2018

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$$p_{\lambda}(\mathbf{z}) = \frac{1}{K}\sum_{k=1}^{K} q_{\phi}(\mathbf{z}|\mathbf{u}_k)$$

Tomczak, J.M., Welling, M. (2018), VAE with a VampPrior, AISTATS 2018

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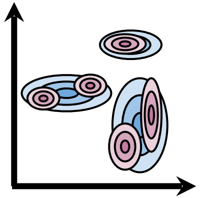

Multi-modal

Tomczak, J.M., Welling, M. (2018), VAE with a VampPrior, AISTATS 2018

VU

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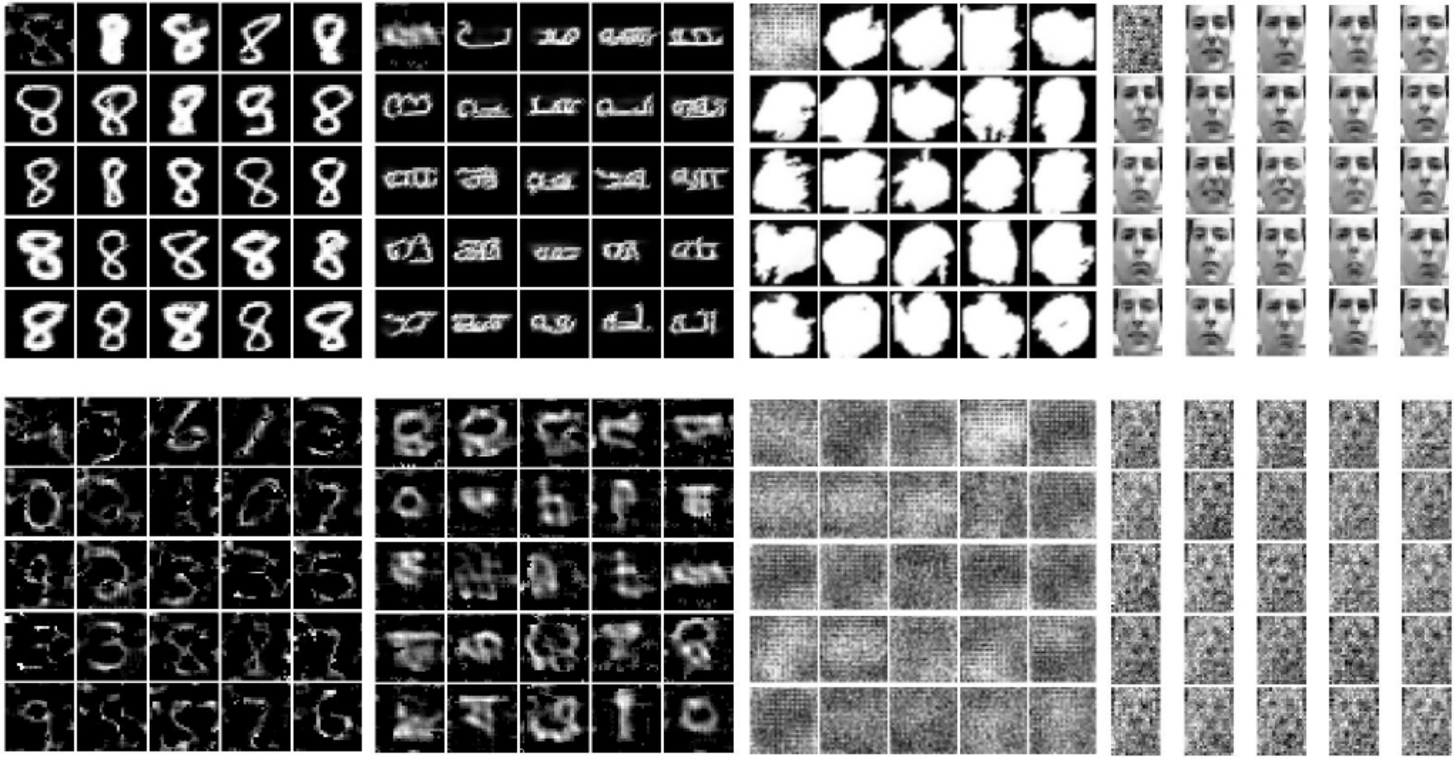
pseudoinputs are trained from scratch by SGD

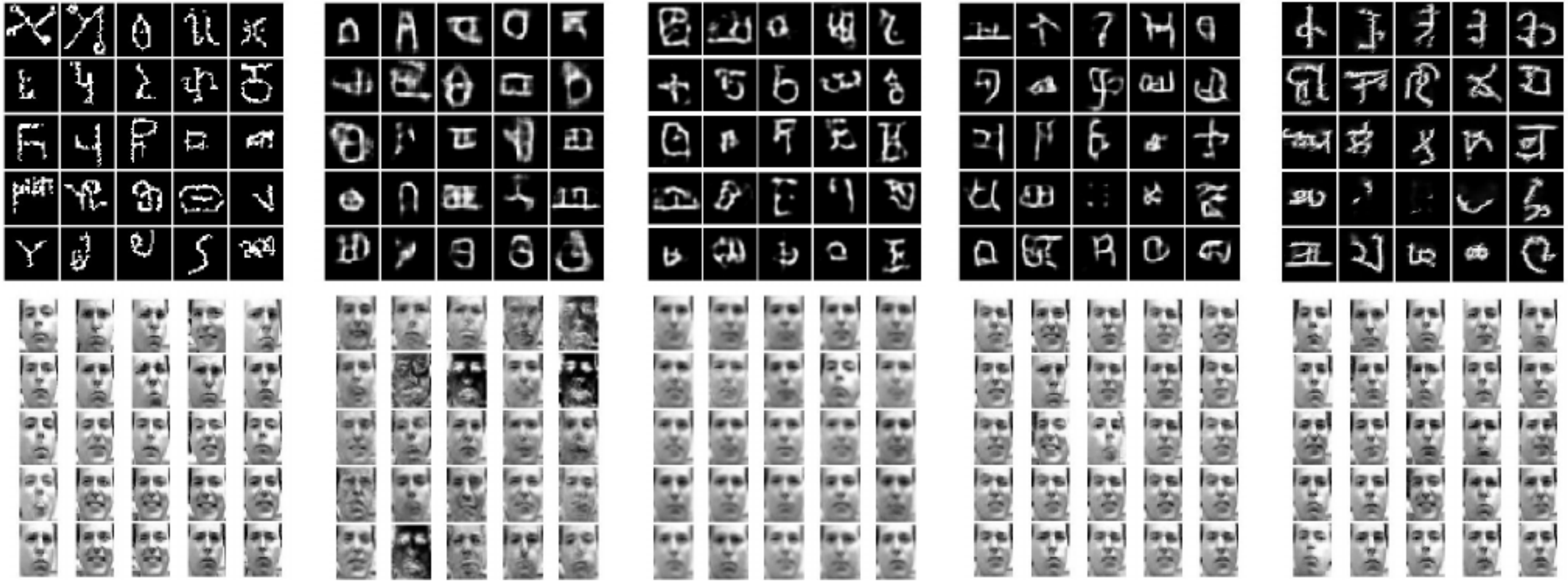
Tomczak, J.M., Welling, M. (2018), VAE with a VampPrior, AISTATS 2018

VAMPPRIOR: EXPERIMENTS (PSEUDOINPUTS)

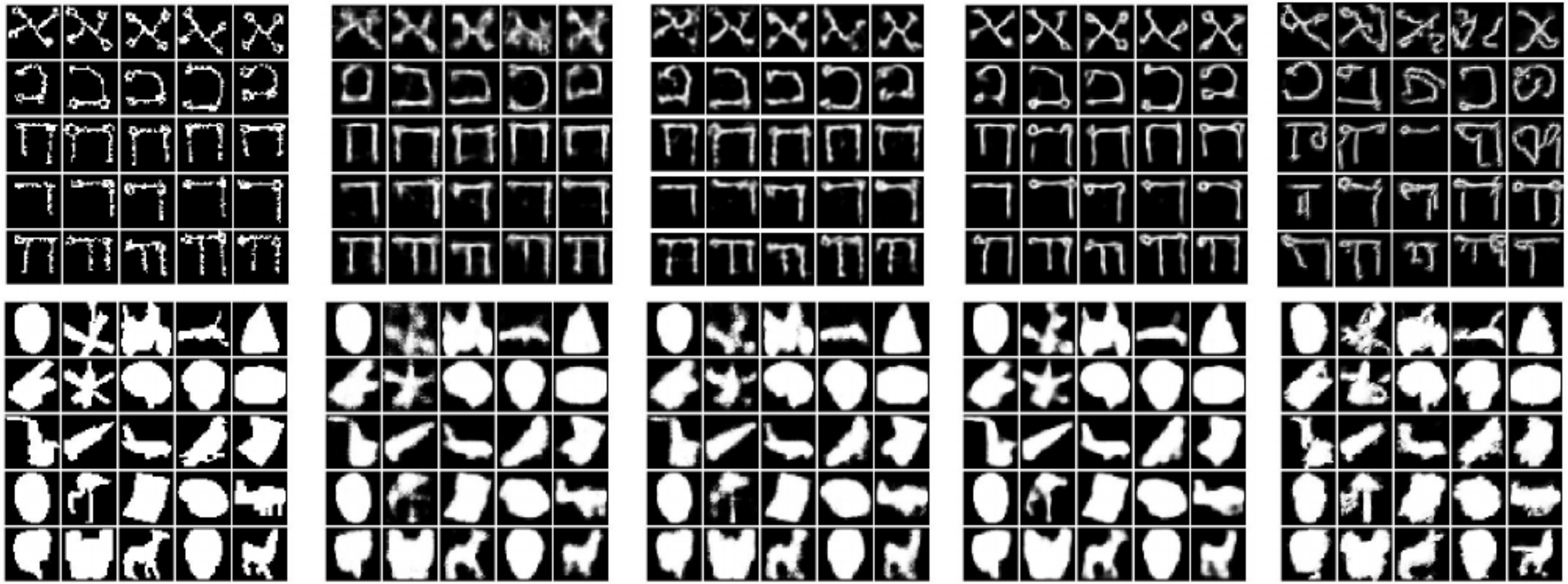


MNIST Omniglot Caltech 101 Silhouettes Frey Faces

VAMPPRIOR: EXPERIMENTS (SAMPLES)


(a) real data (b) VAE (c) HVAE + VampPrior (d) convHVAE + VampPrior (e) PixelHVAE + VampPrior

VAMPPRIOR: EXPERIMENTS (RECONSTRUCTIONS)



(a) real data (b) VAE (c) HVAE + VampPrior (d) convHVAE + VampPrior (e) PixelHVAE + VampPrior

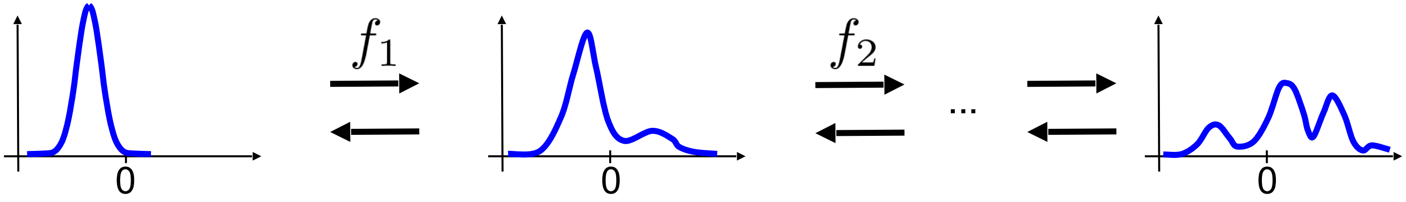
Flow-based models

THE CHANGE OF VARIABLES FORMULA

Let’s recall the change of variables formula with invertible transformations:

$$p(\mathbf{x}) = \pi_0\left(\mathbf{z}_0\right) \prod_{i=1}^{K} \left| \det \frac{\partial f_i(\mathbf{z}_{i-1})}{\partial \mathbf{z}_{i-1}} \right|^{-1}$$

We can think of it as an invertible neural network:



latent space

pixel space

Rippel, O., & Adams, R. P. (2013). High-dimensional probability estimation with deep density models. arXiv preprint arXiv:1302.5125.

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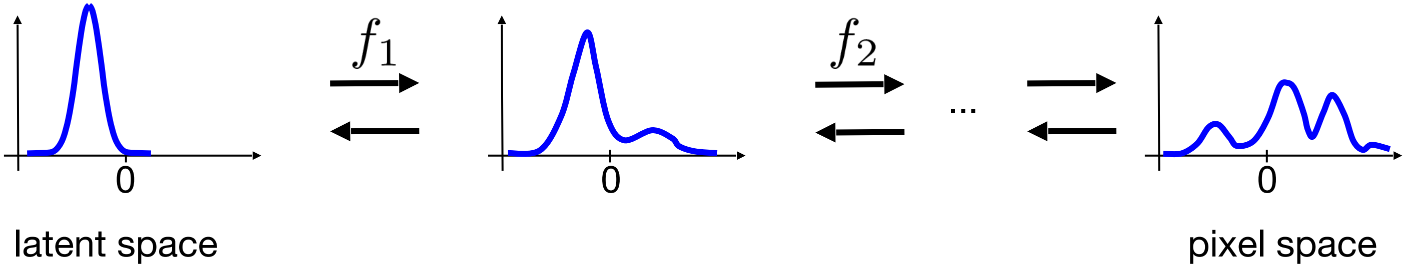

Rippel, O., & Adams, R. P. (2013). High-dimensional probability estimation with deep density models. arXiv preprint arXiv:1302.5125.

REALNVP

Design the invertible transformations as follows:

$$\mathbf{y}_{1:d} = \mathbf{x}_{1:d}$$
$$\mathbf{y}_{d+1:D} = \mathbf{x}_{d+1:D} \odot \exp\left(s\left(\mathbf{x}_{1:d}\right)\right) + t\left(\mathbf{x}_{1:d}\right)$$

Dinh, L., Sohl-Dickstein, J., & Bengio, S. (2016). Density estimation using real nvp. arXiv preprint arXiv:1605.08803.

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Invertible by design:

$$\begin{cases} \mathbf{y}_{1:d} &= \mathbf{x}_{1:d} \\ \mathbf{y}_{d+1:D} &= \mathbf{x}_{d+1:D} \odot \exp\left(s\left(\mathbf{x}_{1:d}\right)\right) + t\left(\mathbf{x}_{1:d}\right) \end{cases} \Leftrightarrow \begin{cases} \mathbf{x}_{1:d} &= \mathbf{y}_{1:d} \\ \mathbf{x}_{d+1:D} &= \left(\mathbf{y}_{d+1:D} - t\left(\mathbf{y}_{1:d}\right)\right) \odot \exp\left(-s\left(\mathbf{y}_{1:d}\right)\right) \end{cases}$$

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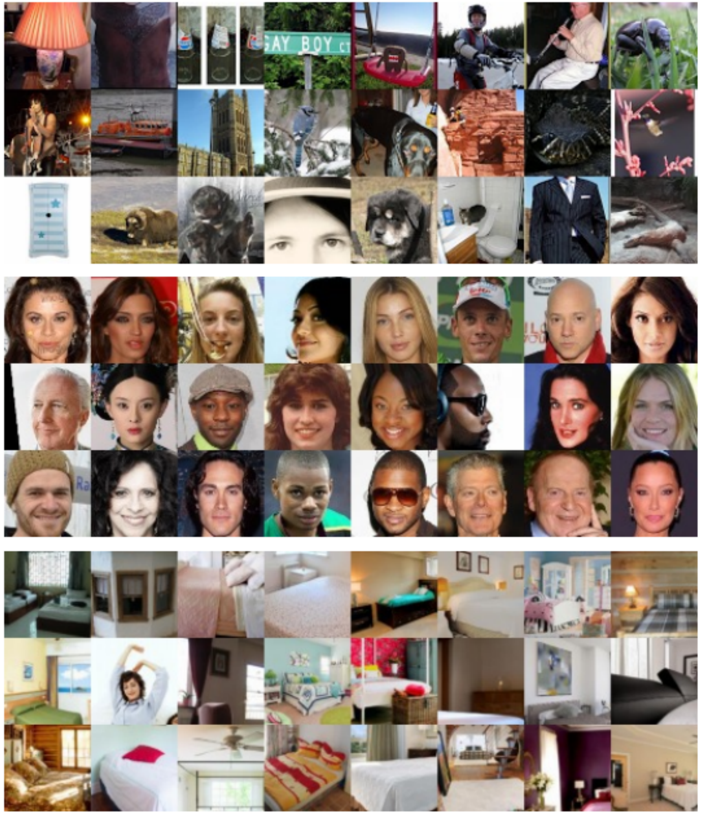
Easy Jacobian:

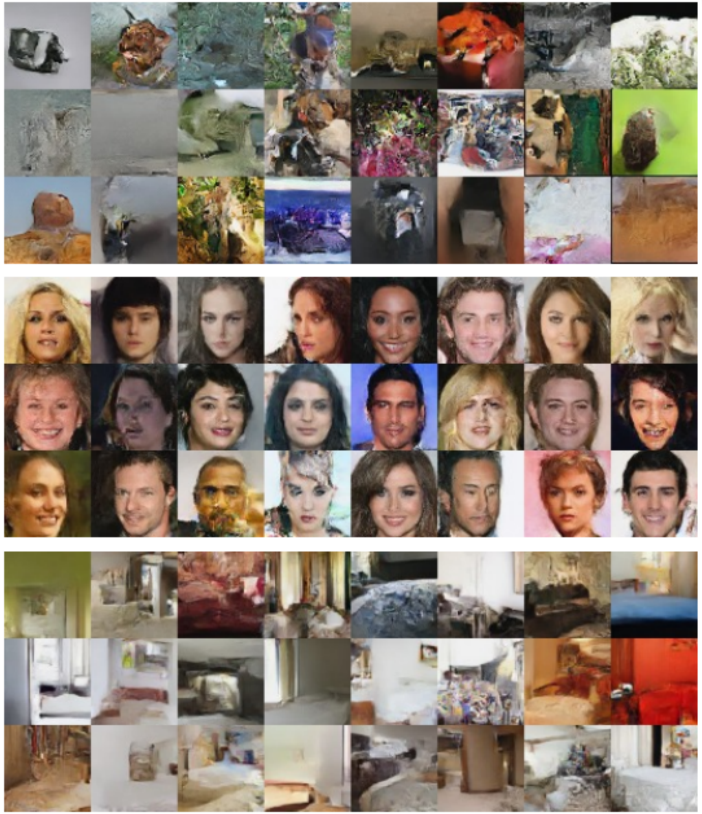
$$\mathbf{J} = \begin{bmatrix} \mathbb{I}_d & \mathbf{0}_{d \times (D-d)} \\ \frac{\partial \mathbf{y}_{d+1:D}}{\partial \mathbf{x}_{1:d}} & \operatorname{diag}\left(\exp\left(s\left(\mathbf{x}_{1:d}\right)\right)\right) \end{bmatrix} \qquad \det(\mathbf{J}) = \prod_{j=1}^{D-d} \exp\left(s\left(\mathbf{x}_{1:d}\right)\right)_j = \exp\left(\sum_{j=1}^{D-d} s\left(\mathbf{x}_{1:d}\right)_j\right)$$

Dinh, L., Sohl-Dickstein, J., & Bengio, S. (2016). Density estimation using real nvp. arXiv preprint arXiv:1605.08803.

RESULTS

RESULTS

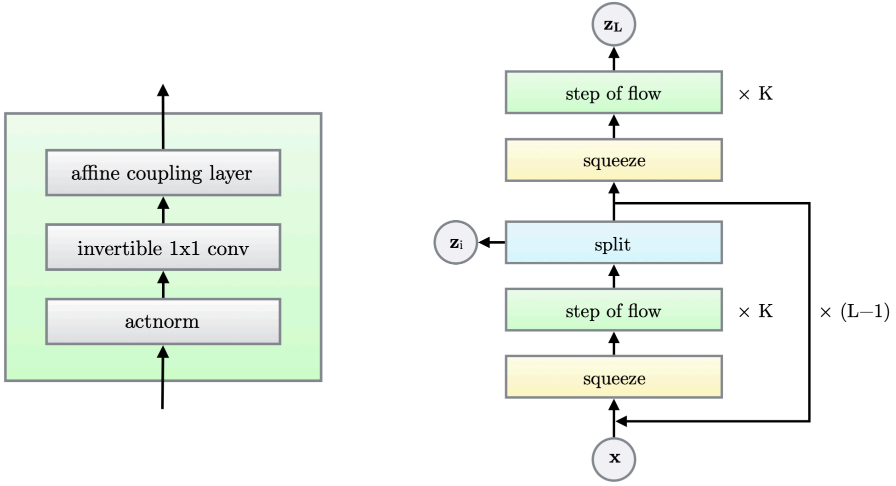




GLOW: REALNVP WITH 1X1 CONVOLUTIONS

A model contains ~1000 convolutions.

A new component: 1x1 convolution instead of a permutation matrix.

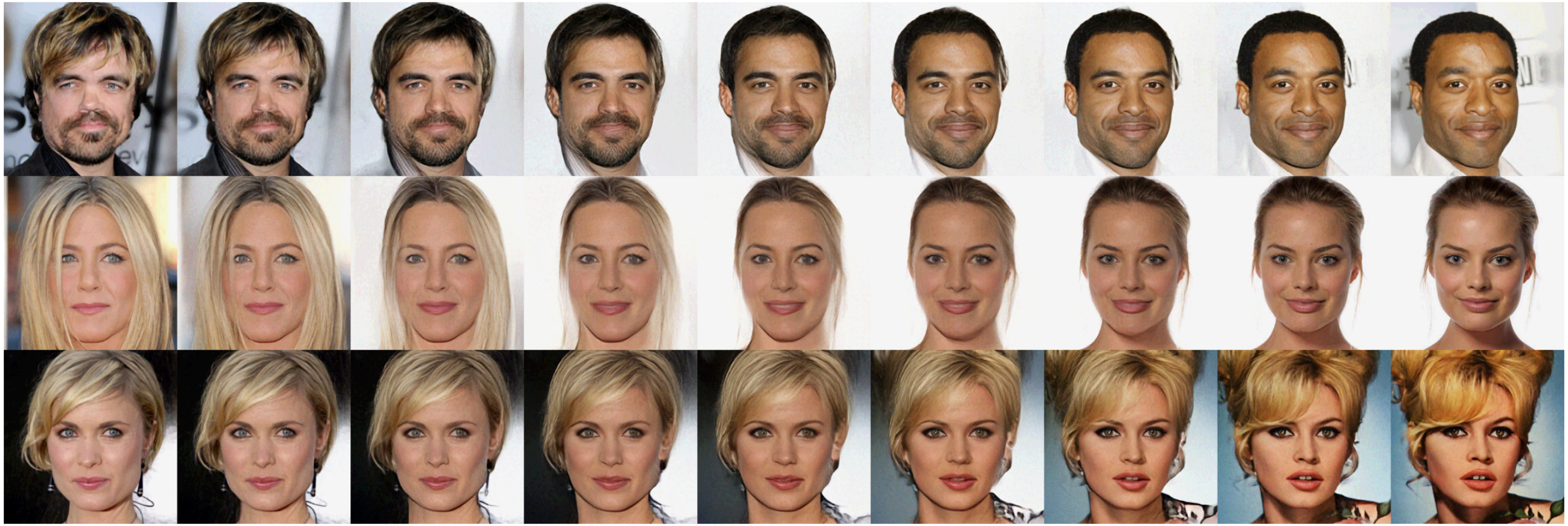


(a) One step of our flow. (b) Multi-scale architecture (Dinh et al., 2016).

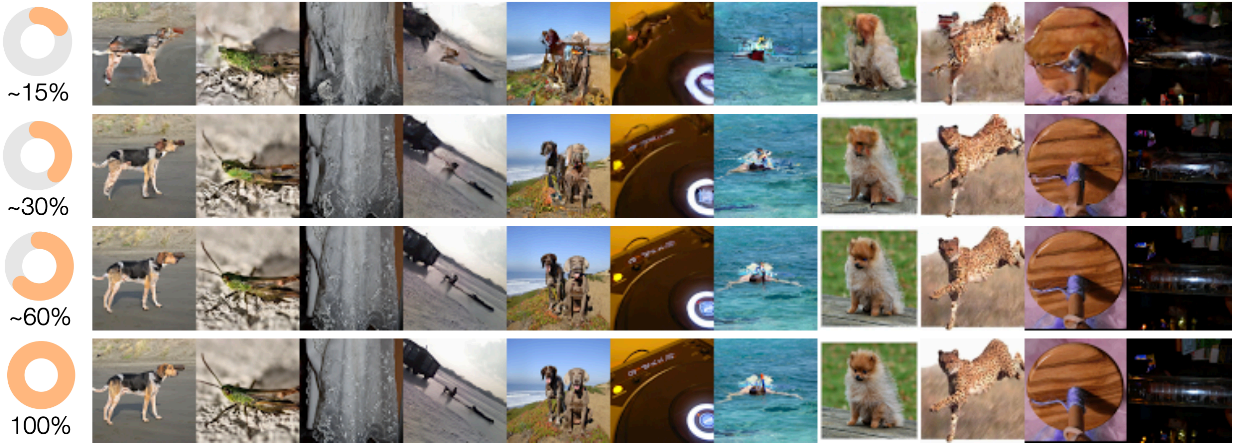
Kingma, D. P., & Dhariwal, P. (2018). Glow: Generative flow with invertible 1x1 convolutions. *NeurIPS 2018*

GLOW: SAMPLES

GLOW: LATENT INTERPOLATION



INTEGER DISCRETE FLOW: NO NEED TO CALCULATE JACOBIAN!



Hoogeboom, E., Peters, J. W., Berg, R. V. D., & Welling, M. (2019). Integer Discrete Flows and Lossless Compression. *NeurIPS 2019*

Future directions

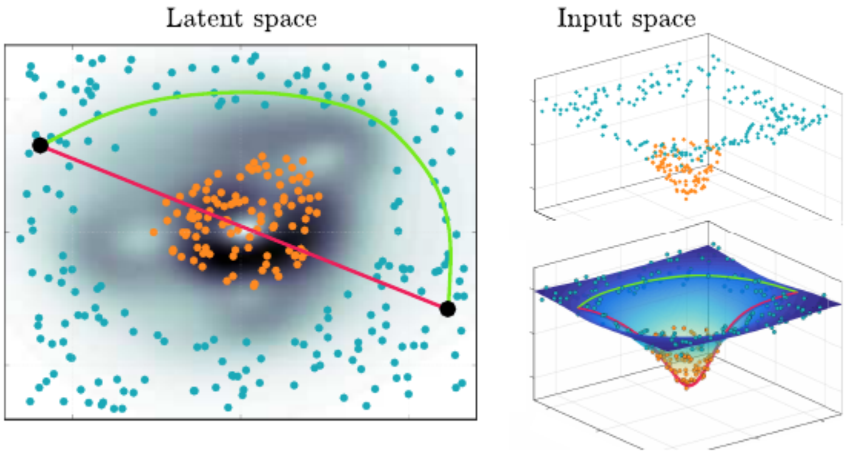
BLURRINESS AND SAMPLING IN VAES

How to avoid sampling from **holes**?

Should we follow **geodesics in the latent space**?

How to use **geometry** of the latent space to build better **decoders**?

How to build **temporal decoders**?



COMPRESSION AND VAES

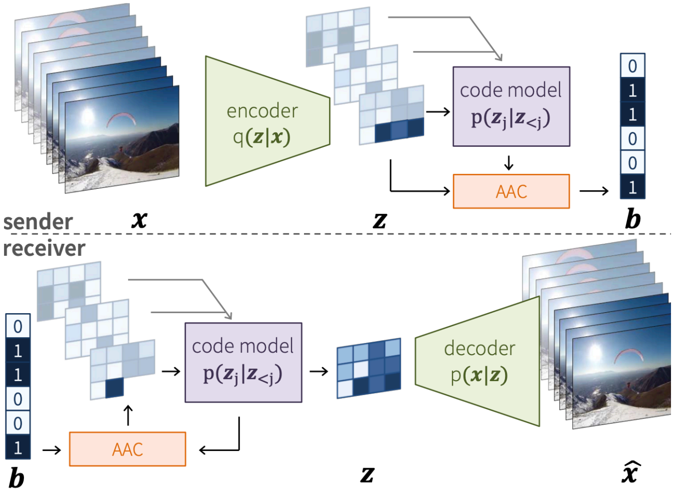
Taking a **deterministic & discrete encoder** allows to simplify the objective.

$$
\begin{aligned}
\mathrm{RE}(x|z) - \mathrm{H}[q(z|x)] - \mathrm{CE}[q(z)||p(z)] \\
= \mathrm{RE}(x|z) - \mathrm{CE}[q(z)||p(z)]
\end{aligned}
$$

It is important to learn a **powerful prior**. This is challenging!

Is it **easier** to learn a prior with **temporal dependencies**?

Can we alleviate some dependencies by using **hypernets**?



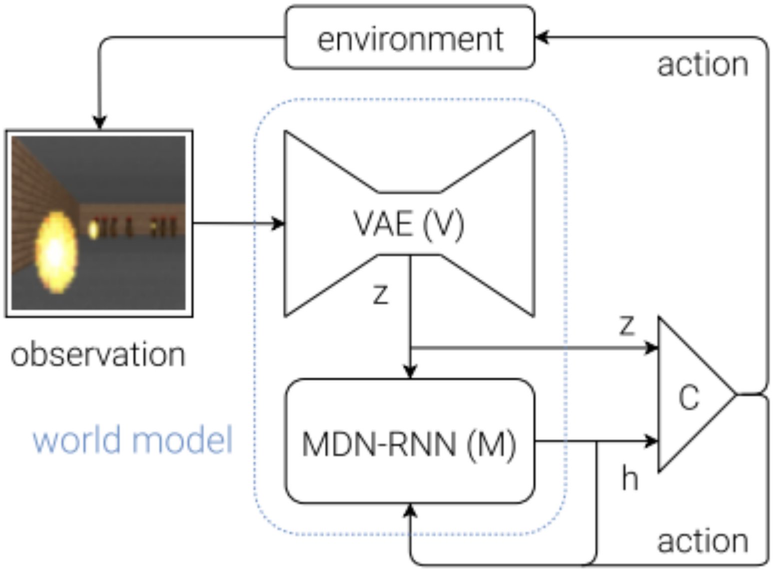
Habibian, A., van Rozendaal, T., Tomczak, J.M., & Cohen, T.S. (2019), Video Compression with Rate-Distortion Autoencoders, ICCV 2019

ACTIVE LEARNING/RL AND VAES

Using **latent representation** to navigate and/or quantify uncertainty.

Formulating **policies** in the latent space entirely.

Do we need a better notion of **sequential dependencies**?



Ha, D., & Schmidhuber, J. (2018). World models. *arXiv preprint arXiv:1803.10122*.

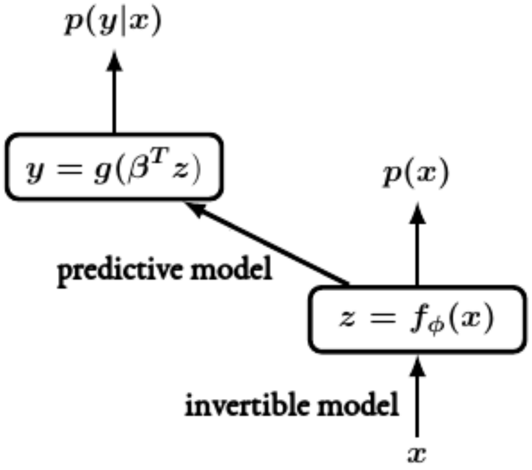
HYBRID AND FLOW-BASED MODELS

We need a **better understanding** of the latent space.

Joining an **invertible model** (flow-based model) with a **predictive model**.

Isn't this model an **overkill**?

How would it work in the **multi-modal learning** scenario?



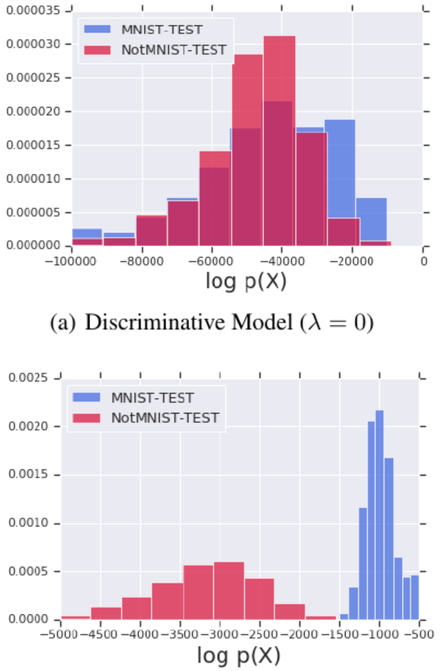
Nalisnick, E., et al. (2019). Hybrid models with deep and invertible features. *arXiv preprint arXiv:1902.02767*.

HYBRID MODELS AND OOD SAMPLE

Going back to first slides, we need a good notion of **p(x)**.

Distinguishing **out-of-distribution (OOD)** samples is very important.

Crucial for **decision making**, **outlier detection**, **policy learning**…



(a) Discriminative Model ($\lambda = 0$)

(b) Hybrid Model

Nalisnick, Eric, et al. "Hybrid models with deep and invertible features." *arXiv preprint arXiv:1902.02767* (2019).

Thank you!

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