

Generative Modeling

Variational Autoencoders

Laboratory for methods of big data analysis



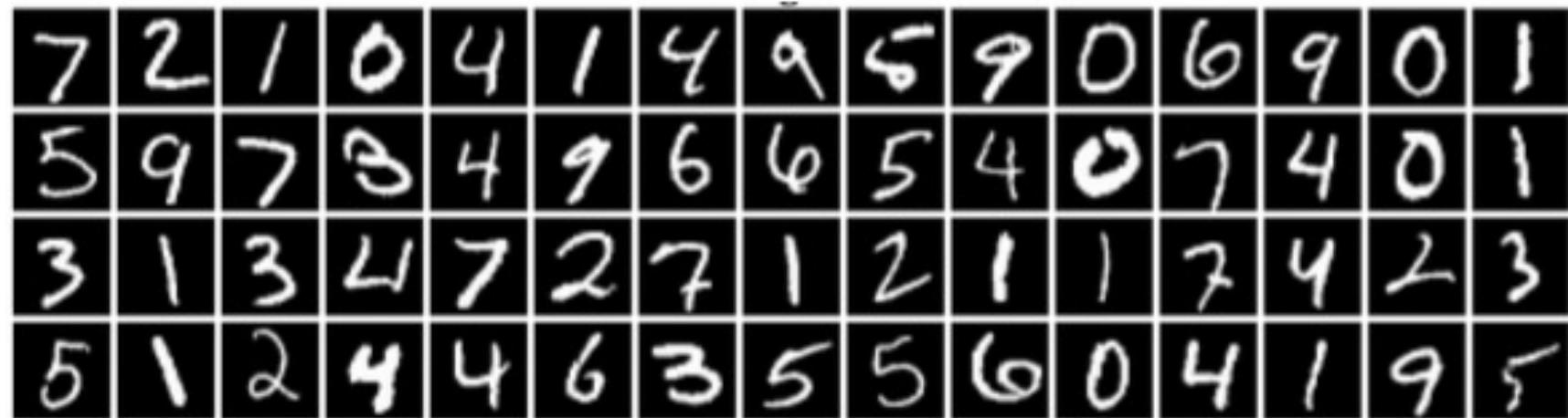
In this Lecture

- ▶ Autoencoders.
- ▶ Gaussian Mixture Models.
- ▶ Variational Autoencoders:
 - Construction.
 - ELBO.
 - Problems.

Idea



Latent variables - MNIST



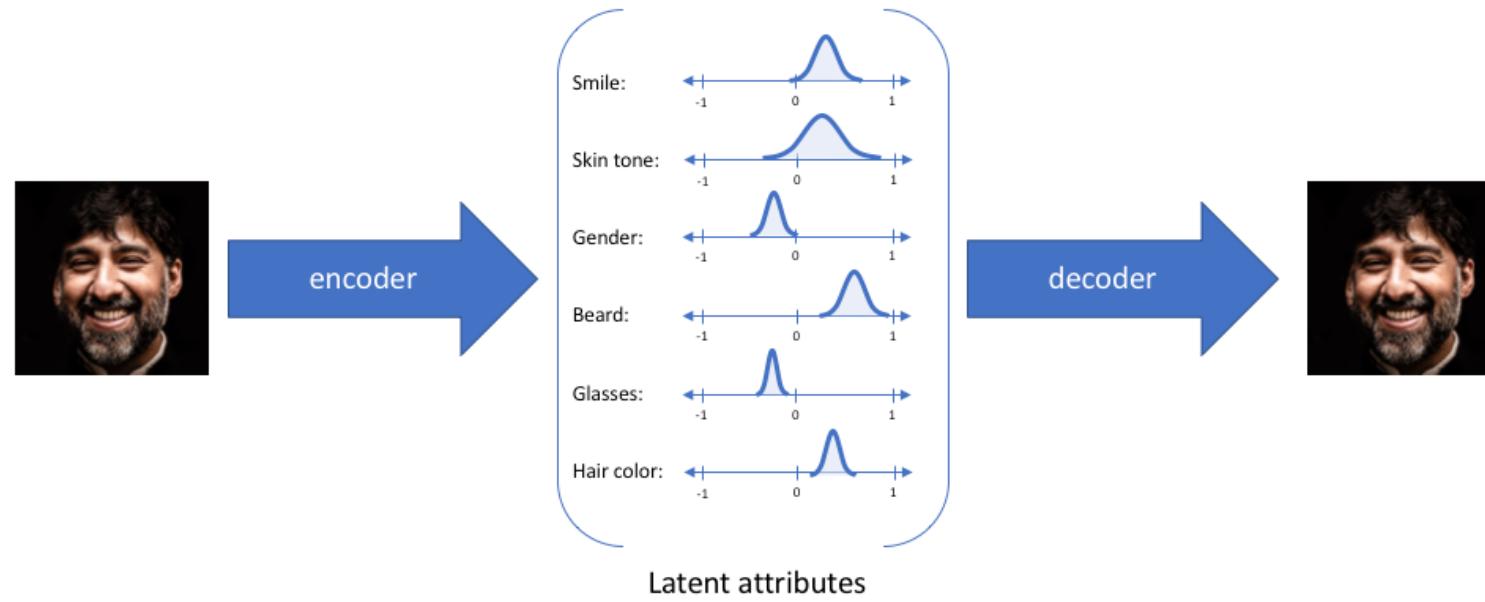
What is common in these images? How can they be characterized?

Latent Variables - Celeb



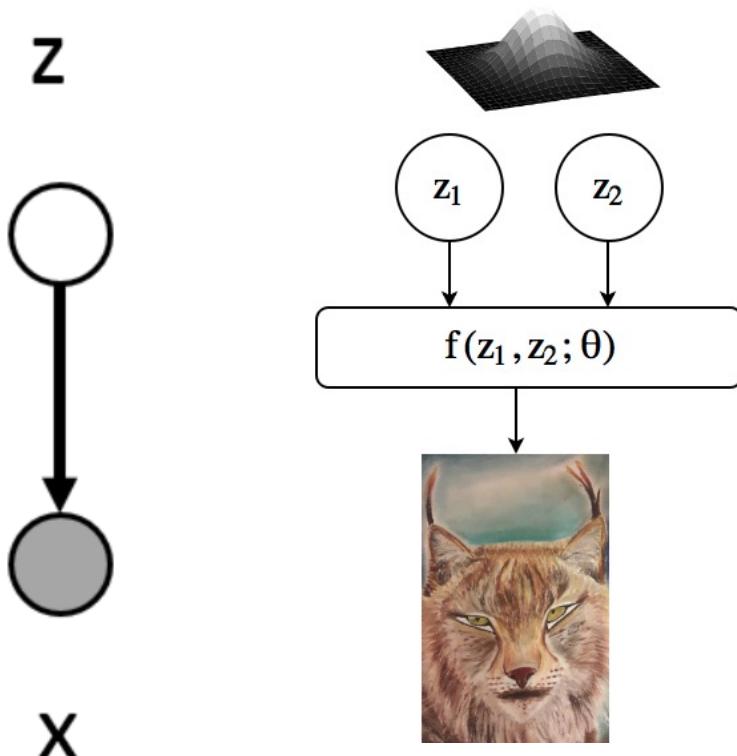
Variability due to eye and hair color, gender, race. However, unless images are annotated, these factors of variation are not explicitly available (latent).

Latent Variables - Celeb



Variability due to eye and hair color, gender, race. However, unless images are annotated, these factors of variation are not explicitly available (latent).

Latent Variable Models: Motivation



- ▶ **Observe** X in the data sample.
Latent observables Z are **hidden**.
- ▶ Knowing latent variable space correctly can be beneficial as $p(x|z)$ can be described **simpler** than $p(x)$.
- ▶ **Hard** to find the real Z space manually, we need unsupervised learning.

Gaussian Mixture Model

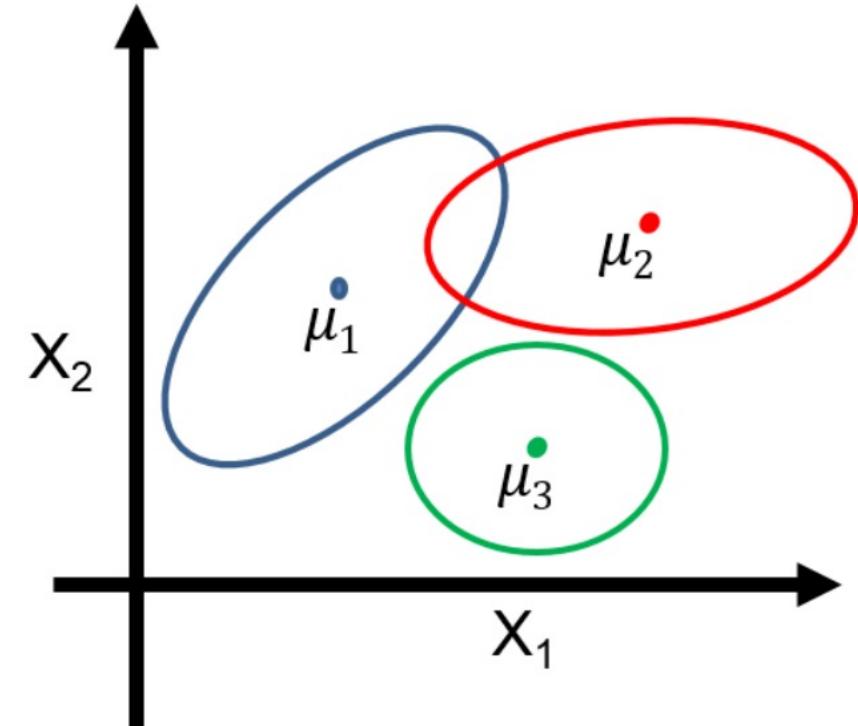
We can use a mixture of distributions (like, Gaussians) to have a better estimate of true PDF. Gaussian Mixture Model proposes:

$$p_{GMM} = \sum_{l=1}^K \pi_l \phi(x; \mu_l, \sigma_l^2),$$

where $\pi_l \geq 0$ are the weights: $\sum \pi_l = 1$. Here the number K is a tuning parameter that specifies the number of Gaussians in our model.

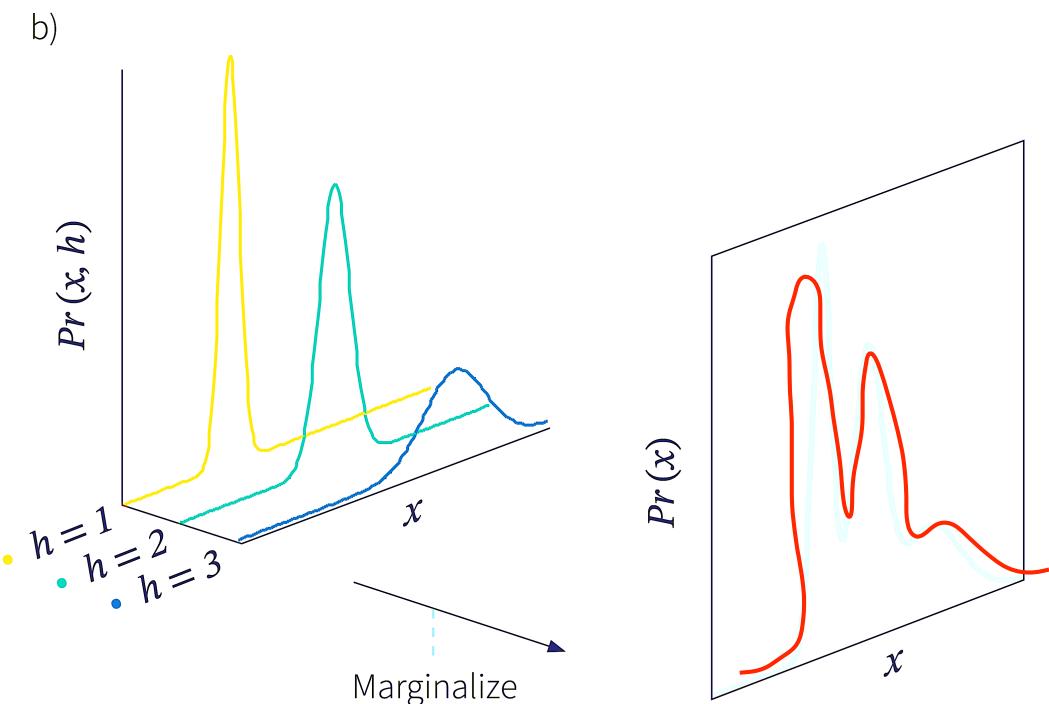
Mixture of Gaussians as Latent Variable Model

- ▶ GMM is a latent variable model.
 - $z \sim \text{Categorical}(1, K)$
 - $p(x|z = k) = N(\mu_k, \Sigma_k)$
- ▶ Generative process
 - Pick a mixture component k by sampling z .
 - Generate a data point by sampling from that Gaussian.



Combination of $p(x)$

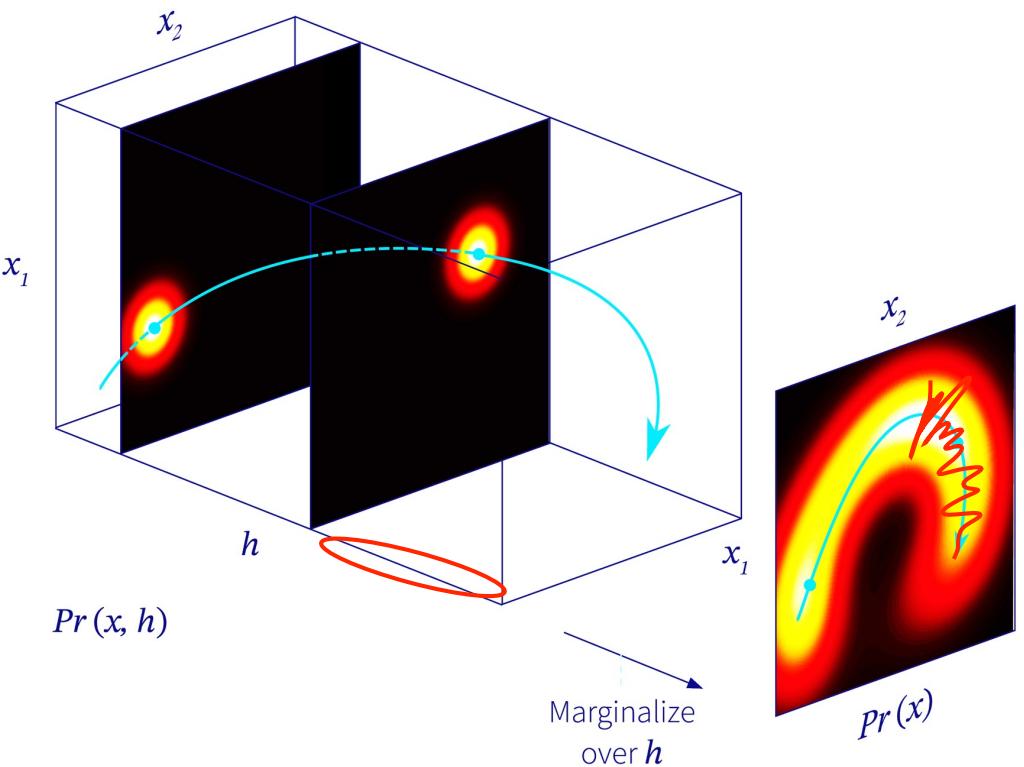
- ▶ Combine simple models into a more complex and expressive one.
- ▶ Obtain PDF using simple formula.



$$p(x) = \sum_{all z} p(x, z) = \sum_{all z} p(z)p(x|z) = \sum_{k=1}^K p(z = k)N(x; \mu_k, \Sigma_k)$$

Combination of $p(x)$

- ▶ Combine simple models into a more complex and expressive one.
- ▶ Obtain PDF using simple formula.
- ▶ What if we have a continuous observable?



$$p(x) = \sum_{\text{all } z} p(x, z) = \sum_{\text{all } z} p(z)p(x|z) = \sum_{k=1}^K p(z = k)N(x; \mu_k, \Sigma_k)$$

$$p(x; \theta) = \int_z p(x, z; \theta) dz = \int_z p(x; \theta|z)p(z) dz$$

Finding parameters θ

How do we find the parameters θ ? The most natural way is to maximise the log likelihood:

$$\log \prod_{i=1}^D p(x^i; \theta) = \sum_{x \in D} \log p(x; \theta)$$

In the following we will need to:

- › define a loss function to optimize
- › calculate gradients of the loss function with respect to the parameters θ .
- › apply a variant of stochastic gradient descent.

Maximizing the likelihood

Consider one sample, x . Then to maximize the likelihood, we need to calculate:

$$p(x; \theta) = \int_z p(x, z; \theta) dz = \int_z p(x; \theta|z)p(z) dz$$

- ▶ Easy to calculate in special cases:
 - in case of independent observables $x|z \perp z$.
 - special cases of conjugation.
- ▶ In general, x depends heavily on z (by construction).
- ▶ Integral is intractable.

Estimating likelihood: Naive Monte-Carlo

We can use the same algorithm as we have seen in GMM:

$$p(x; \theta) = \sum_{all z} p(x, z; \theta) = |Z| \mathbb{E}_{z \sim Uniform(z)}(p(x, z; \theta)).$$

For this, we can fix the distribution followed by z .

This is really only tractable when x is relatively low-dimensional. In case of image, we run into the curse of dimensionality, where we need to grab many samples to get an accurate view of x .

Wrap-up

- ▶ Problems:
 - We can't calculate $p(x)$.
 - We can't write the maximum-likelihood objective.
- ▶ We need a different approach or objective function. Idea:
 - if we can't write likelihood, let's instead derive a lower bound on it.
 - If the lower bound is tractable, then we can optimize the parameters with respect to the lower bound.
 - If we are making the lower bound larger, we are making the likelihood larger.

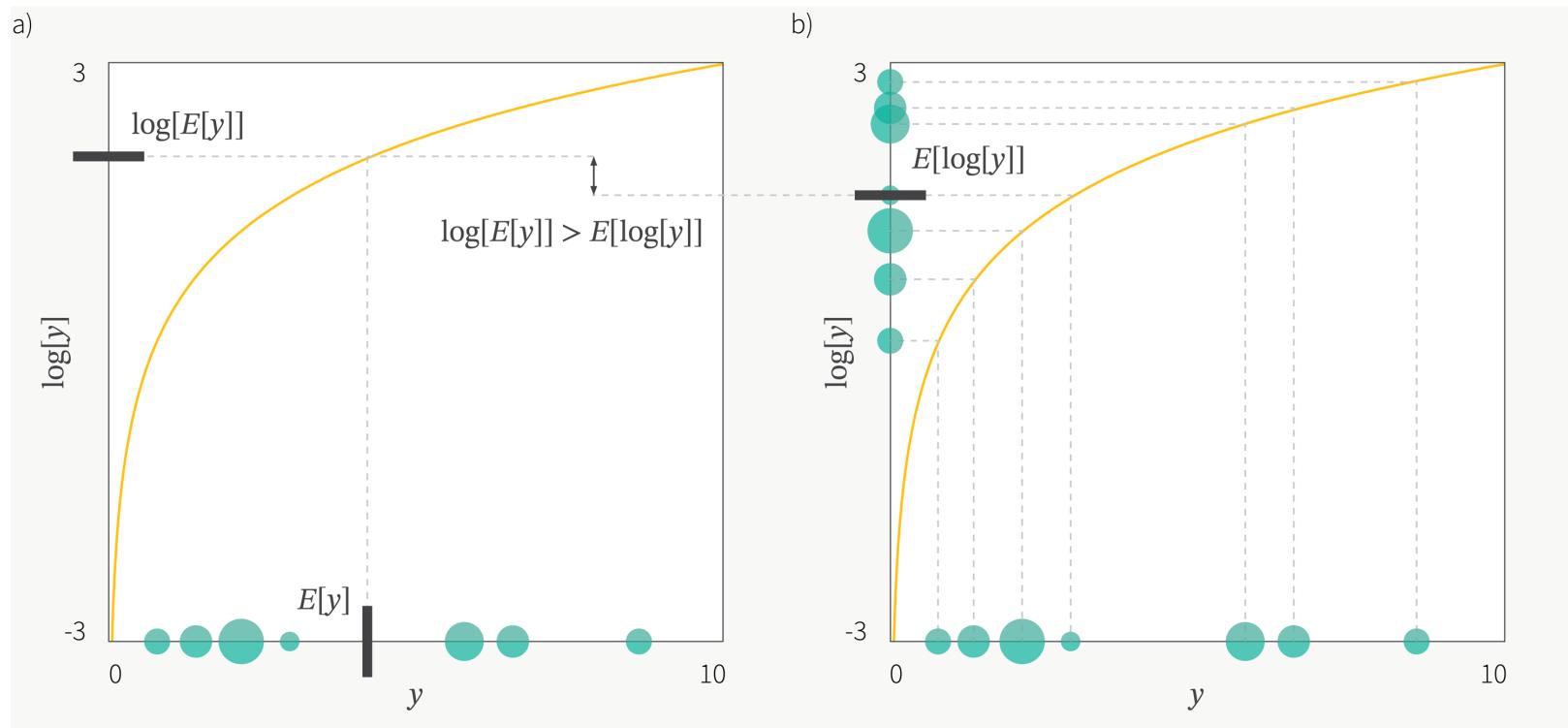
Evidence Lower Bound



Jensen's inequality

For concave function $g(\cdot)$:

$$g[\mathbb{E}[y]] \geq \mathbb{E}[g[y]].$$



$$\log \int p(y)y dy \geq \int p(y) \log y dy .$$

Figure: BorelisAI

Deriving the Evidence Lower BOund

- ▶ Start multiplying and dividing $q(z)$ (arbitrary function):

$$\log p(x; \theta) = \log \int p(x, z; \theta) dz = \log \int q(z) \frac{p(x, z; \theta)}{q(z)} dz.$$

- ▶ Jensen's inequality for convex functions (\log):

$$\log \int q(z) \frac{p(x, z; \theta)}{q(z)} dz \geq \int q(z) \log \frac{p(x, z; \theta)}{q(z)} dz.$$

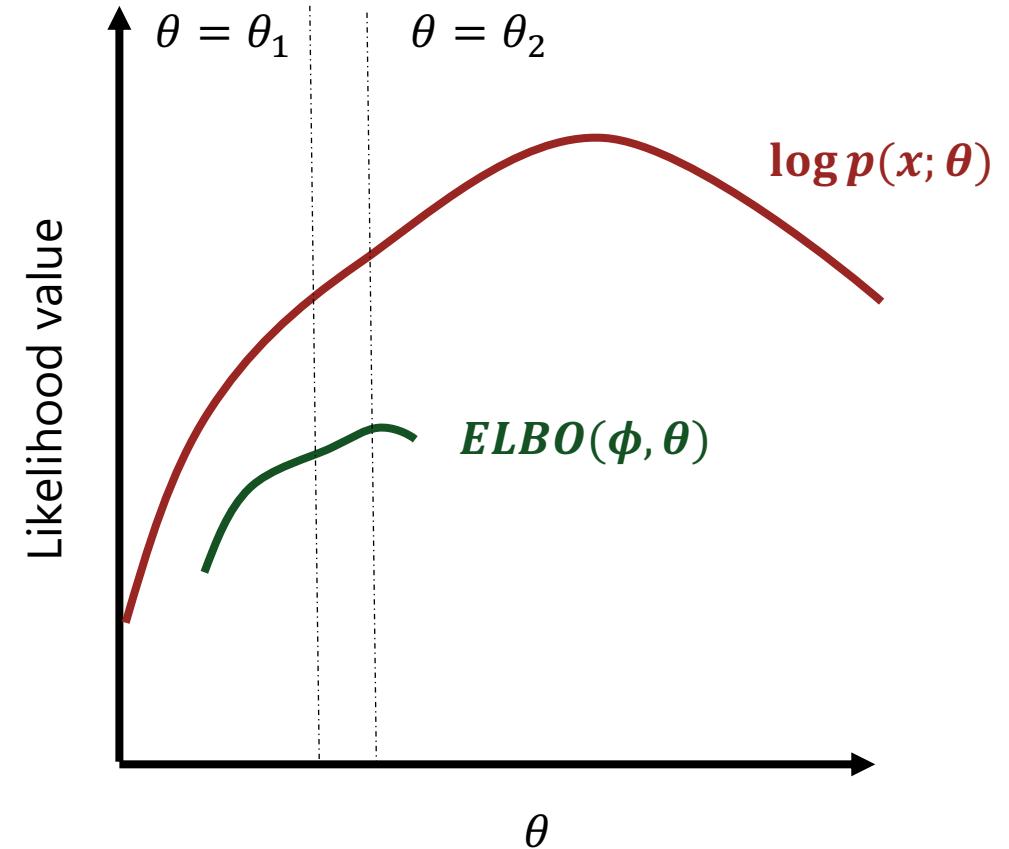
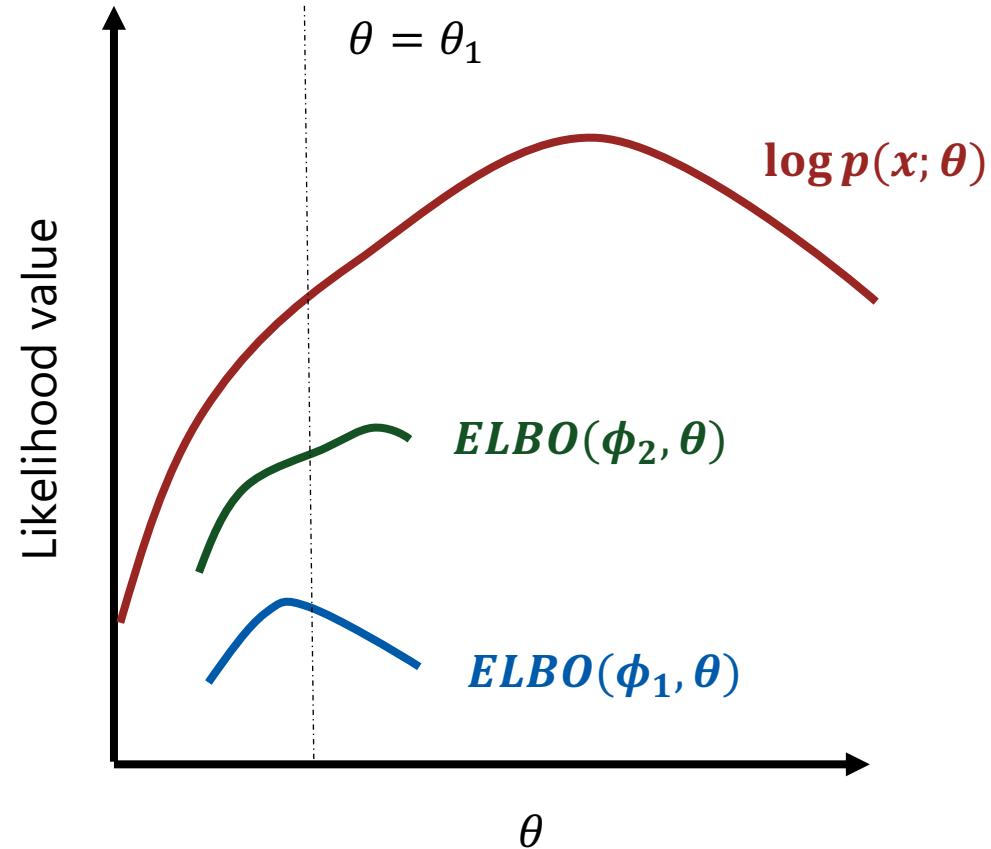
The rhs is **evidence lower bound**

- ▶ $q(z)$ has different set of parameters, ϕ

$$ELBO(\phi, \theta) = \int q(z; \phi) \log \frac{p(x, z; \theta)}{q(z; \phi)} dz$$

ELBO so far

$$ELBO(\phi, \theta) = \int q(z; \phi) \log \frac{p(x, z; \theta)}{q(z; \phi)} dz$$



Tightness of bound

$$ELBO(\phi, \theta) = \int q(z; \phi) \log \frac{p(x, z; \theta)}{q(z; \phi)} dz$$

- We use chain rule

$$ELBO(\phi, \theta) = \int q(z; \phi) \log \frac{p(x; \theta)p(z|x; \theta)}{q(z; \phi)} dz$$

- Separate part independent on z :

$$= \int q(z; \phi) \log p(x; \theta) dz + \int q(z; \phi) \log \frac{p(z|x; \theta)}{q(z; \phi)} dz =$$

$$= \log p(x; \theta) + \int q(z; \phi) \log \frac{p(z|x; \theta)}{q(z; \phi)} dz =$$

- Definition of KL divergence:

$$= \log p(x; \theta) - KL(q(z; \phi) || p(z|x; \theta)).$$

- Bound is tight iff $KL = 0$.

M. Hoffman, M. Johnson, ELBO surgery, NIPS2016

Variational Autoencoder



Dependence on prior on z

- ▶ We use chain rule

$$ELBO(\phi, \theta) = \int q(z; \phi) \log \frac{p(z)p(x|z; \theta)}{q(z; \phi)} dz =$$

- ▶ Separate KL divergence part:

$$= \int q(z; \phi) \log p(x|z; \theta) dz + \int q(z; \phi) \log \frac{p(z)}{q(z; \phi)} dz =$$

- ▶ Definition of KL

$$= \int q(z; \phi) \log p(x|z; \theta) dz - KL(q(z; \phi) || p(z)).$$

Reconstruction loss

Latent Parametrization agreement

Latent Parametrization Agreement

- ▶ Measures the degree to which the auxiliary distribution, $q(h, \theta)$, matches the prior $p(z)$:

$$KL(q(z; \phi) || p(z)).$$

- ▶ The KL divergence has closed form if both are distributions are known parametric (e.g., Gaussian):

$$q(z; \phi) = N_z(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

$$p(z) = N_z(\mathbf{0}, \mathbf{I}).$$

- ▶ In this case:

$$KL[q(z|x, \theta), p(z)] = 12(Tr[\boldsymbol{\Sigma}] + \boldsymbol{\mu}^T \boldsymbol{\mu} - D - \log[\det[\boldsymbol{\Sigma}]])$$

D. Kingma et al. Auto-Encoding Variational Bayes, ICLR 2014

Latent Parametrization Agreement: training

- ▶ Measures the degree to which the auxiliary distribution, $q(h, \theta)$, matches the prior $p(z)$:

$$KL(q(z; \phi) || p(z)).$$

- ▶ The KL divergence has closed form if both distributions are known parametric (e.g., Gaussian):

$$q(z|x; \phi) = N_z(g_{\mu}(x; \phi), g_{\sigma}(x; \phi));$$

$$p(z) = N_z(\mathbf{0}, I).$$

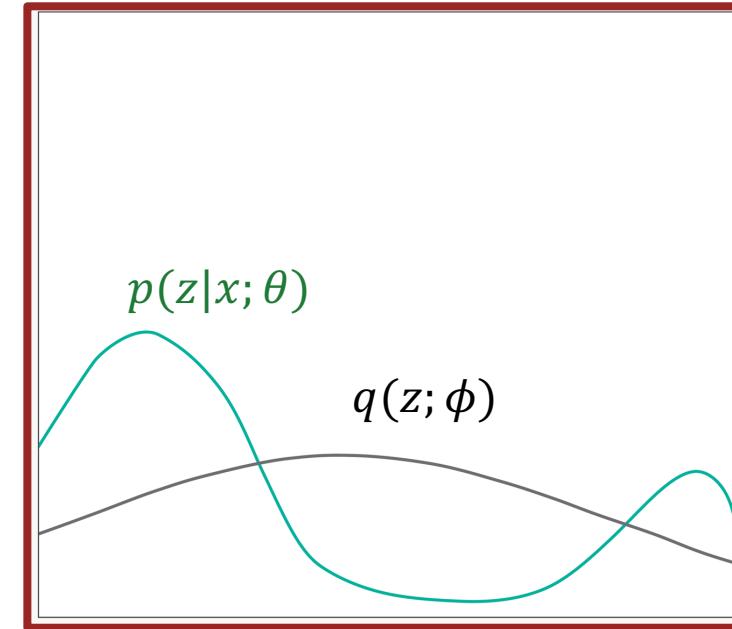
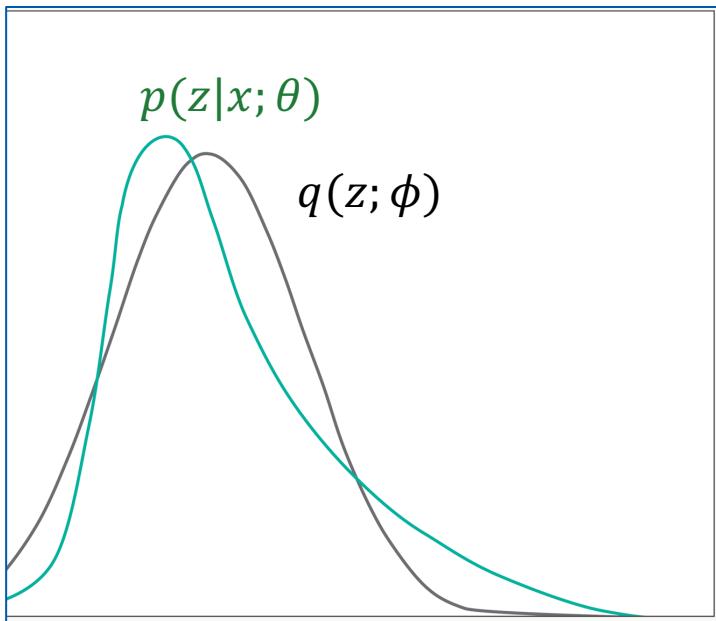
- ▶ In this case:

$$KL[q(z|x, \theta), p(z)] = \frac{1}{2} (Tr[\Sigma] + \mu^T \mu - D - \log[\det[\Sigma]])$$

Problems of parametrization choice

- ▶ For tightness of bound:

$$KL(q(z; \phi) || p(z|x; \theta)) \rightarrow 0.$$



- ▶ The tight bound might be unreachable.

Figure: BorelisAI

Reconstruction Loss

- ▶ Reconstruction loss:

$$\int q(z|x; \phi) \log p(x|z; \theta) dz.$$

- ▶ Still troubles to compute directly, we can approximate it with mathematical expectation (even with one sample z^*) and thus have:

$$\begin{aligned} ELBO(\theta, \phi) &= \int q(z; \phi) \log p(x|z; \theta) dz - KL(q(z; \phi) || p(z)) \approx \\ &\approx \log[p(x|z^*; \phi)] - KL[q(z|x, \theta), p(z)]. \end{aligned}$$

Variational Autoencoder

Maximize

$$\mathcal{L}_{VAE} = \mathbb{E}_z \log[p(x|z; \theta)] - KL[q(z|x, \phi), p(z)]$$

Autoencoder, as we reconstruct $x \rightarrow z \rightarrow x$.

Variational, as it constructs Gaussian approximation to the posterior distribution.

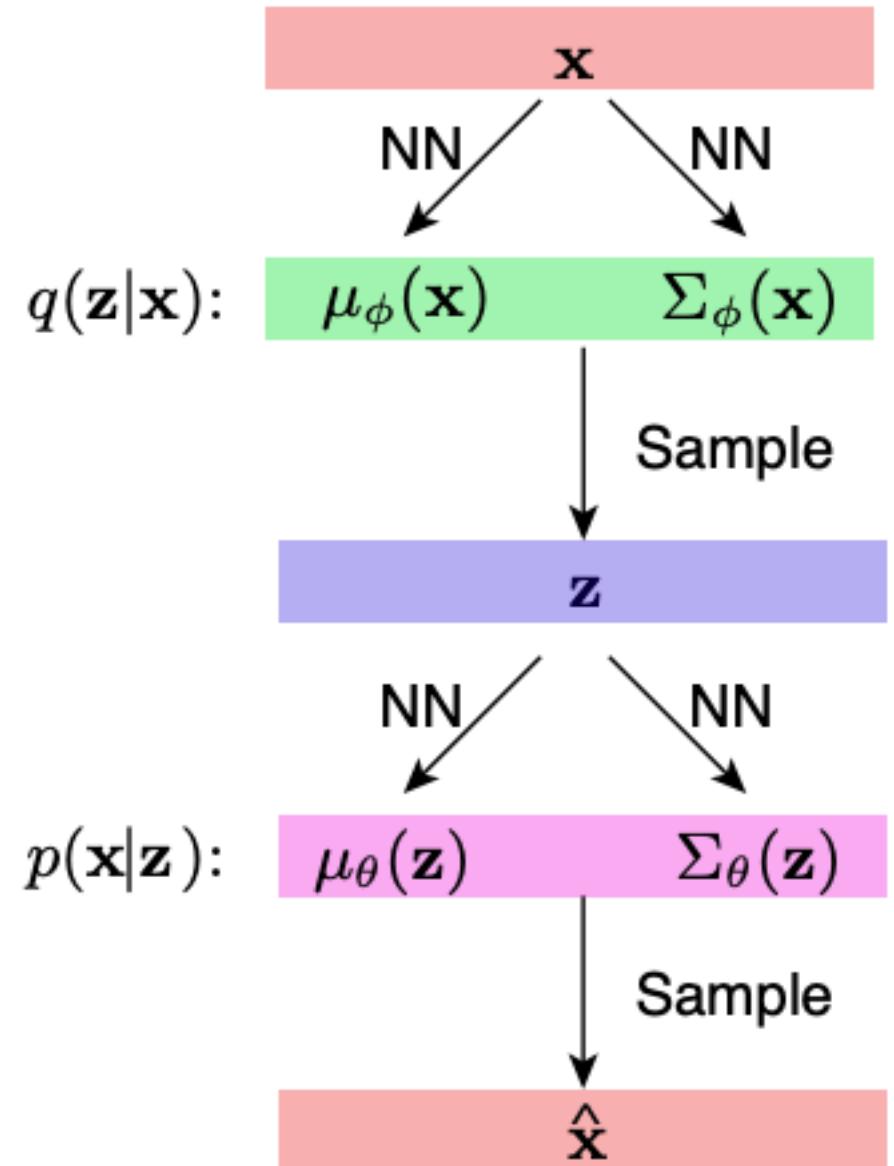


Fig: Kao UCLA DL lectures

Training VAE

We can estimate gradients for ELBO:

- › gradient wrt θ is easy:

$$\nabla_{\theta} \mathcal{L}(x; \theta, \phi) = \nabla_{\theta} \log p(x, z; \theta)$$

and can be done using a simple MC estimation.

- › for ϕ situation is much more tricky, since we calculate expectation over q :

$$\nabla_{\phi} \mathcal{L}(x; \theta, \phi) = \nabla_{\phi} \mathbb{E}_{q(z|x;\phi)} [\log p(x, z; \theta) - \log q(z|x; \phi)].$$

luckily, we can use reparameterization.

Reparameterization trick

- ▶ Sampling:

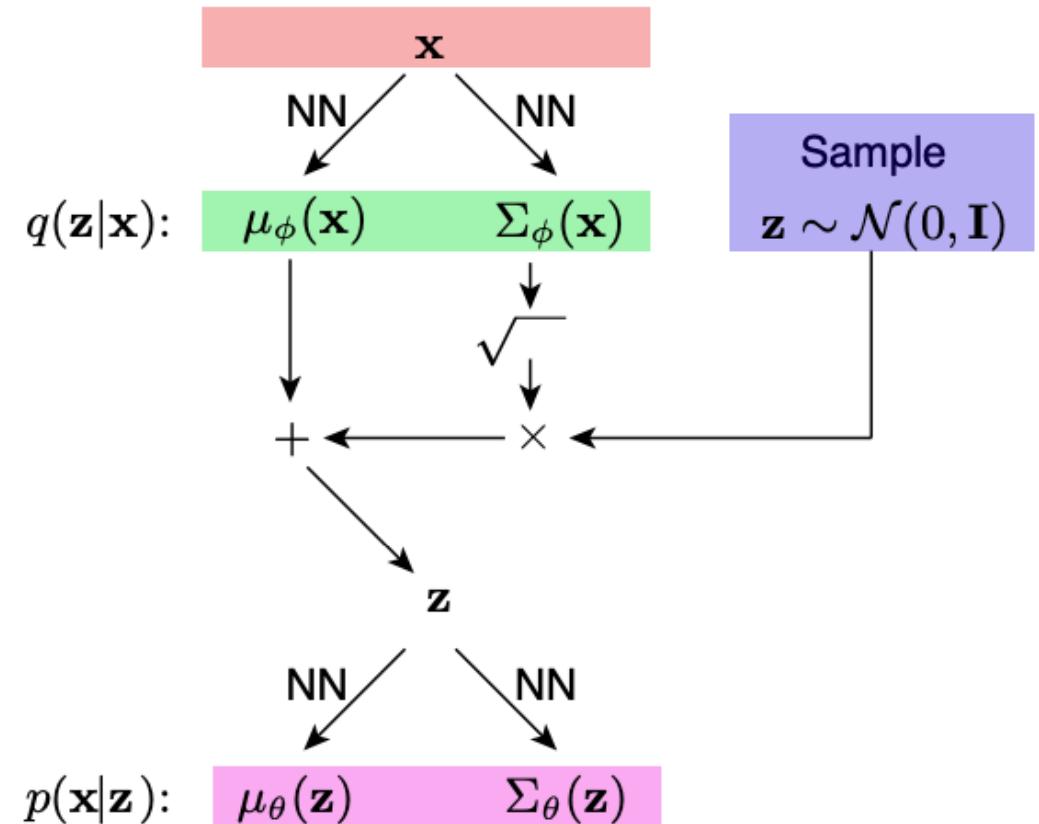
$$z \sim q(z|x)$$

- ▶ Can be done:

$$\varepsilon \sim N(0, I);$$

$$z = \mu_\phi(x) + \Sigma^{\frac{1}{2}}(x)\varepsilon.$$

- ▶ Backpropagation now does not pass through sampling.



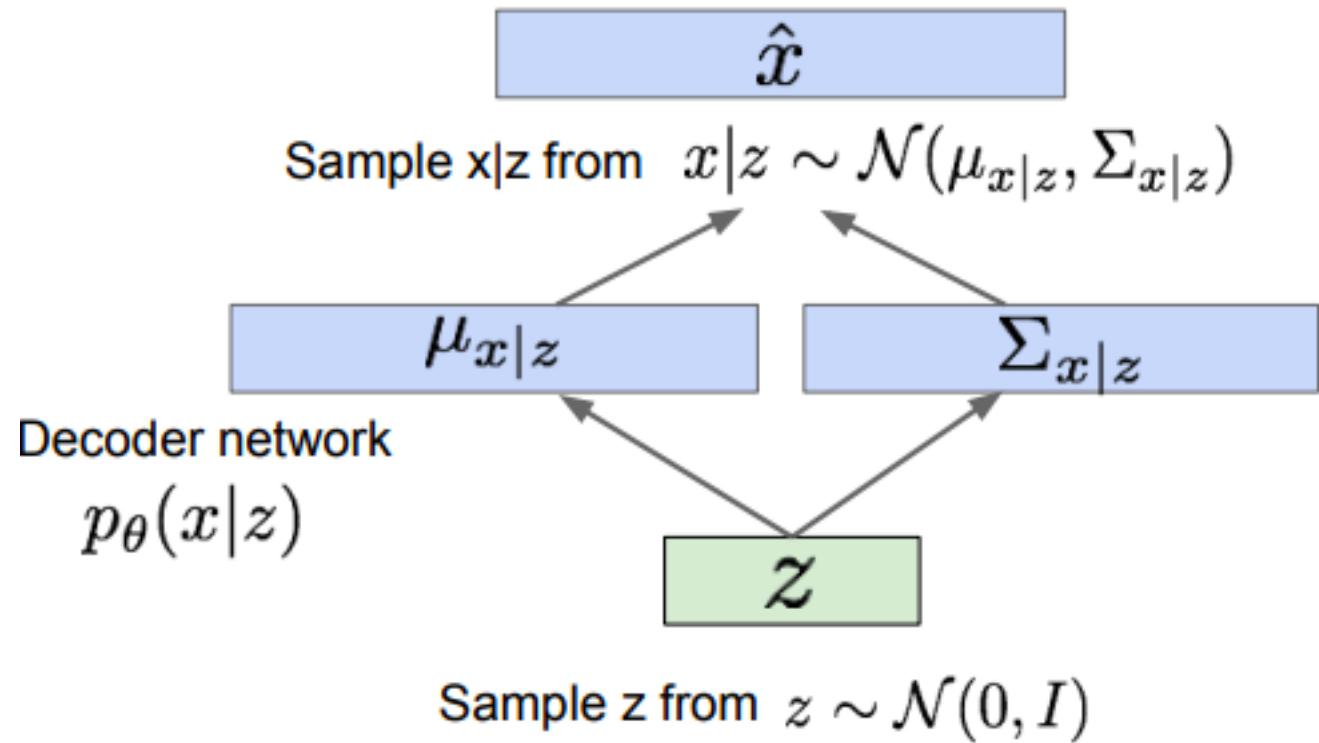
Final Per-event Objective and Results

- ▶ Write out
$$\mathcal{L}_{VAE}(x_i; \theta, \phi) = \mathbb{E}_{z \sim p(\varepsilon)} \log[p(x_i|z; \theta)] - KL[q(z|x_i, \phi), p(z)]$$
- ▶ We can even use a single noise sample:

$$\mathcal{L}_{VAE}(x_i; \theta, \phi) = \log[p(x_i|z; \theta)] - KL[q(z|x_i, \phi), p(z)]$$

- ▶ Note that the gradient estimates from per-event ELBO will be unbiased.

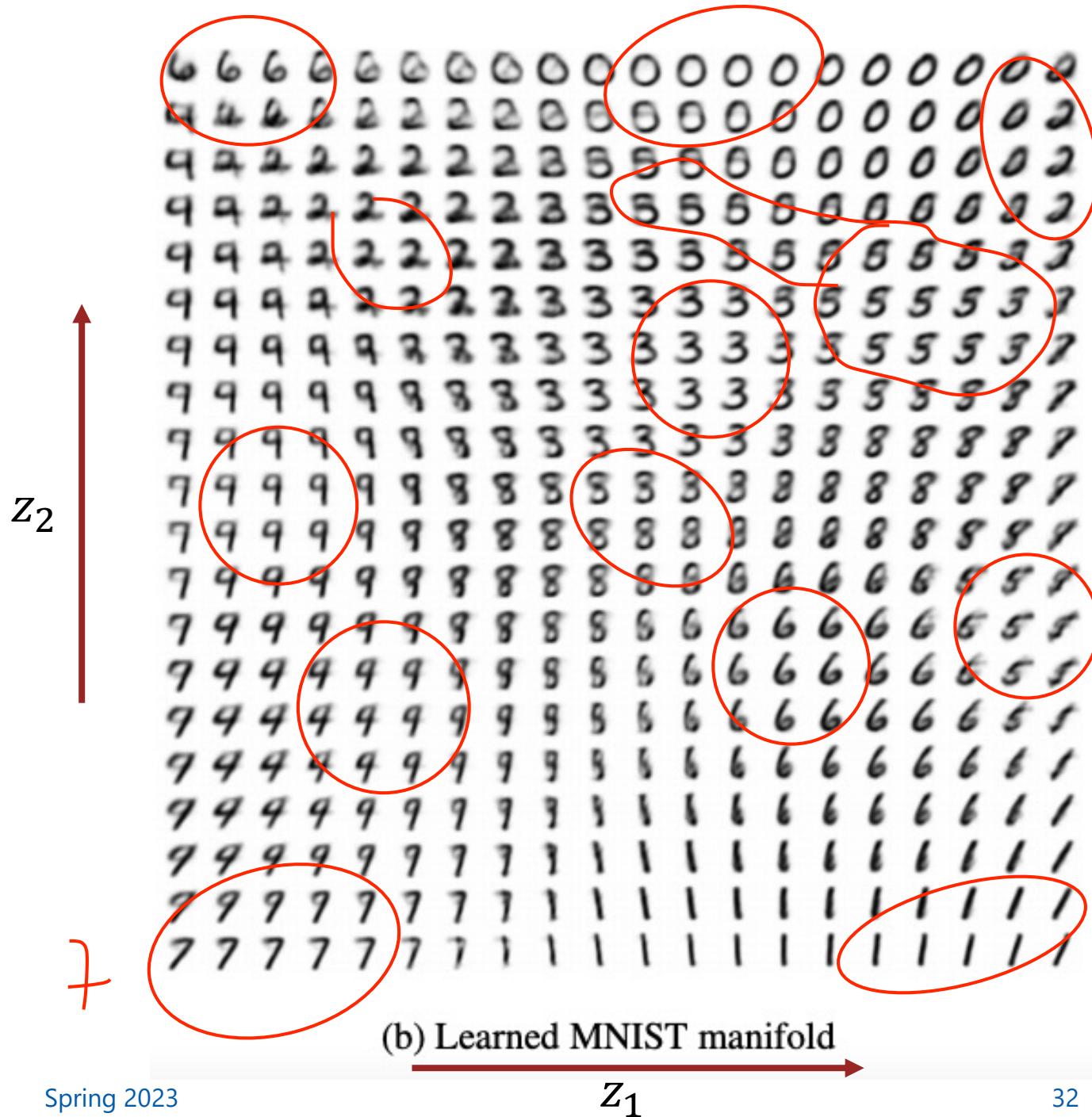
Sampling



- ▶ We now can use the same idea like in GMM.
- ▶ Sampling from prior.

Results

- ▶ The latent space is well organized.
- ▶ The results are good.



Results

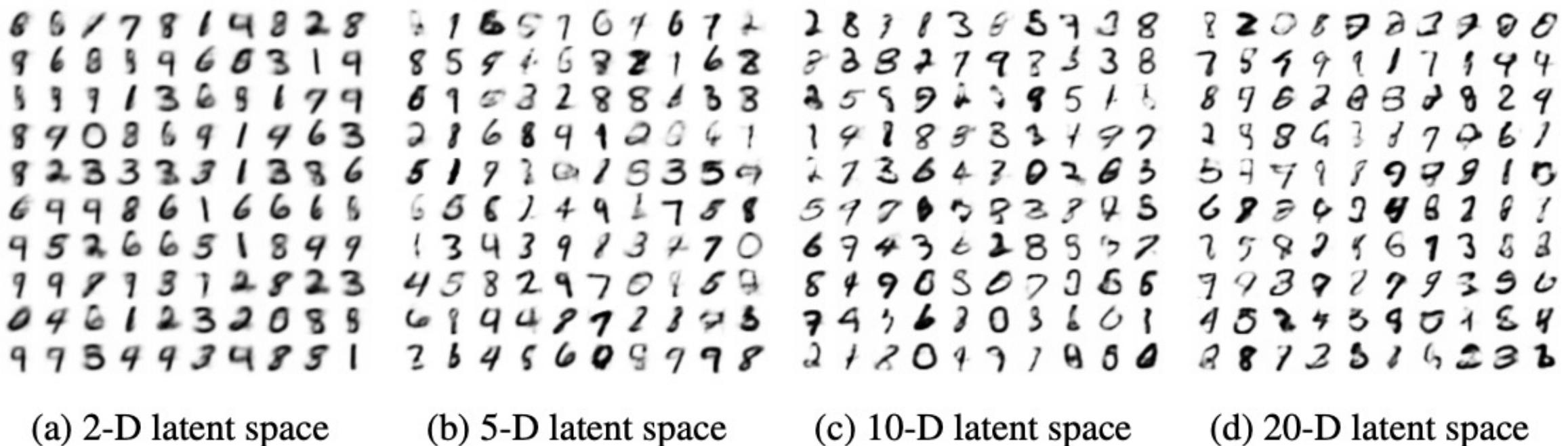
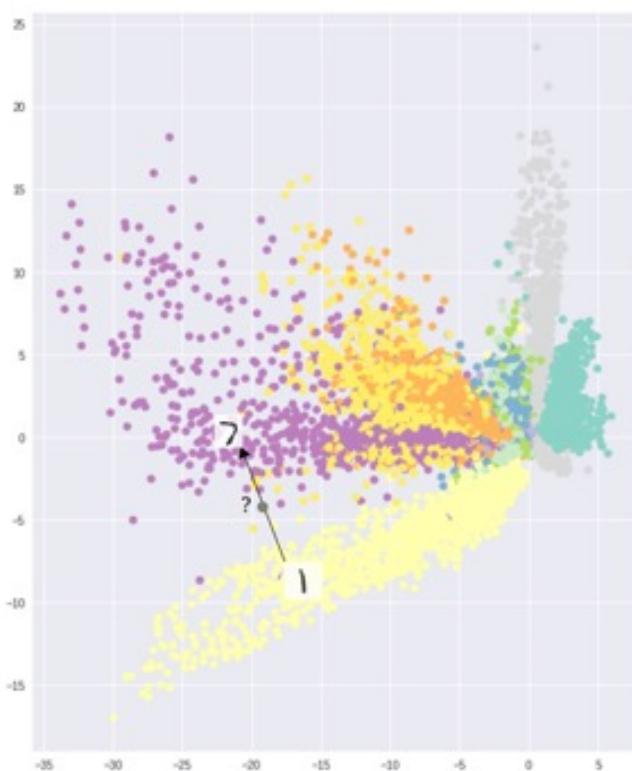


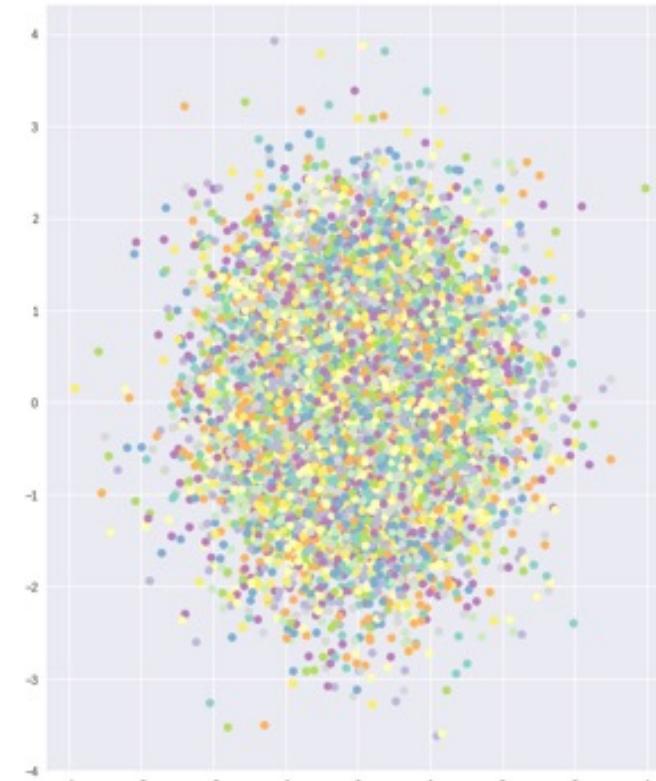
Figure 5: Random samples from learned generative models of MNIST for different dimensionalities of latent space.

Results Discussed

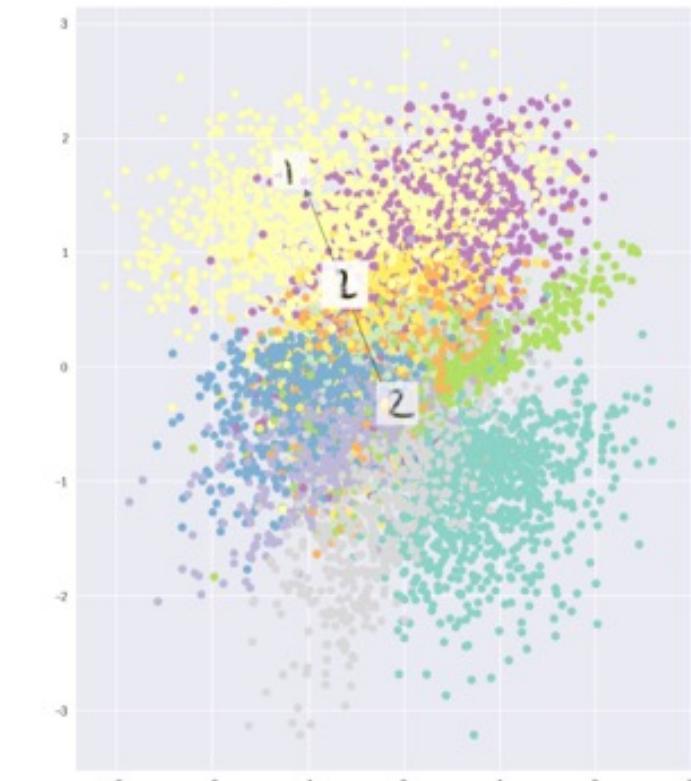
Only reconstruction loss



Only KL divergence



Combination



[Shafkat's blog](#)

Amortized Inference

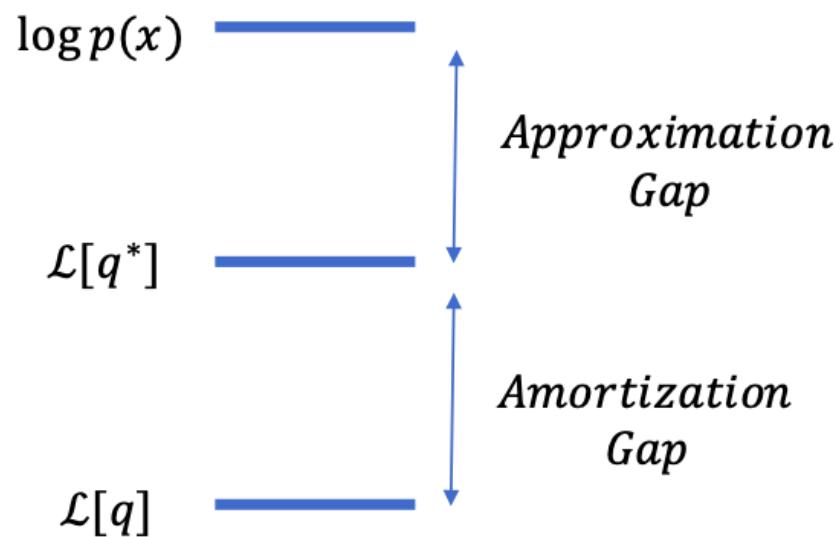


Figure 1. Gaps in Inference

- ▶ variational parameters ϕ_i should be calculated for every data point x_i ;
- ▶ for big datasets this is unsustainable;
- ▶ forget about it and make a single model.

Cremer et al Inference Suboptimality in Variational Autoencoders, ICML 2018

Images for Amortization Gap

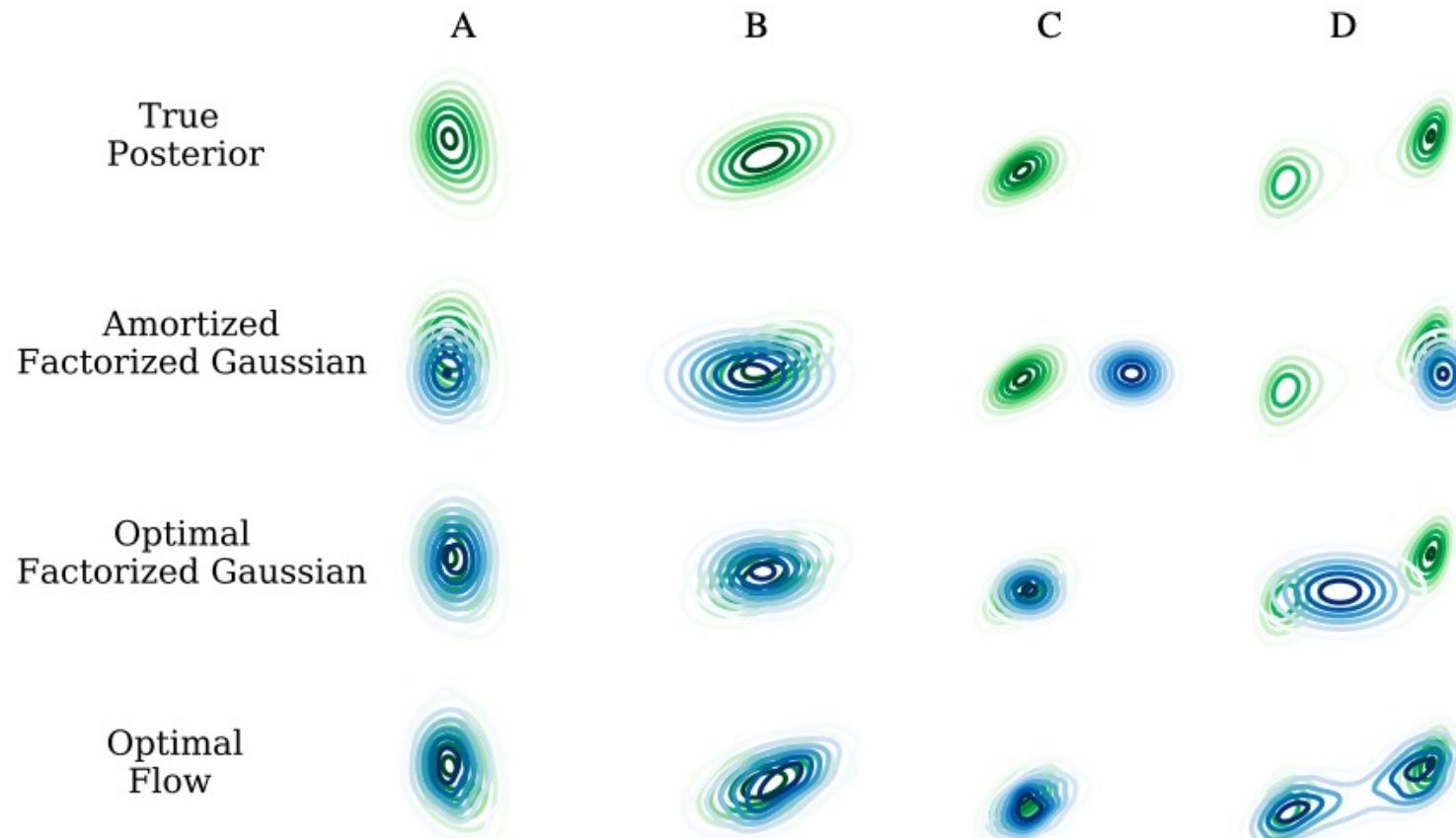


Figure 2. True Posterior and Approximate Distributions of a VAE with 2D latent space. The columns represent four different datapoints. The green distributions are the true posterior distributions, highlighting the mismatch with the blue approximations. Amortized: Variational parameters learned over the entire dataset. Optimal: Variational parameters optimized for each individual datapoint. Flow: Using a flexible approximate distribution.

VAE: starting optimization problem

- ▶ Stochastic optimization can get stuck:
 - in the beginning, likelihood term $\log p(x|z)$ is relatively weak, such that an initially attractive state is where $q(z|x) \approx p(z)$.
- ▶ Several ideas possible:
 - optimization schedule - gradually increase weight of KL.
 - free bits - ensure that on average, a certain minimum number of bits of information are encoded per latent variable.

VAE: posterior collapse



Can happen to weak encoders or noisy data.

The sampling does not depend on the latent model.

An averaged figures are produced.

KL-divergence term annealing is proposed.

Fig: J. Chou Generated Loss and Augmented Training of MNIST VAE

VAE: blurred problem

Due to minimization of KL
 $KL(q(z; \phi) \| p(z|x; \theta)) \rightarrow 0.$

Can be countered by choosing a sufficiently flexible inference model, and/or a sufficiently flexible generative model.



VQ-VAE



Latent Spaces

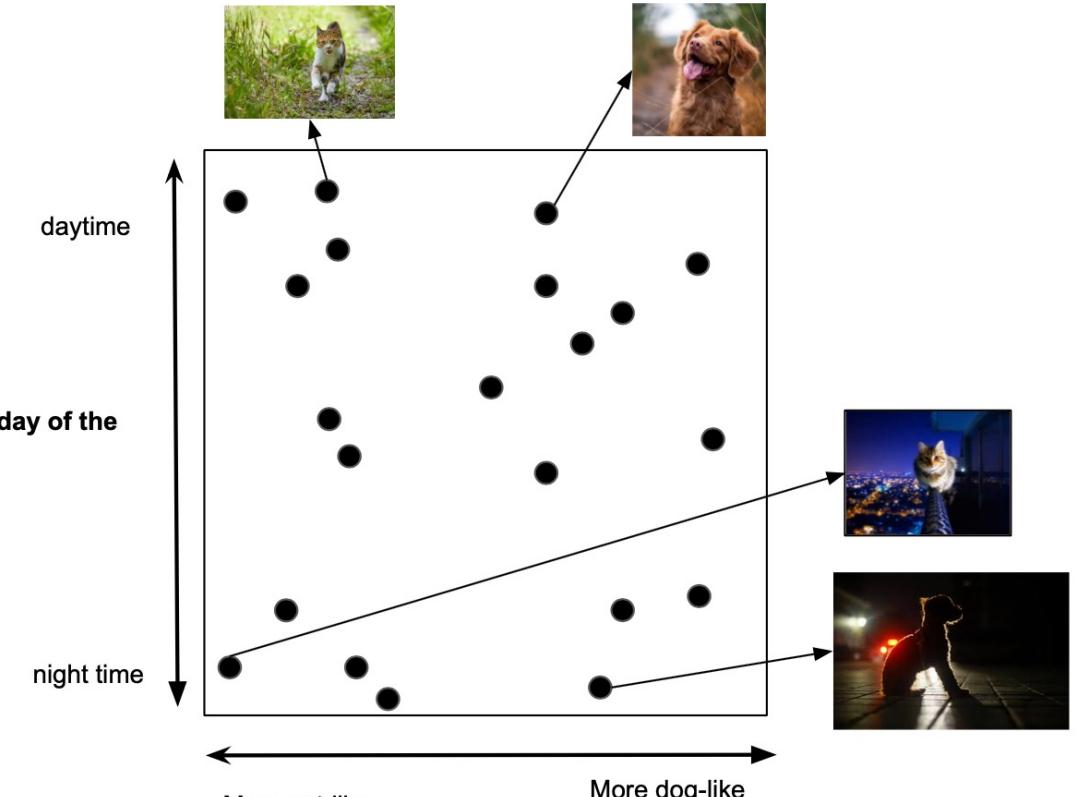
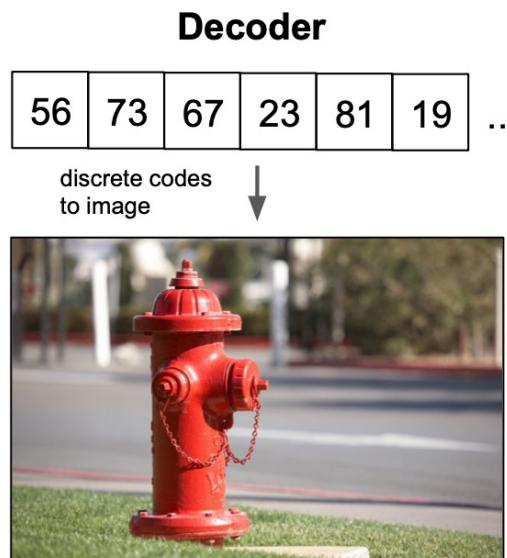
An Oversimplified Example of a Cat/Dog Image Latent Space

VAE gives a good representations

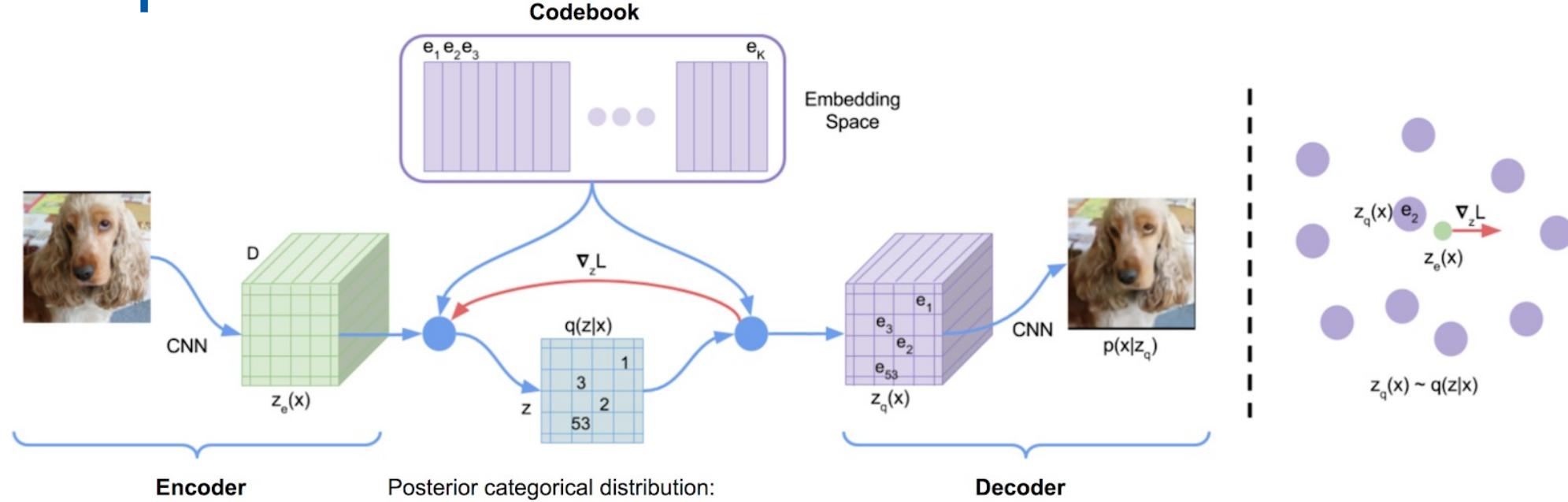
Can we study it?



56	73	67	23	81	19	...
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Latent Space Quantization



- ▶ Reconstruction loss:

$$z_q(x) = \operatorname{argmin}_i \|z_e(x) - e_i\|$$

$z_e(x)$ - encoder vector for some raw input x

e_i - i-th codebook vector

$z_q(x)$ - resulting quantized vector that is passed as input to the decoder

VQ-VAE results

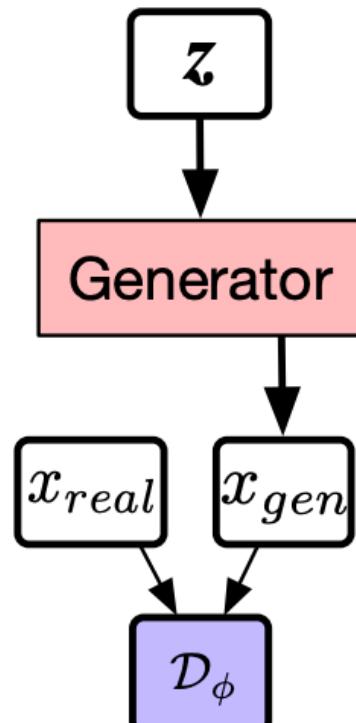


Figure 2: Left: ImageNet 128x128x3 images, right: reconstructions from a VQ-VAE with a 32x32x1 latent space, with K=512.

VAE+GAN



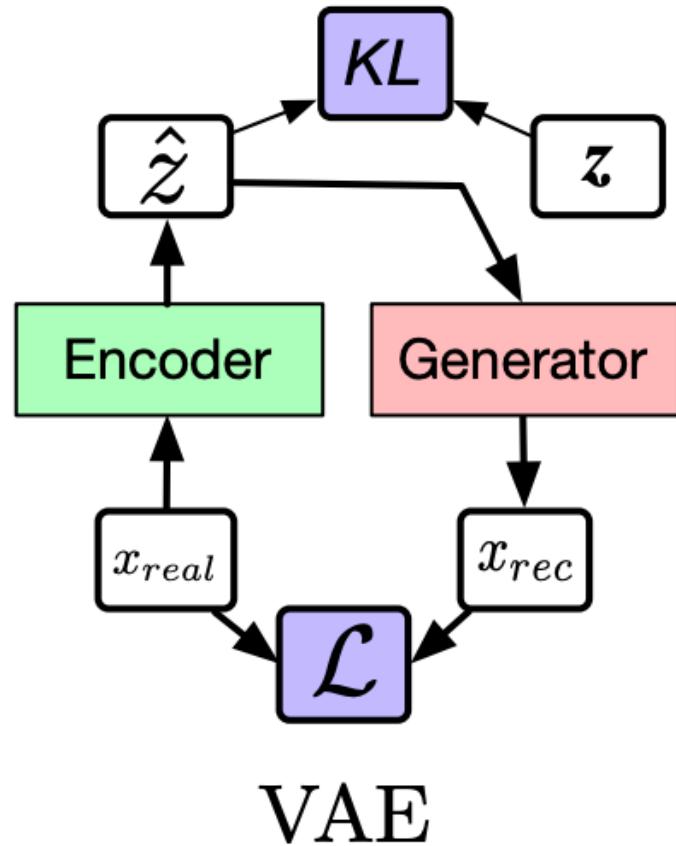
Improving GANs



DCGAN

- ▶ Main problems with GAN:
 - mode collapse;
 - intractable likelihood.
- ▶ Idea:
 - use likelihood-based mode;
 - have easier inference;
 - diversify sampling.

Reminder: VAE structure



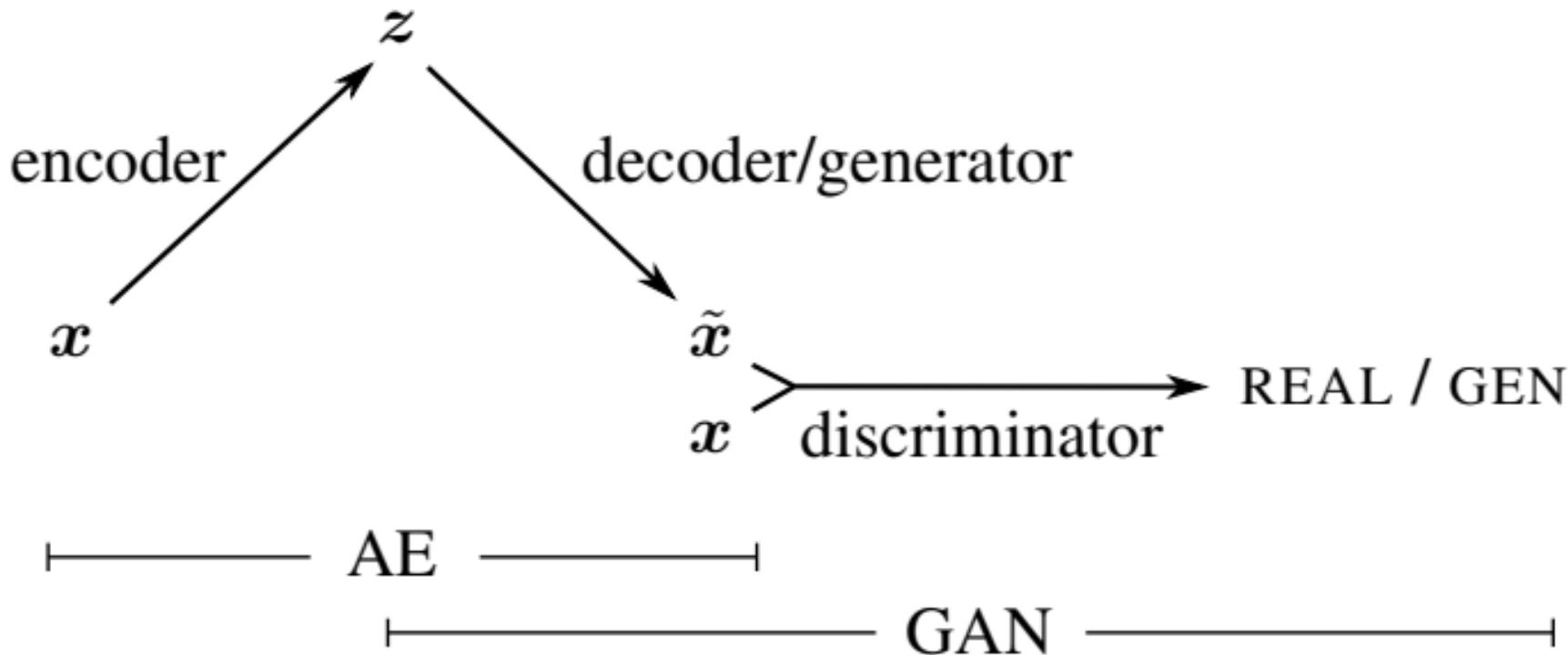
$$\mathcal{L}_{prior} = KL(q_n(z|x)||p(z))$$

+

$$-\mathcal{L}_{pixel} = \mathbb{E}_{q_n(z|x)}(\log p_\theta(x|z))$$

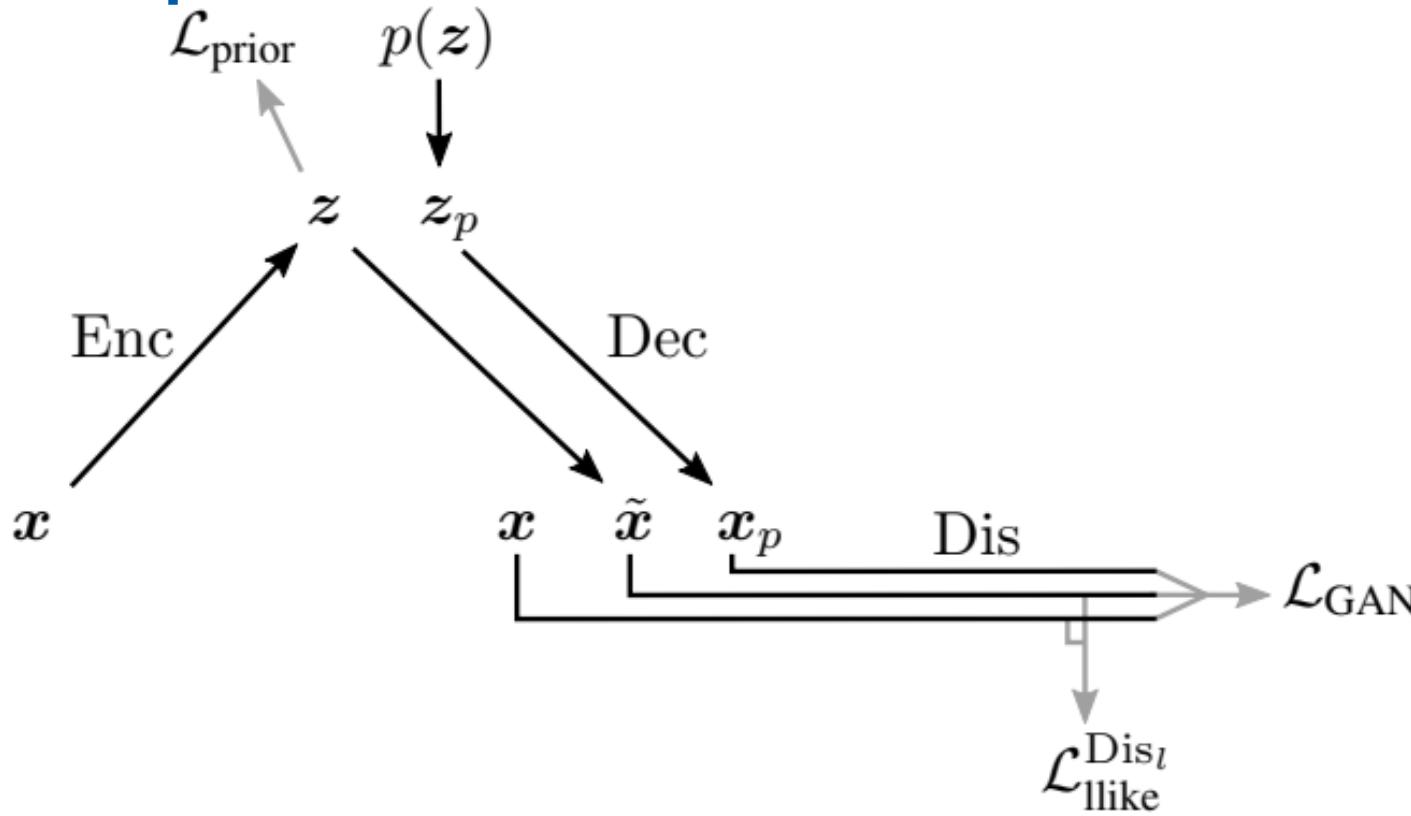
$$= \mathcal{L}_{VAE}$$

VAE+GAN



- ▶ problem of VAE is blurry output
- ▶ GAN overcomes due to the use of discriminator
- ▶ add GAN loss to VAE

VAE+GAN expanded

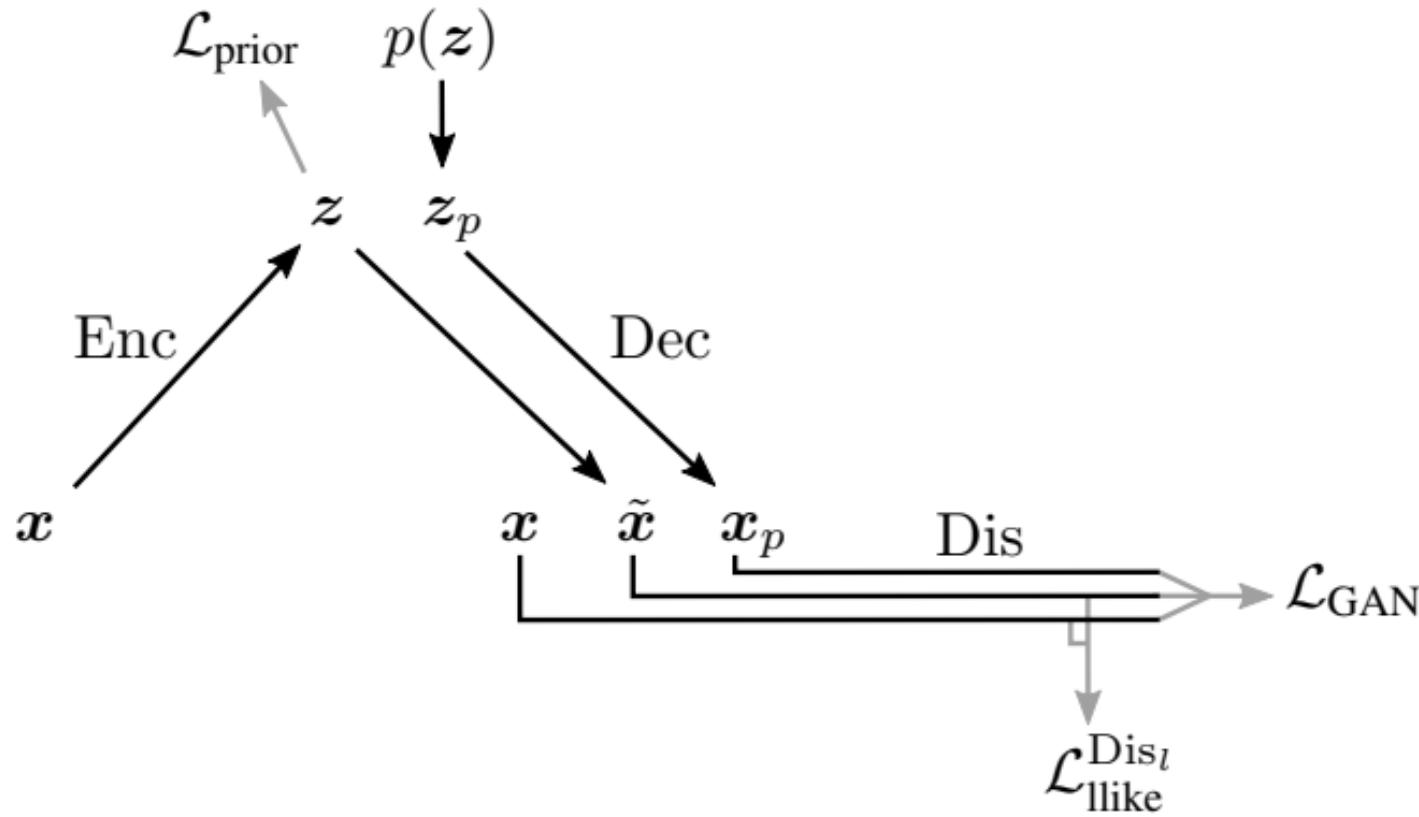


- ▶ Consider image as a whole:

$$-\mathcal{L}_{DIS} = \mathbb{E}_{q_n(z|x)} p(Dis_l(x)|z) = \mathbb{E}_{q_n(z|x)} N(Dis_l(x)|Dis_l(\tilde{x}), I), \quad \tilde{x} \sim Dec(z)$$

where $Dis_l(x)$ denote the hidden representation of the l -th layer of the discriminator.

VAE+GAN final loss



$$\mathcal{L}_{GAN+VAE} = \underbrace{\mathcal{L}_{prior}}_{\text{Image}} + \underbrace{\mathcal{L}_{DIS}}_{\text{Image}} + \underbrace{\mathcal{L}_{GAN}}_{\text{Style}}$$

VAE+GAN results

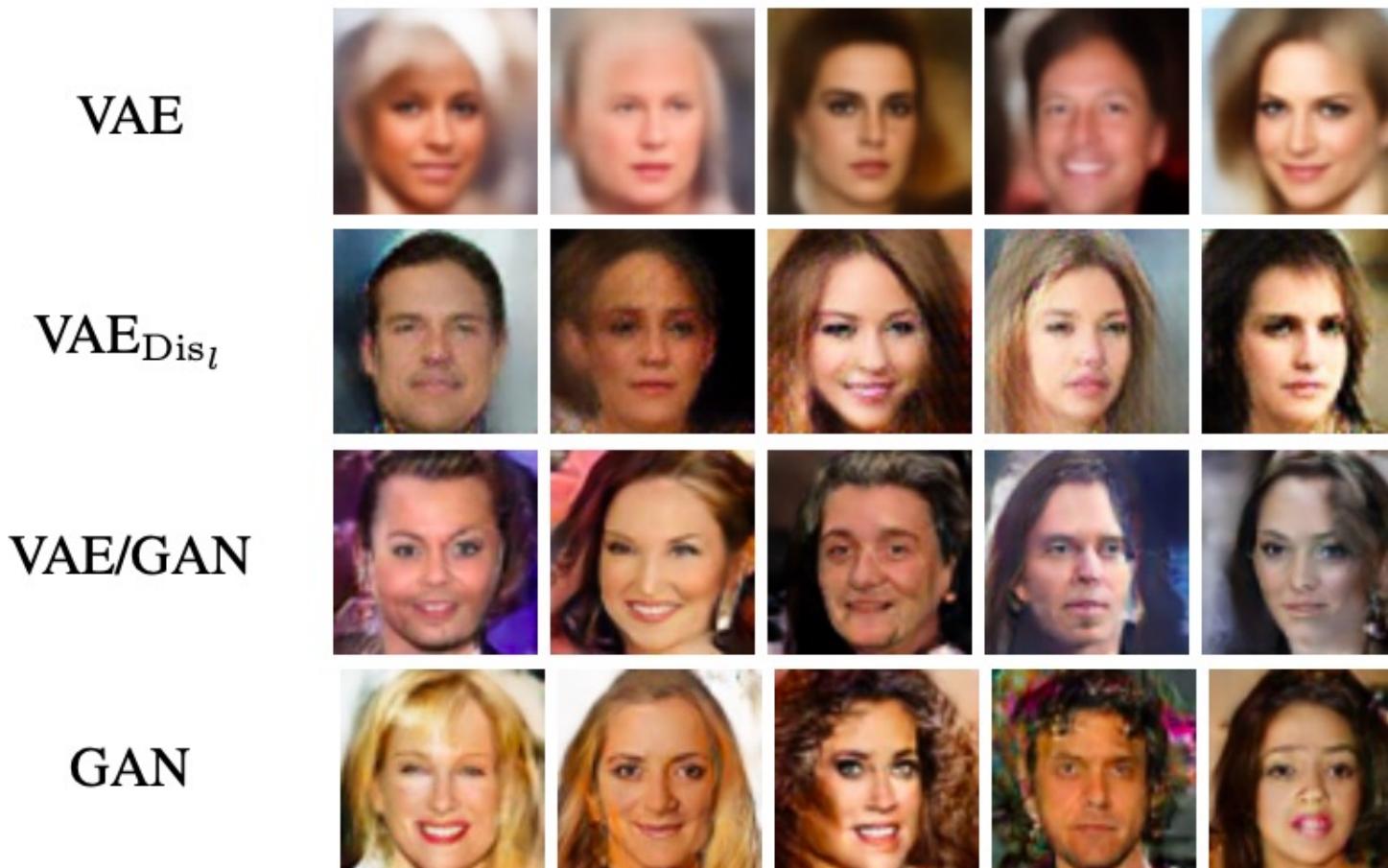


Figure 3. Samples from different generative models.

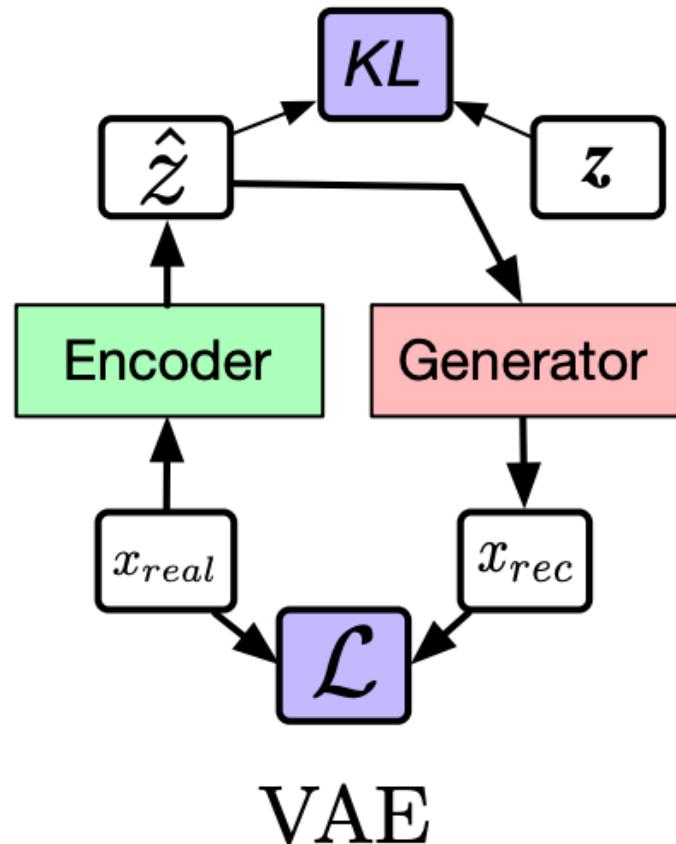
Wrap-up

- ▶ Benefits from combined loss and combined architecture.
- ▶ Better images than VAE or GAN standalone.
- ▶ Can be viewed as extension of VAE with adversarial selection.
- ▶ Can be viewed as extension of GAN with better latent space construction.

More VAEGANs



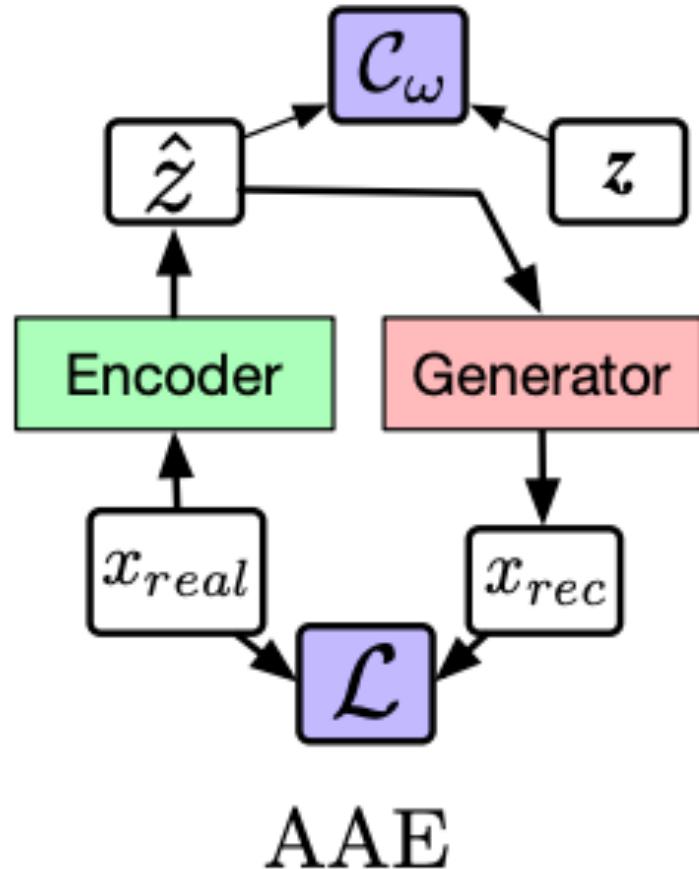
VAE structure



- ▶ KL divergence is considered as one of blurriness causes.
- ▶ We can switch this objective to GAN-like.

<https://arxiv.org/pdf/1511.05644.pdf>

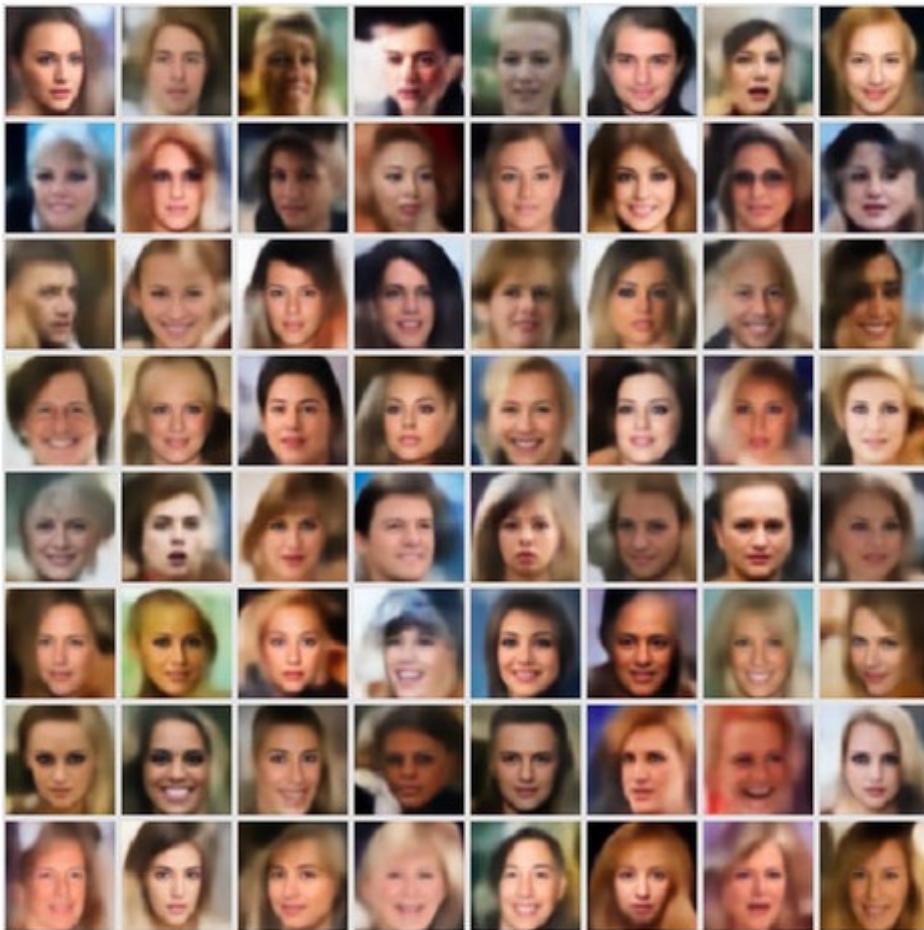
AAE structure



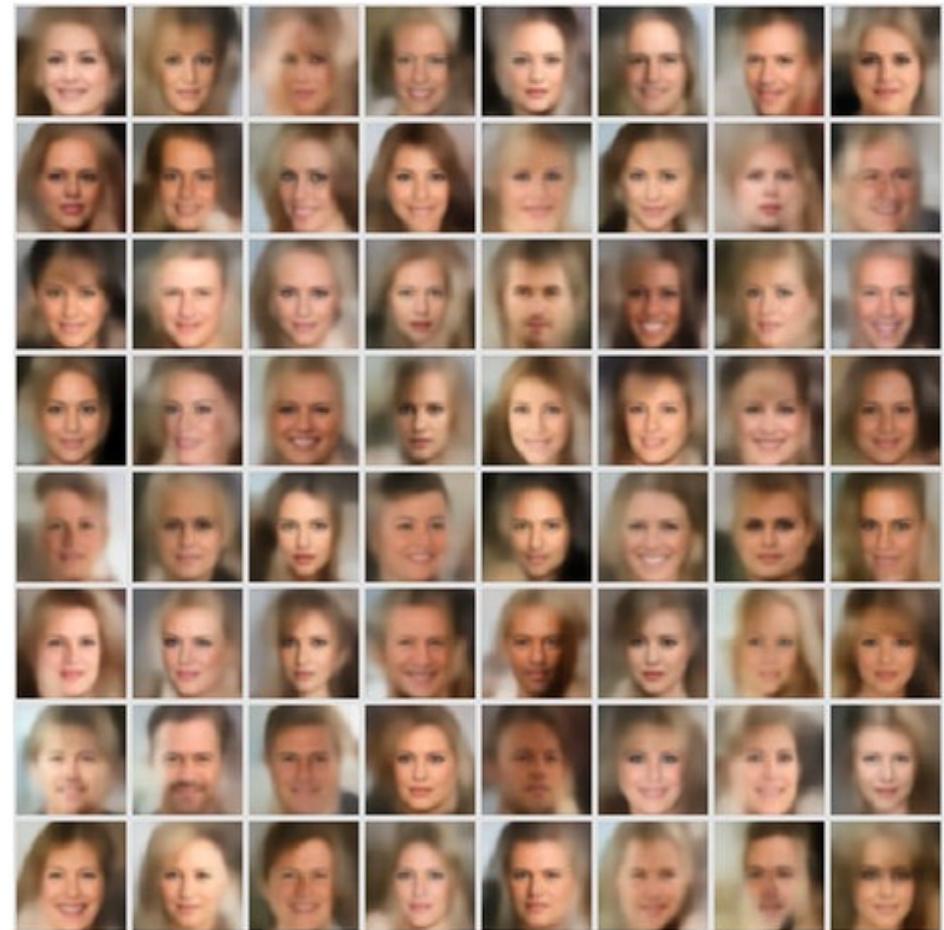
- ▶ KL divergence is considered as one of blurriness causes.
- ▶ We can switch this objective to GAN-like.
- ▶ Price to pay: ELBO becomes less constrained.

<https://arxiv.org/pdf/1511.05644.pdf>

AAE results



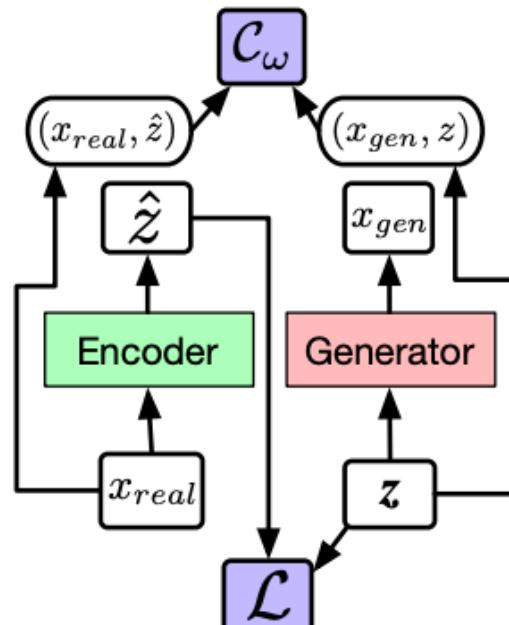
(b) VAE samples



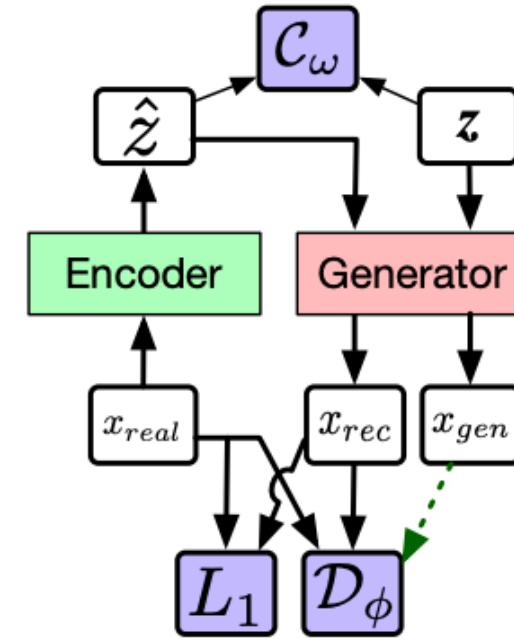
(c) AAE samples

<https://arxiv.org/pdf/1802.06847.pdf>

VEEGAN and VGH



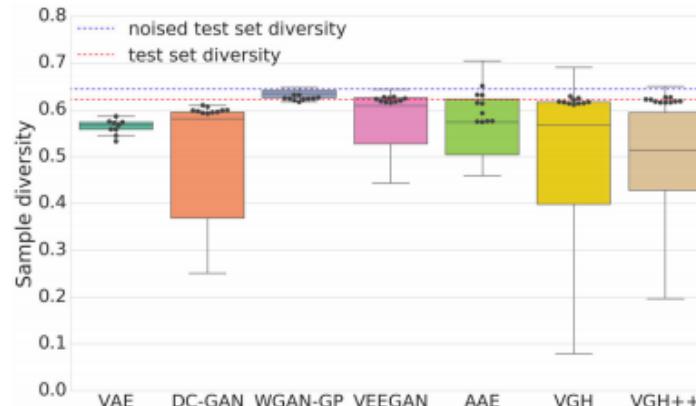
VEEGAN



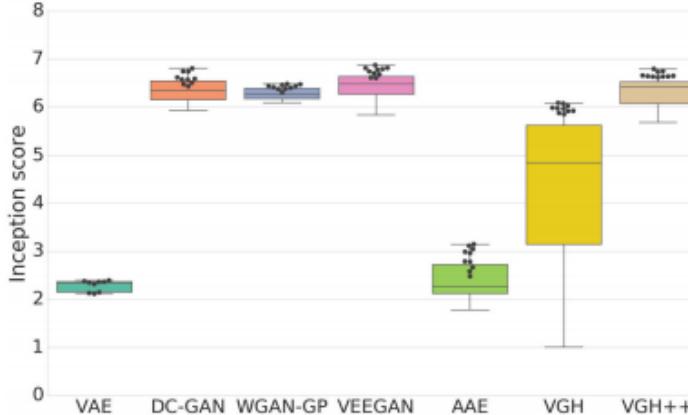
VGH/VGH++

- ▶ VGH: Marginal matching and implicit distributions using GANs both in latent and visible space;
- ▶ VEEGAN: Directly match in joint space.

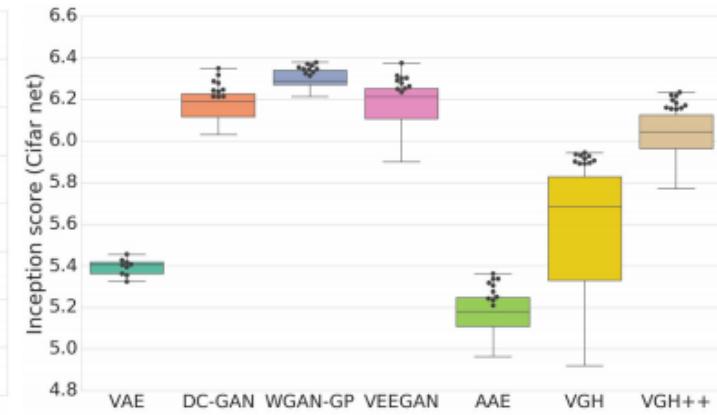
VAE+GAN merged



(a) Diversity score (CelebA)



(b) Inception score (ImageNet)



(c) Inception score (CIFAR)

Figure 8: (Left) Sample diversity on CelebA, and is viewed relative to test set: too much diversity shows failure to capture the data distribution, too little is indicative of mode collapse. We also report the diversity obtained on a noised-version of the test set, which has a higher diversity than the test set. (Middle) Inception scores on CIFAR-10. (Right) Inception scores computed using a VGG-style network on CIFAR-10. For inception scores, higher values are better. For test data, diversity score: 0.621, inception score: 11.25, inception score (using CIFAR-10 trained net): 9.18. Best results are shown with black dots, and box plots show the hyperparameter sensitivity.

- ▶ Our aim was to improve GAN mode collapse and VAE blurriness.
- ▶ The results are yet to be improved.

Conclusions

- ▶ VAE is one of the strong generative models that is used in current days.
- ▶ Several attempts were made to merge strong points of GANs and VAE.
- ▶ Work is ongoing.