



# VAE with a VampPrior

Jakub Tomczak

Tübingen, 22nd of March 2018

# Generative modeling

Modeling in a high-dimensional space is difficult.

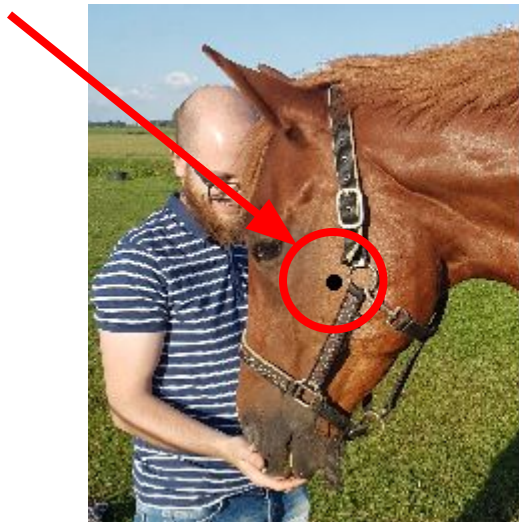
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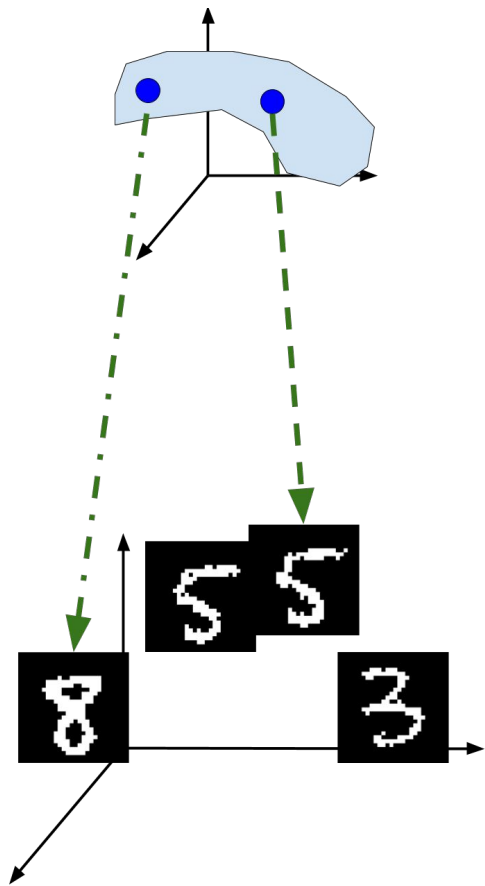
Very inefficient!

A possible **solution**? → **Models with latent variables**

# Latent Variable Models

Latent variable model:

$$p(\mathbf{x}) = \int p_{\theta}(\mathbf{x}|\mathbf{z}) p_{\lambda}(\mathbf{z}) d\mathbf{z}$$





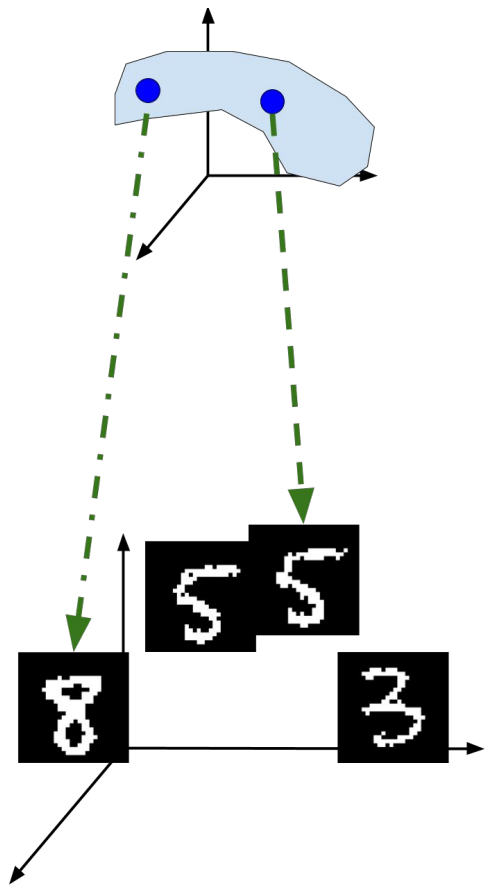
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First sample  $\mathbf{z}$ .

Second sample  $\mathbf{x}$  for given  $\mathbf{z}$ .



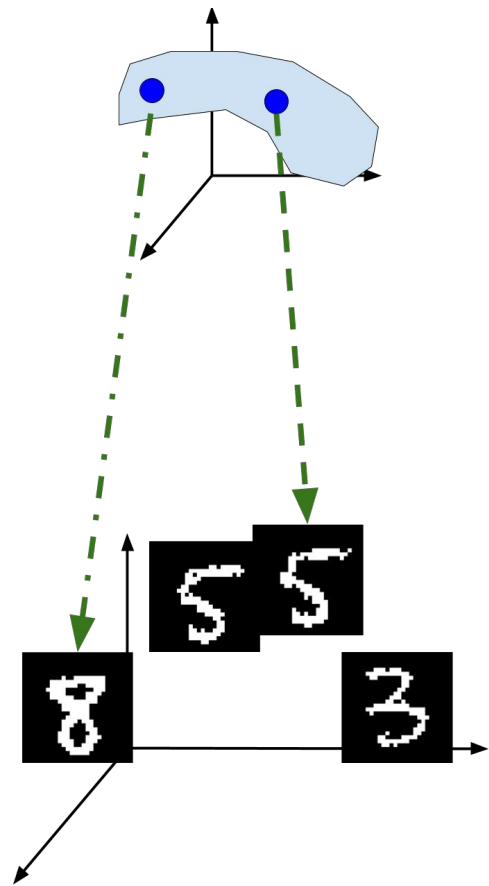
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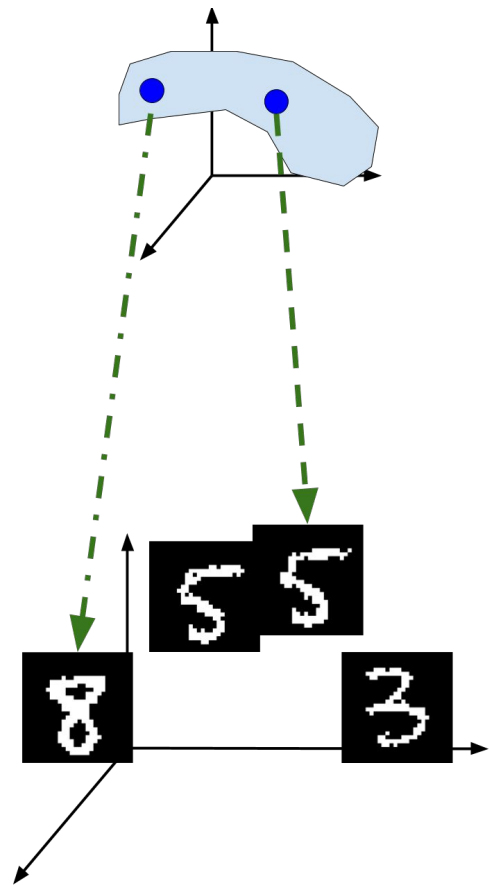
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**How to calculate this integral?**

If  $p_{\theta}(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\mathbf{W}\mathbf{z} + \mathbf{b}, \Psi)$  and  $p_{\lambda}(\mathbf{z}) = \mathcal{N}(\mu_0, \Sigma_0)$ ,  
then we get **Factor Analysis**.

What if we take a **non-linear transformation** of  $\mathbf{z}$ ?  
→ **an infinite mixture of Gaussians**



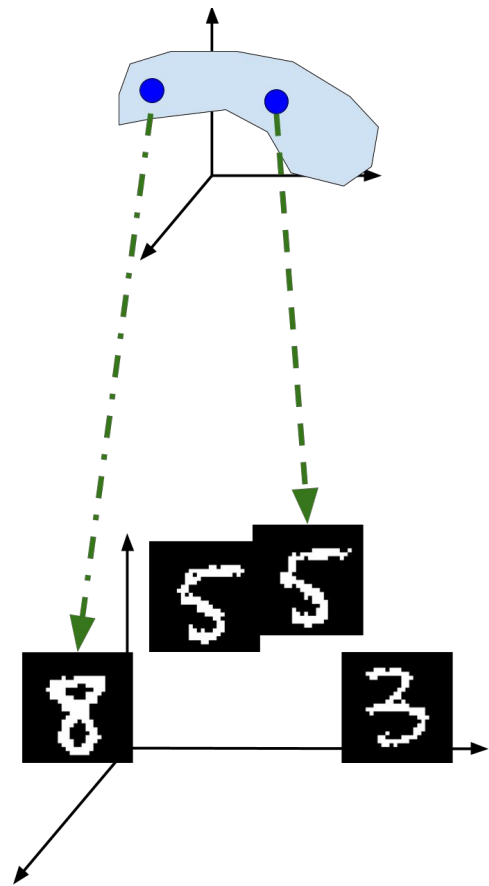
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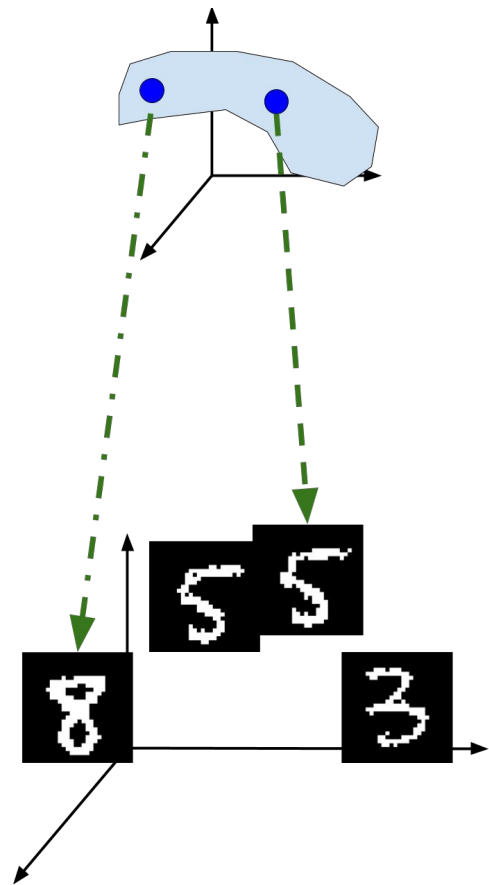
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Convenient but limiting!

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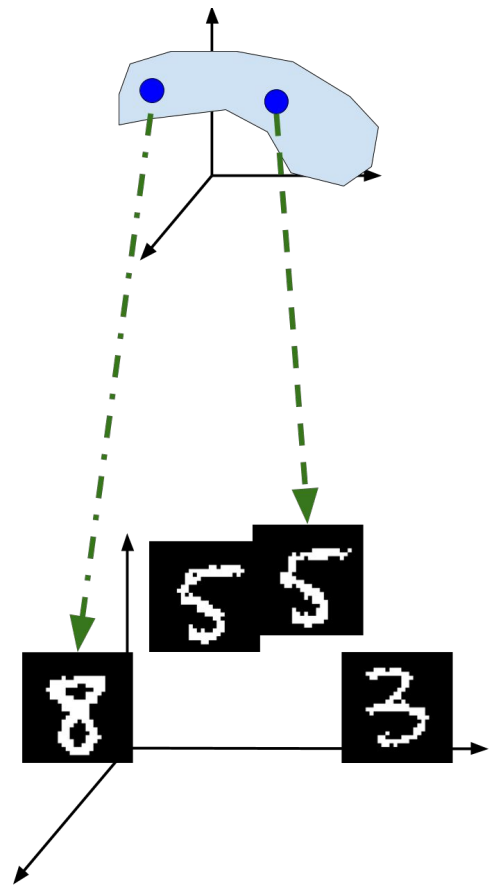
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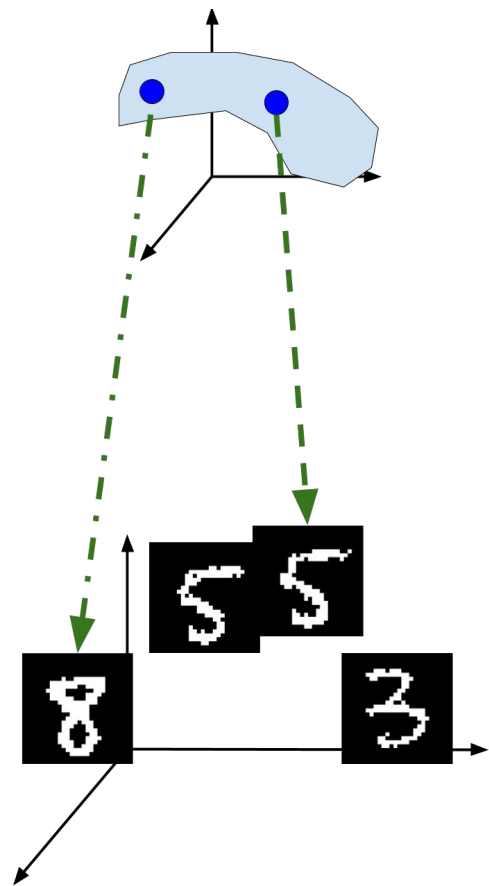
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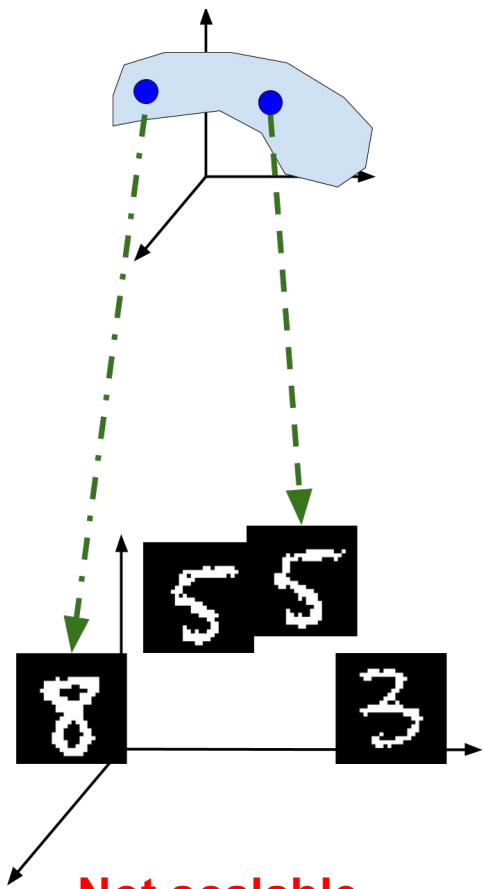
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**Not scalable...**





# Variational inference for Latent Variable Models

$$\begin{aligned}\log p(\mathbf{x}) &= \log \int p_{\theta}(\mathbf{x}|\mathbf{z}) p_{\lambda}(\mathbf{z}) \, d\mathbf{z} \\ &= \log \int \frac{q_{\phi}(\mathbf{z}|\mathbf{x})}{q_{\phi}(\mathbf{z}|\mathbf{x})} p_{\theta}(\mathbf{x}|\mathbf{z}) p_{\lambda}(\mathbf{z}) \, d\mathbf{z} \\ &\geq \int q_{\phi}(\mathbf{z}|\mathbf{x}) \log \frac{p_{\theta}(\mathbf{x}|\mathbf{z}) p_{\lambda}(\mathbf{z})}{q_{\phi}(\mathbf{z}|\mathbf{x})} \, d\mathbf{z} \\ &= \mathbb{E}_{\mathbf{z} \sim q_{\phi}(\mathbf{z}|\mathbf{x})} [\log p_{\theta}(\mathbf{x}|\mathbf{z})] - \text{KL}[q_{\phi}(\mathbf{z}|\mathbf{x}) || p_{\lambda}(\mathbf{z})]\end{aligned}$$

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Variational posterior

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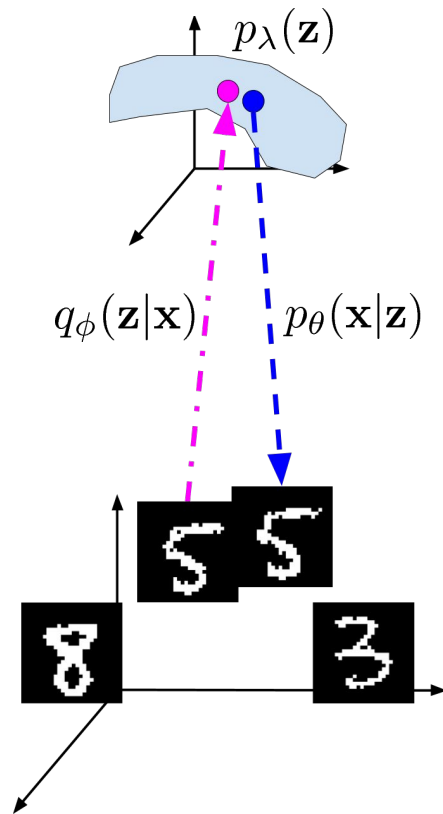
# Variational Auto-Encoder

Let us assume the following distributions:

$$q_{\phi}(\mathbf{z}|\mathbf{x}) = \mathcal{N}(\mathbf{z}|\boldsymbol{\mu}, \text{diag}(\boldsymbol{\sigma}^2)) \quad \text{encoder}$$

$$p_{\theta}(\mathbf{x}|\mathbf{z}) = \text{Bern}(\theta(\mathbf{z})) \quad \text{decoder}$$

$$p_{\lambda}(\mathbf{z}) = \mathcal{N}(\mathbf{0}, \mathbf{I}) \quad \text{prior}$$



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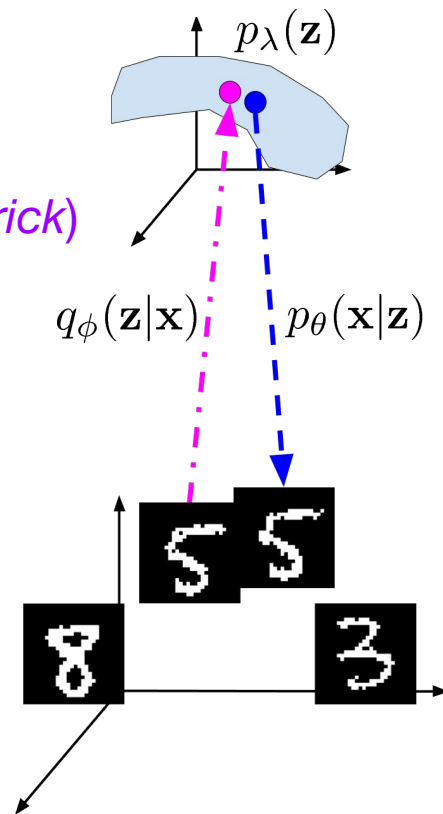
decoder

$$p_{\lambda}(\mathbf{z}) = \mathcal{N}(0, \mathbf{I})$$

prior

sampling is easy  
(reparameterization trick)

$$\mathbf{z} = \boldsymbol{\mu} + \boldsymbol{\sigma} \odot \boldsymbol{\varepsilon}$$



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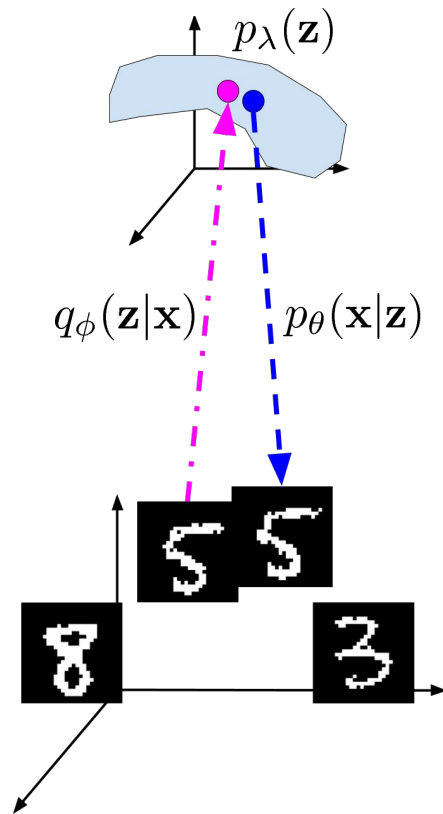
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or any other  
distribution



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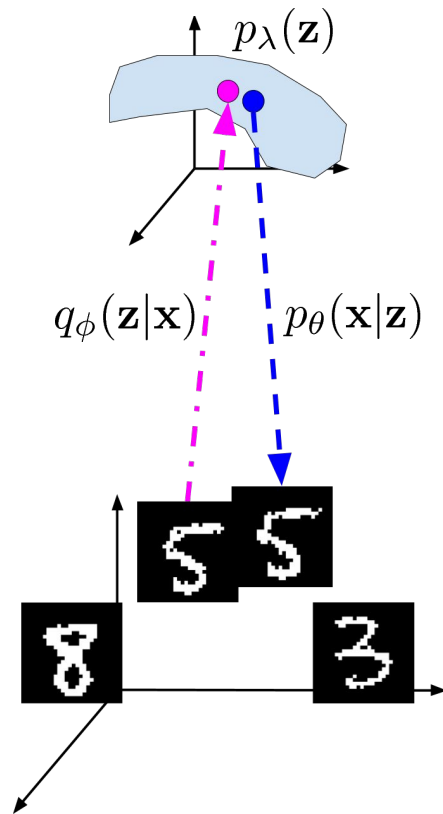
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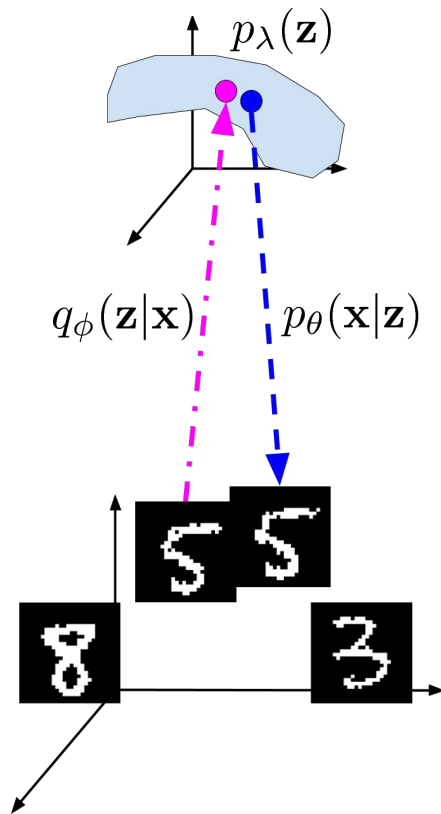
simplest case





# Variational Auto-Encoder

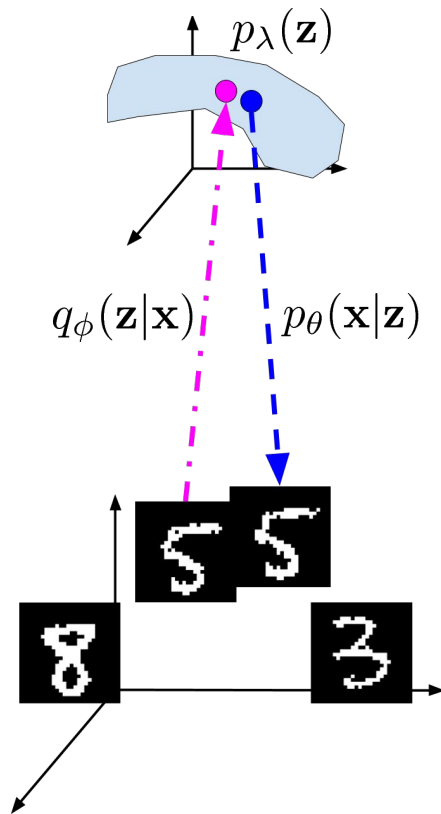
$$q_{\phi}(\mathbf{z}|\mathbf{x}) \propto p_{\theta}(\mathbf{x}|\mathbf{z}) p_{\lambda}(\mathbf{z})$$



# Variational Auto-Encoder

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

Fully-connected  
ConvNets  
PixelCNN

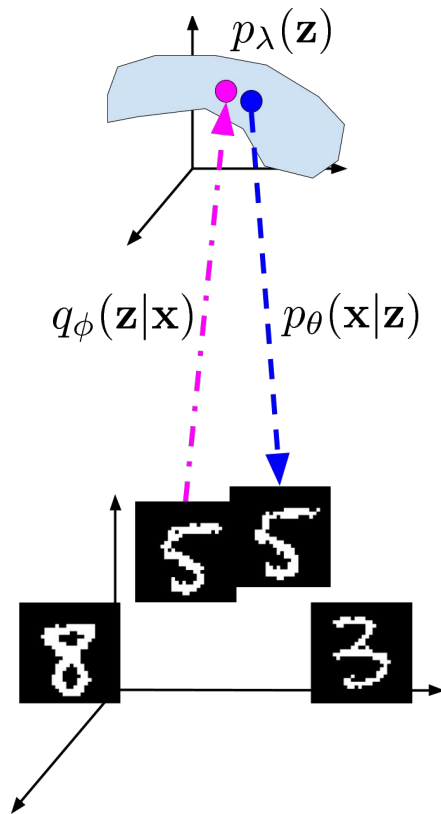


# Variational Auto-Encoder

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

Normalizing flows  
Volume-preserving flows

Fully-connected  
ConvNets  
PixelCNN



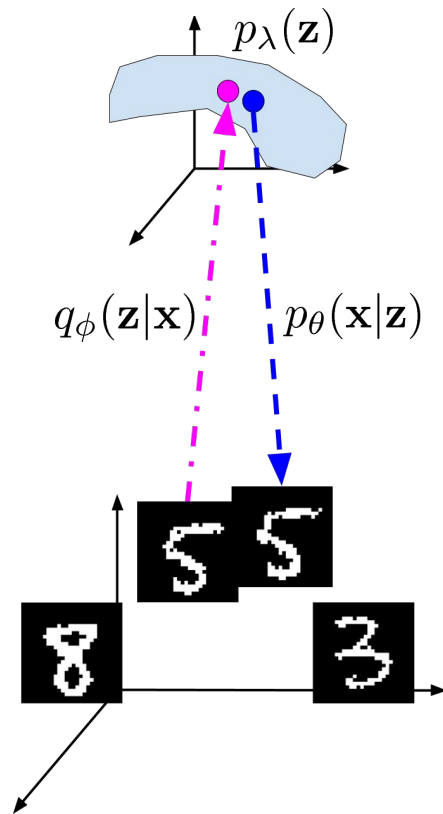
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ConvNets  
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Autoregressive Prior  
Objective Prior  
Stick-Breaking Prior  
VampPrior



# Variational Auto-Encoder

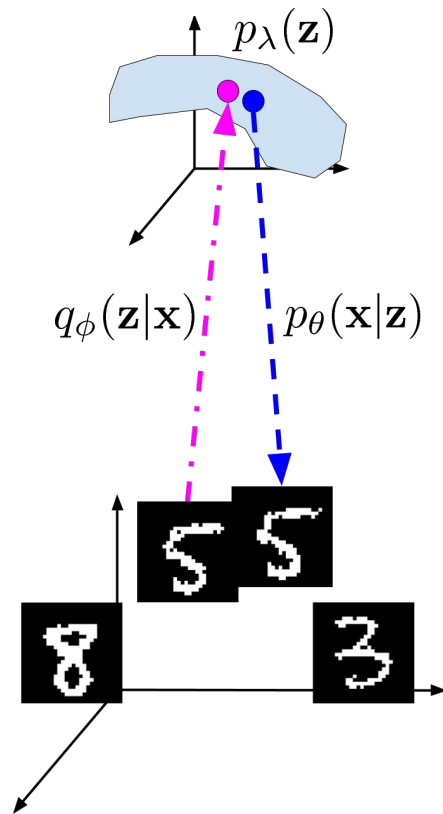
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Normalizing flows  
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Importance Weighted AE  
Renyi Divergence  
Stein Divergence

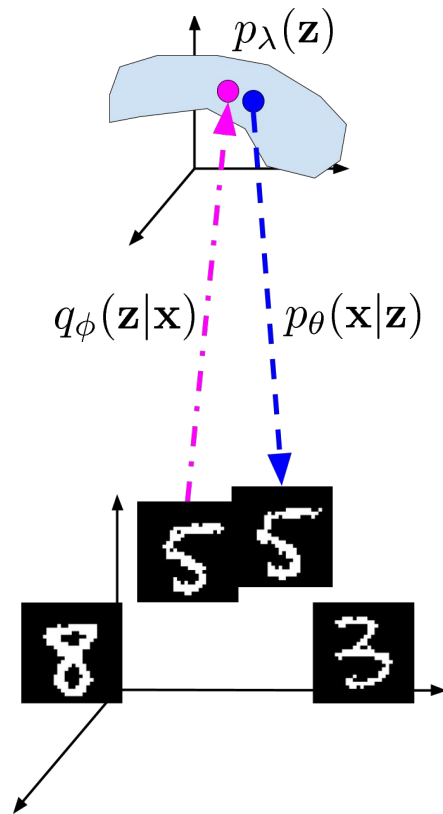
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Autoregressive Prior  
Objective Prior  
Stick-Breaking Prior  
**VampPrior**



# New Prior

- Let's re-write the ELBO:

$$\begin{aligned}\mathbb{E}_{\mathbf{x} \sim q(\mathbf{x})} [\ln p(\mathbf{x})] &\geq \mathbb{E}_{\mathbf{x} \sim q(\mathbf{x})} [\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} [\ln p_\theta(\mathbf{x}|\mathbf{z})]] + \\ &\quad + \mathbb{E}_{\mathbf{x} \sim q(\mathbf{x})} [\mathbb{H}[q_\phi(\mathbf{z}|\mathbf{x})]] + \\ &\quad - \mathbb{E}_{\mathbf{z} \sim q(\mathbf{z})} [-\ln p_\lambda(\mathbf{z})]\end{aligned}$$

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Empirical distribution



# New Prior

- Let's re-write the ELBO:

Reconstruction error

$$\begin{aligned}\mathbb{E}_{\mathbf{x} \sim q(\mathbf{x})} [\ln p(\mathbf{x})] \geq & \underbrace{\mathbb{E}_{\mathbf{x} \sim q(\mathbf{x})} [\mathbb{E}_{q_{\phi}(\mathbf{z}|\mathbf{x})} [\ln p_{\theta}(\mathbf{x}|\mathbf{z})]]}_{\text{Reconstruction error}} + \\ & + \mathbb{E}_{\mathbf{x} \sim q(\mathbf{x})} [\mathbb{H}[q_{\phi}(\mathbf{z}|\mathbf{x})]] + \\ & - \mathbb{E}_{\mathbf{z} \sim q(\mathbf{z})} [-\ln p_{\lambda}(\mathbf{z})]\end{aligned}$$

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**Aggregated posterior**

$$\begin{aligned}q(\mathbf{z}) &= \mathbb{E}_{q(\mathbf{x})} [q_\phi(\mathbf{z}|\mathbf{x})] \\ &= \frac{1}{N} \sum_{n=1}^N q_\phi(\mathbf{z}|\mathbf{x}_n)\end{aligned}$$

# New Prior

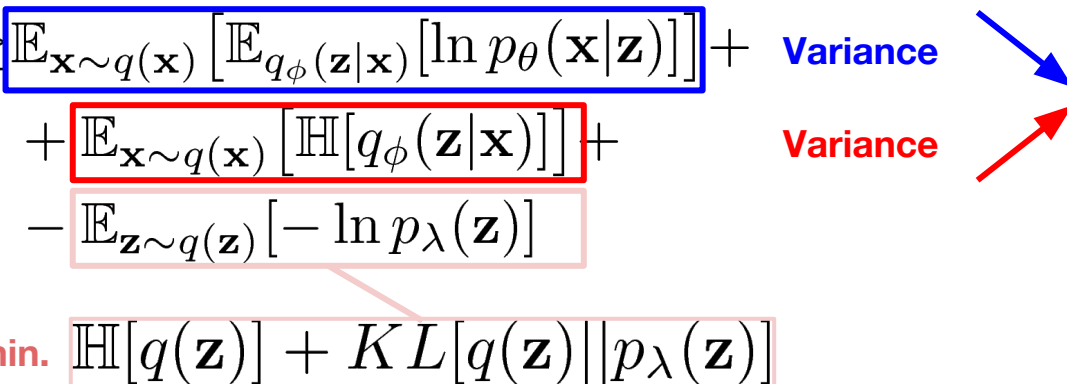
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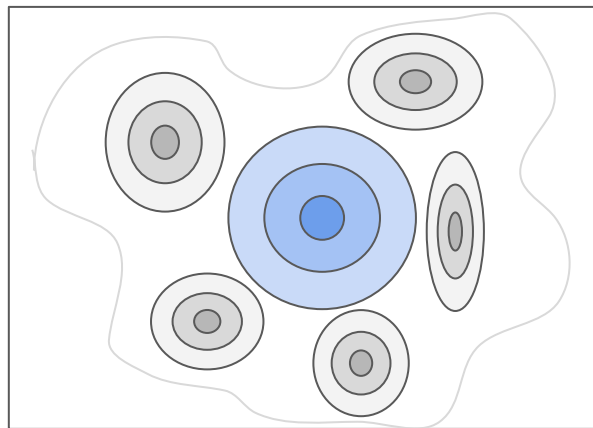
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# New Prior

$$\min. \mathbb{H}[q(\mathbf{z})] + KL[q(\mathbf{z})||p_{\lambda}(\mathbf{z})]$$

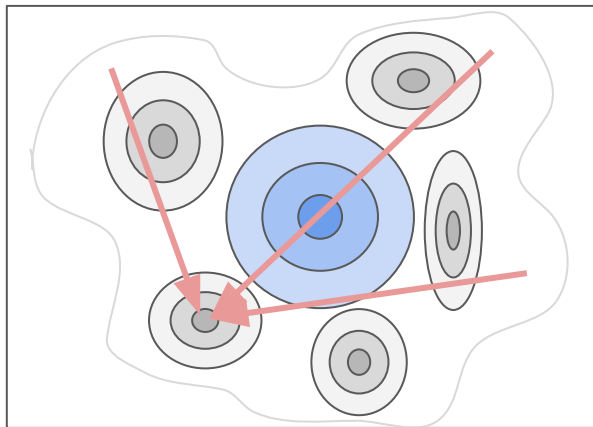


Prior

Aggregated  
posterior

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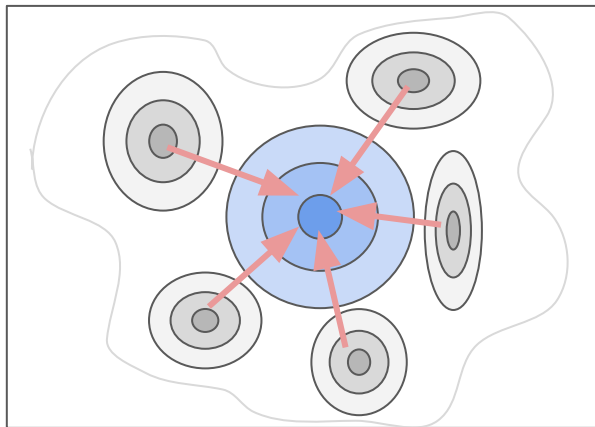
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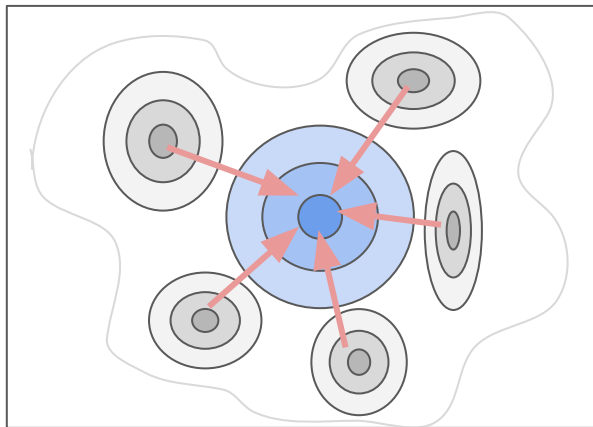
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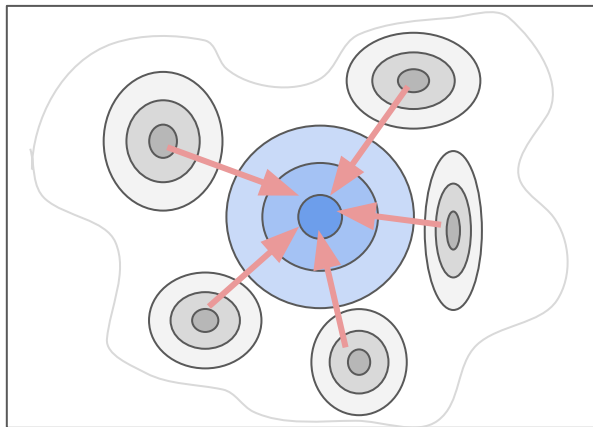
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Standard prior is too strong and overregularizes the encoder.

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Standard prior is too strong and overregularizes the encoder.

What is the “optimal” prior?

# New Prior (**V**ariational **M**ixture of **P**osteriors **P**rior)

- We look for **the optimal prior** using the Lagrange function:

$$\max_{p_\lambda(\mathbf{z})} -\mathbb{E}_{\mathbf{z} \sim q(\mathbf{z})} [-\ln p_\lambda(\mathbf{z})] + \beta \left( \int p_\lambda(\mathbf{z}) d\mathbf{z} - 1 \right)$$

- The solution is simply **the aggregated posterior**.
- We approximate it using  $K$  **pseudo-inputs** instead of  $N$  observations:

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

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# New Prior (Variational Mixture of Posteriors Prior)

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- The solution is simply **the aggregated posterior**.

$$p_\lambda^*(\mathbf{z}) = \frac{1}{N} \sum_{n=1}^N q_\phi(\mathbf{z} | \mathbf{x}_n)$$

- We approximate it using  $K$  pseudo-inputs instead of  $N$  observations:

**infeasible**

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

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**they are trained from scratch**



# New Prior (Variational Mixture of Posteriors Prior)

- Is the VampPrior different than the Mixture of Gaussians?  $p_\lambda(\mathbf{z}) = \frac{1}{K} \sum_{k=1}^K \mathcal{N}(\mu_k, \text{diag}(\sigma_k^2))$
- VampPrior: the prior and the posterior must “cooperate” during training.

VampPrior

$$\frac{1}{K} \sum_{k=1}^K \left\{ \left( \frac{q_\phi(\mathbf{z}_\phi^{(l)} | \mathbf{x}) \frac{\partial}{\partial \phi_i} q_\phi(\mathbf{z}_\phi^{(l)} | \mathbf{u}_k) - q_\phi(\mathbf{z}_\phi^{(l)} | \mathbf{u}_k) \frac{\partial}{\partial \phi_i} q_\phi(\mathbf{z}_\phi^{(l)} | \mathbf{x})}{\frac{1}{K} \sum_{k=1}^K q_\phi(\mathbf{z}_\phi^{(l)} | \mathbf{u}_k) q_\phi(\mathbf{z}_\phi^{(l)} | \mathbf{x})} \right) + \right. \\ \left. + \left( \frac{(q_\phi(\mathbf{z}_\phi^{(l)} | \mathbf{x}) \frac{\partial}{\partial \mathbf{z}_\phi} q_\phi(\mathbf{z}_\phi^{(l)} | \mathbf{u}_k) - q_\phi(\mathbf{z}_\phi^{(l)} | \mathbf{u}_k) \frac{\partial}{\partial \mathbf{z}_\phi} q_\phi(\mathbf{z}_\phi^{(l)} | \mathbf{x})) \frac{\partial}{\partial \phi_i} \mathbf{z}_\phi^{(l)}}{\frac{1}{K} \sum_{k=1}^K q_\phi(\mathbf{z}_\phi^{(l)} | \mathbf{u}_k) q_\phi(\mathbf{z}_\phi^{(l)} | \mathbf{x})} \right) \right\}$$

standard/  
MoG

$$\frac{1}{p_\lambda(\mathbf{z}_\phi^{(l)}) q_\phi(\mathbf{z}_\phi^{(l)} | \mathbf{x})} \left( q_\phi(\mathbf{z}_\phi^{(l)} | \mathbf{x}) \frac{\partial}{\partial \mathbf{z}_\phi} p_\lambda(\mathbf{z}_\phi^{(l)}) - p_\lambda(\mathbf{z}_\phi^{(l)}) \frac{\partial}{\partial \mathbf{z}_\phi} q_\phi(\mathbf{z}_\phi^{(l)} | \mathbf{x}) \right) \frac{\partial}{\partial \phi_i} \mathbf{z}_\phi^{(l)}$$

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MoG

$$\frac{1}{p_\lambda(\mathbf{z}_\phi^{(l)}) q_\phi(\mathbf{z}_\phi^{(l)} | \mathbf{x})} \left( q_\phi(\mathbf{z}_\phi^{(l)} | \mathbf{x}) \frac{\partial}{\partial \mathbf{z}_\phi} p_\lambda(\mathbf{z}_\phi^{(l)}) - p_\lambda(\mathbf{z}_\phi^{(l)}) \frac{\partial}{\partial \mathbf{z}_\phi} q_\phi(\mathbf{z}_\phi^{(l)} | \mathbf{x}) \right) \frac{\partial}{\partial \phi_i} \mathbf{z}_\phi^{(l)}$$

# New Prior (**V**ariational **M**ixture of **P**osteriors **P**rior)

- VampPrior is closely related to the **Empirical Bayes**.
  - We propose a new approach that learns parameters of the prior and combines the variational inference with the EB approach.
- VampPrior is closely related to the **Information Bottleneck**.
  - The aggregated posterior naturally plays the role of the prior.
  - The VampPrior brings the VAE and the IB formulations together.

# Hierarchical VampPrior VAE

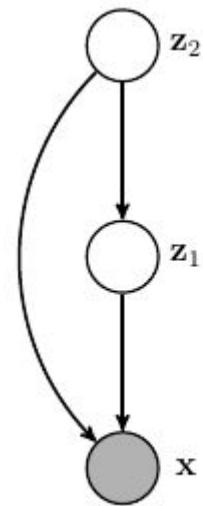
Typical issue in hierarchical VAE: **inactive stochastic units**

$$p(\mathbf{z}_2) = \frac{1}{K} \sum_{k=1}^K q_{\psi}(\mathbf{z}_2 | \mathbf{u}_k),$$

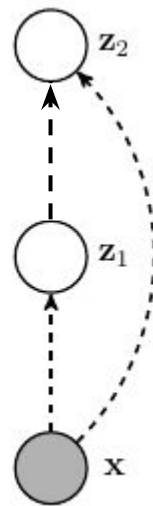
$$p_{\lambda}(\mathbf{z}_1 | \mathbf{z}_2) = \mathcal{N}(\mathbf{z}_1 | \mu_{\lambda}(\mathbf{z}_2), \text{diag}(\sigma_{\lambda}^2(\mathbf{z}_2))),$$

$$q_{\phi}(\mathbf{z}_1 | \mathbf{x}, \mathbf{z}_2) = \mathcal{N}(\mathbf{z}_1 | \mu_{\phi}(\mathbf{x}, \mathbf{z}_2), \text{diag}(\sigma_{\phi}^2(\mathbf{x}, \mathbf{z}_2))),$$

$$q_{\psi}(\mathbf{z}_2 | \mathbf{x}) = \mathcal{N}(\mathbf{z}_2 | \mu_{\psi}(\mathbf{x}), \text{diag}(\sigma_{\psi}^2(\mathbf{x})))$$



generative part



variational part

# Hierarchical VampPrior VAE

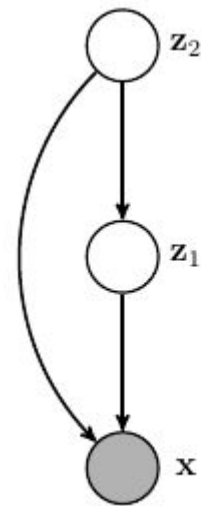
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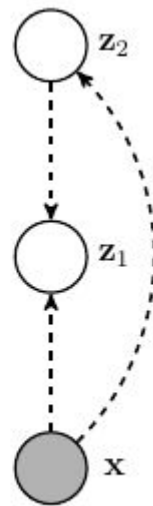
$$p_{\lambda}(\mathbf{z}_1 | \mathbf{z}_2) = \mathcal{N}(\mathbf{z}_1 | \mu_{\lambda}(\mathbf{z}_2), \text{diag}(\sigma_{\lambda}^2(\mathbf{z}_2))),$$

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# Hierarchical VampPrior VAE

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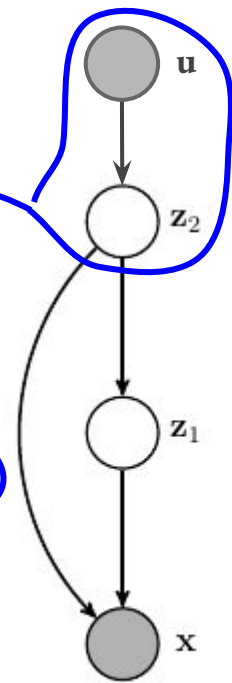
$$p(\mathbf{z}_2) = \frac{1}{K} \sum_{k=1}^K q_{\psi}(\mathbf{z}_2 | \mathbf{u}_k),$$

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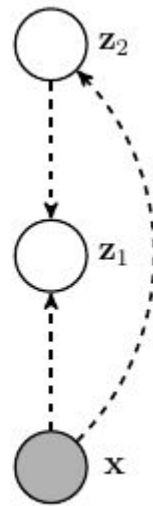
$$q_{\phi}(\mathbf{z}_1 | \mathbf{x}, \mathbf{z}_2) = \mathcal{N}(\mathbf{z}_1 | \mu_{\phi}(\mathbf{x}, \mathbf{z}_2), \text{diag}(\sigma_{\phi}^2(\mathbf{x}, \mathbf{z}_2))),$$

$$q_{\psi}(\mathbf{z}_2 | \mathbf{x}) = \mathcal{N}(\mathbf{z}_2 | \mu_{\psi}(\mathbf{x}), \text{diag}(\sigma_{\psi}^2(\mathbf{x})))$$

**It counteracts inactive stochastic hidden units problem!**



generative part



variational part

# Experiments

DATASET	VAE ( $L = 1$ )		HVAE ( $L = 2$ )		CONVHVAE ( $L = 2$ )		PIXELHVAE ( $L = 2$ )	
	standard	VampPrior	standard	VampPrior	standard	VampPrior	standard	VampPrior
staticMNIST	-88.56	- <b>85.57</b>	-86.05	- <b>83.19</b>	-82.41	- <b>81.09</b>	-80.58	- <b>79.78</b>
dynamicMNIST	-84.50	- <b>82.38</b>	-82.42	- <b>81.24</b>	-80.40	- <b>79.75</b>	-79.70	- <b>78.45</b>
Omniglot	-108.50	- <b>104.75</b>	-103.52	- <b>101.18</b>	-97.65	- <b>97.56</b>	-90.11	- <b>89.76</b>
Caltech 101	-123.43	- <b>114.55</b>	-112.08	- <b>108.28</b>	-106.35	- <b>104.22</b>	- <b>85.51</b>	-86.22
Frey Faces	4.63	<b>4.57</b>	4.61	<b>4.51</b>	4.49	<b>4.45</b>	4.43	<b>4.38</b>
Histopathology	6.07	<b>6.04</b>	5.82	<b>5.75</b>	5.59	<b>5.58</b>	4.84	<b>4.82</b>

# Experiments

Table 2: Test LL for static MNIST.

MODEL	LL
VAE ( $L = 1$ ) + NF [32]	-85.10
VAE ( $L = 2$ ) [6]	-87.86
IWAE ( $L = 2$ ) [6]	-85.32
HVAE ( $L = 2$ ) + SG	-85.89
HVAE ( $L = 2$ ) + MoG	-85.07
HVAE ( $L = 2$ ) + VAMPprior <i>data</i>	-85.71
HVAE ( $L = 2$ ) + VAMPprior	<b>-83.19</b>
AVB + AC ( $L = 1$ ) [28]	-80.20
VLAE [7]	<b>-79.03</b>
VAE + IAF [18]	-79.88
CONVHVAE ( $L = 2$ ) + VAMPprior	-81.09
PIXELHVAE ( $L = 2$ ) + VAMPprior	-79.78

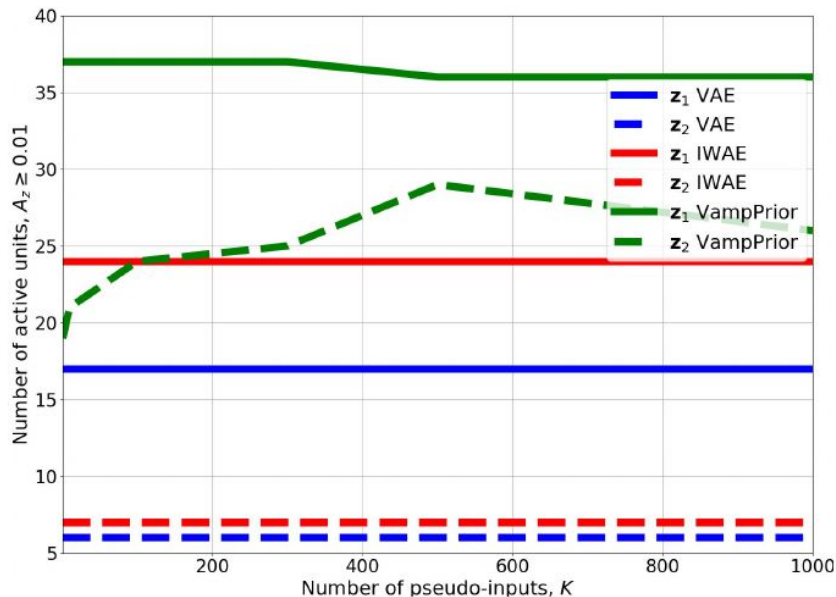


Figure 3: A comparison between two-level VAE and IWAE with the standard normal prior and theirs VampPrior counterpart in terms of number of active units for varying number of pseudo-inputs on static MNIST.



# Experiments

Table 3: Test LL for dynamic MNIST.

MODEL	LL
VAE ( $L = 2$ ) + VGP [40]	-81.32
CAGEM-0 ( $L = 2$ ) [25]	-81.60
LVAE ( $L = 5$ ) [36]	-81.74
HVAE ( $L = 2$ ) + VAMPrior <i>data</i>	-81.71
HVAE ( $L = 2$ ) + VAMPrior	<b>-81.24</b>
VLAE [7]	-78.53
VAE + IAF [18]	-79.10
PIXELVAE [15]	-78.96
CONVHVAE ( $L = 2$ ) + VAMPrior	-79.78
PIXELHVAE ( $L = 2$ ) + VAMPrior	<b>-78.45</b>

Table 4: Test LL for OMNIGLOT.

MODEL	LL
VR-MAX ( $L = 2$ ) [24]	-103.72
IWAE ( $L = 2$ ) [6]	-103.38
LVAE ( $L = 5$ ) [36]	-102.11
HVAE ( $L = 2$ ) + VAMPrior	<b>-101.18</b>
VLAE [7]	-89.83
CONVHVAE ( $L = 2$ ) + VAMPrior	-97.56
PIXELHVAE ( $L = 2$ ) + VAMPrior	<b>-89.76</b>

Table 5: Test LL for Caltech 101 Silhouettes.

MODEL	LL
IWAE ( $L = 1$ ) [24]	-117.21
VR-MAX ( $L = 1$ ) [24]	-117.10
HVAE ( $L = 2$ ) + VAMPrior	<b>-108.28</b>
VLAE [7]	<b>-78.53</b>
CONVHVAE ( $L = 2$ ) + VAMPrior	-104.22
PIXELHVAE ( $L = 2$ ) + VAMPrior	-86.22

# Experiments

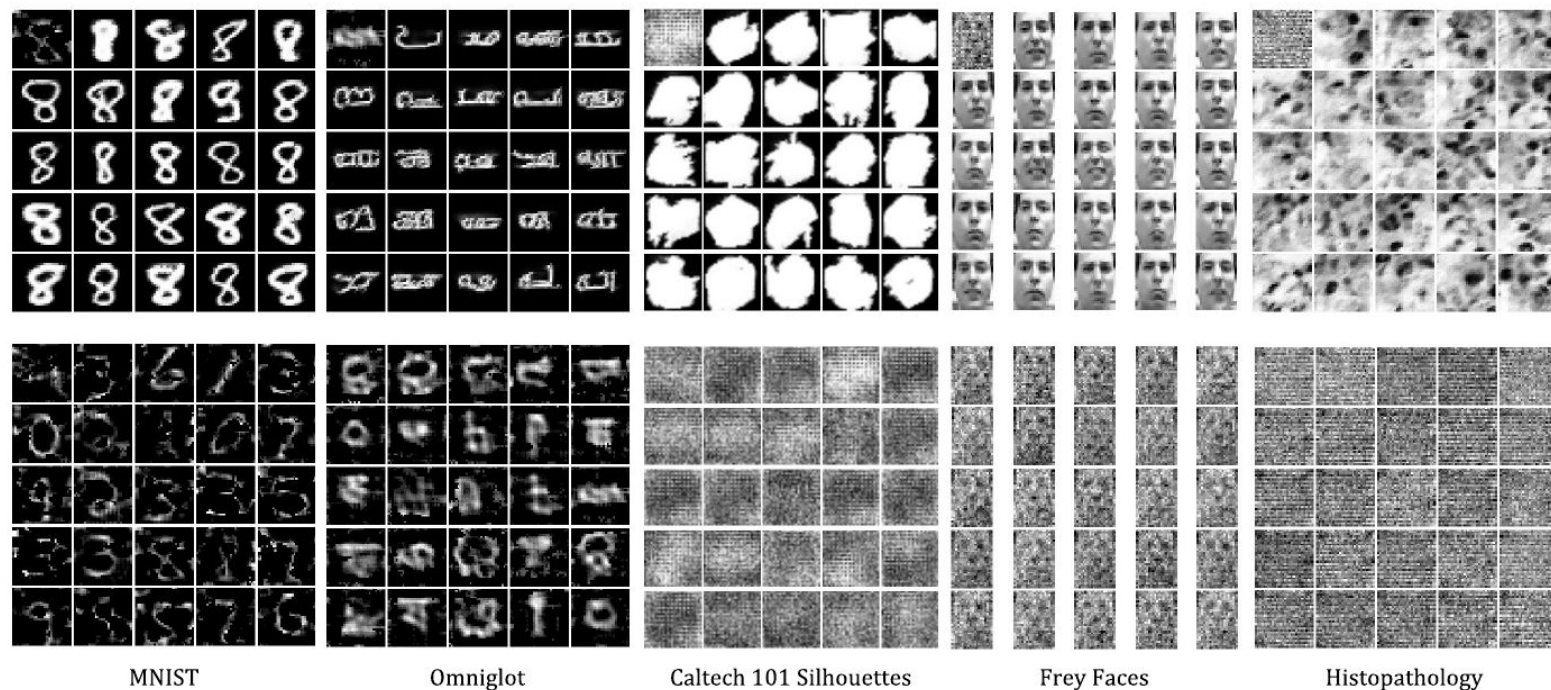


Figure 4: (*top row*) Images generated by PIXELHVAE + VAMPPRIOR for chosen pseudo-input in the left top corner. (*bottom row*) Images represent a subset of trained pseudo-inputs for different datasets.

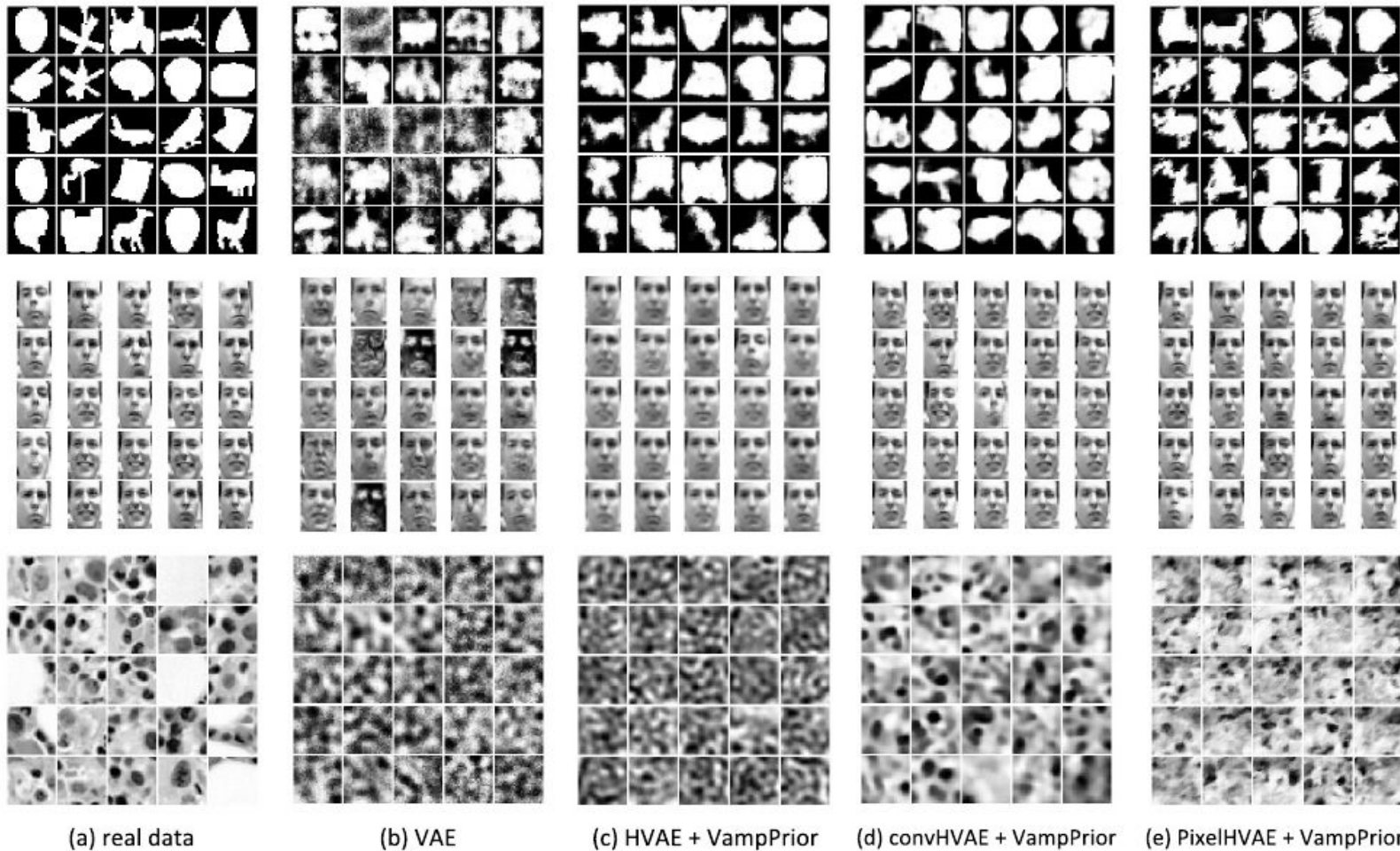


Figure 5: (a) Real images from test sets and images generated by (b) the vanilla VAE, (c) the HVAE ( $L = 2$ ) + VampPrior, (d) the convHVAE ( $L = 2$ ) + VampPrior and (e) the PixelHVAE ( $L = 2$ ) + VampPrior.

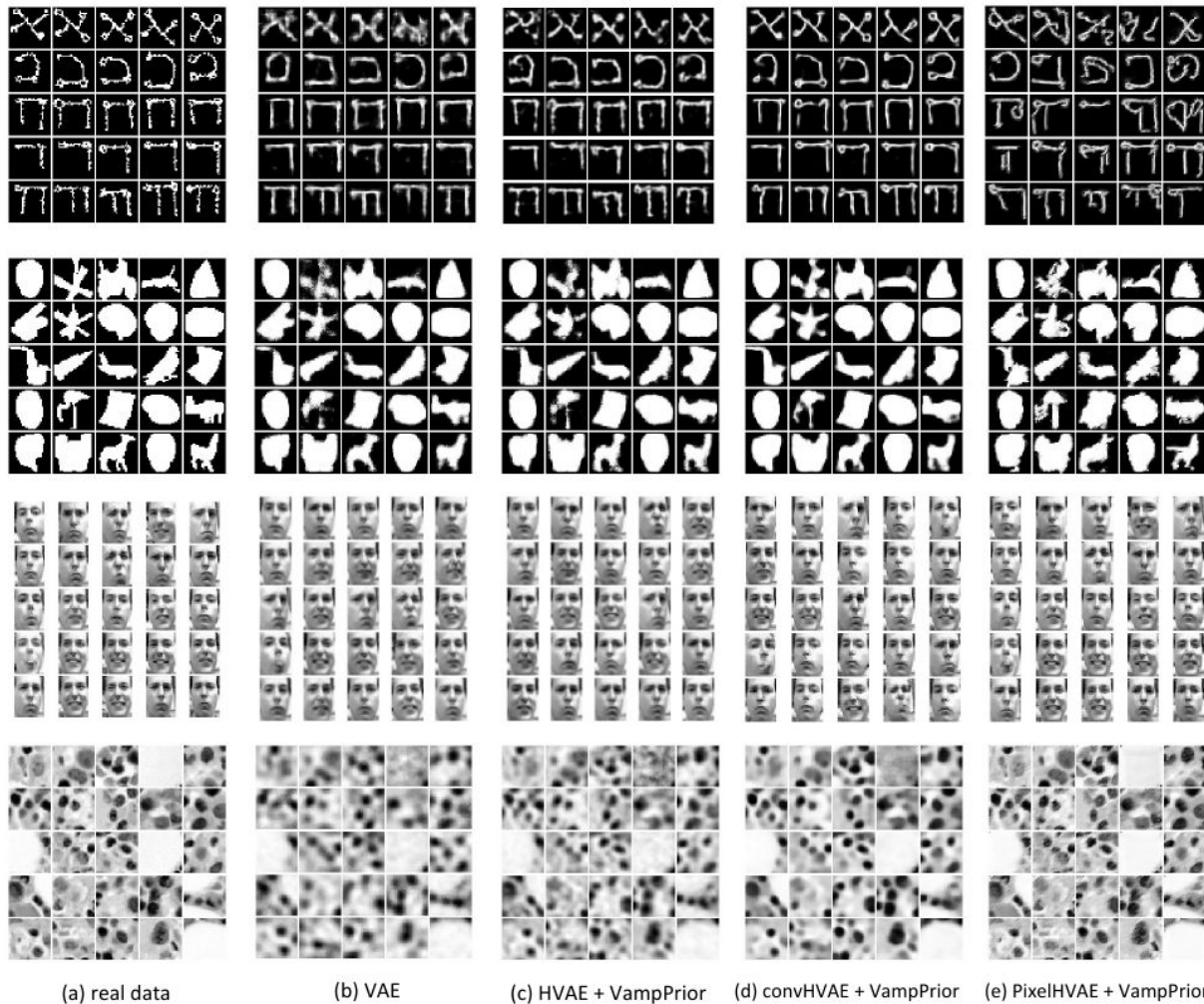


Figure 6: (a) Real images from test sets, (b) reconstructions given by the vanilla VAE, (c) the HVAE ( $L = 2$ ) + VampPrior, (d) the convHVAE ( $L = 2$ ) + VampPrior and (e) the PixelHVAE ( $L = 2$ ) + VampPrior.

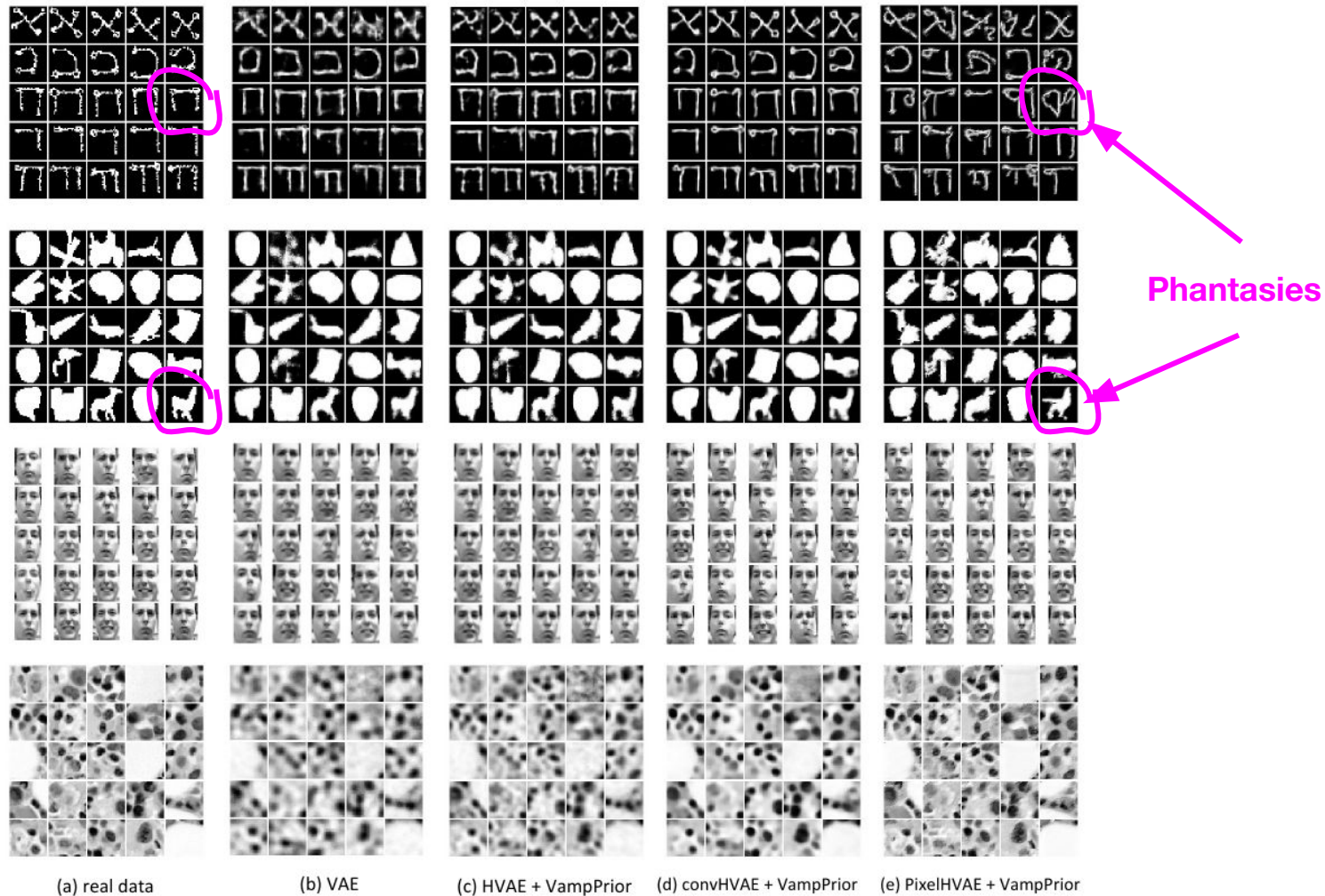


Figure 6: (a) Real images from test sets, (b) reconstructions given by the vanilla VAE, (c) the HVAE ( $L = 2$ ) + VampPrior, (d) the convHVAE ( $L = 2$ ) + VampPrior and (e) the PixelHVAE ( $L = 2$ ) + VampPrior.

# Conclusion



The **prior** in VAE is extremely important.

**VampPrior** = approximated aggregated posterior as the optimal prior

Hierarchical VampPrior VAE  
→ **less** inactive stochastic units.

Multimodal prior → **better** generative process



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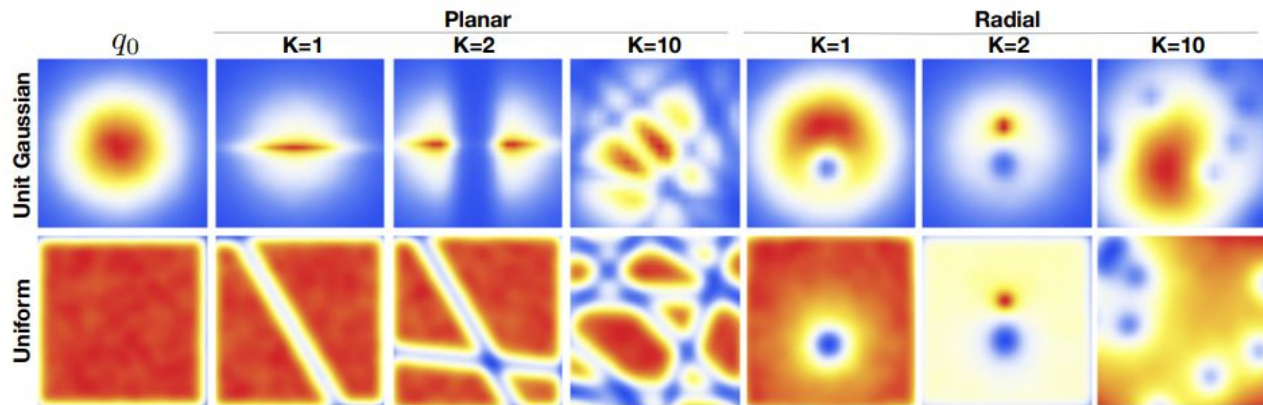
**VampPrior** = approximated aggregated posterior as the **optimal prior**

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# Future directions

VampPrior +  
Normalizing flows



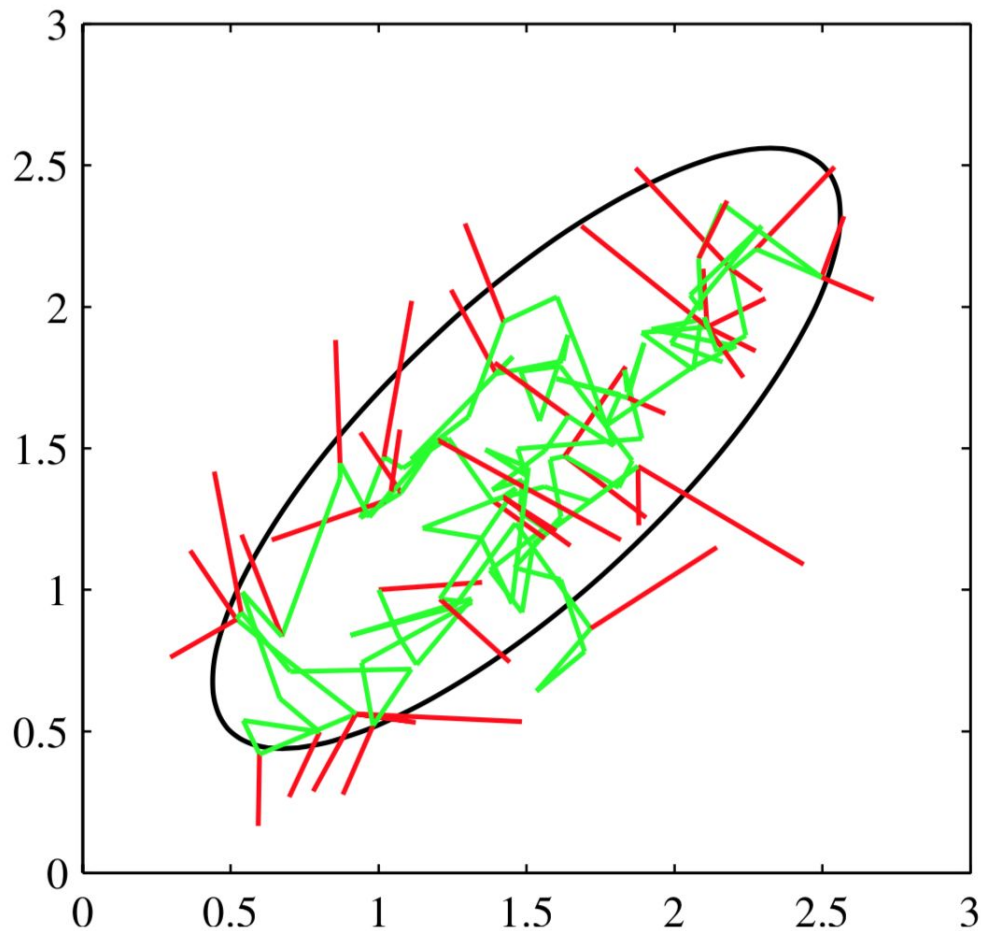


## Future directions

How to (better) learn  
pseudoinputs?

→MCMC?

→Wake-Sleep?



**Webpage:**

<https://jmtomczak.github.io/>

**Code on github:**

<https://github.com/jmtomczak/>

**Contact:**

[jakubmkt@gmail.com](mailto:jakubmkt@gmail.com)