VAE variants

Hao Dong

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VAE variants

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Representation learning:
- Convolutional VAE
- Conditional VAE
- β-VAE
- IWAE

Hierarchical representation learning:
- Ladder VAE
- Progressive + Fade-in VAE

Temporal representation learning:
- VAE in speech
- Temporal Difference VAE (TD-VAE)

VAE variants

- Convolutional VAE
- Conditional VAE
- IWAE
- β-VAE
- Ladder VAE
- Progressive + Fade-in VAE
- VAE in speech
- Temporal Difference VAE (TD-VAE)

Representation learning: IWAE, β-VAE

Hierarchical representation learning: Ladder VAE, Progressive + Fade-in VAE

Temporal representation learning: VAE in speech, Temporal Difference VAE (TD-VAE)

Convolutional Variational Autoencoder

- **Limitations of vanilla VAE**
  - The size of weight of fully connected layer == input size x output size
  - If VAE uses fully connected layers only, will lead to curse of dimensionality when the input dimension is large (e.g., image).

- **Solution**

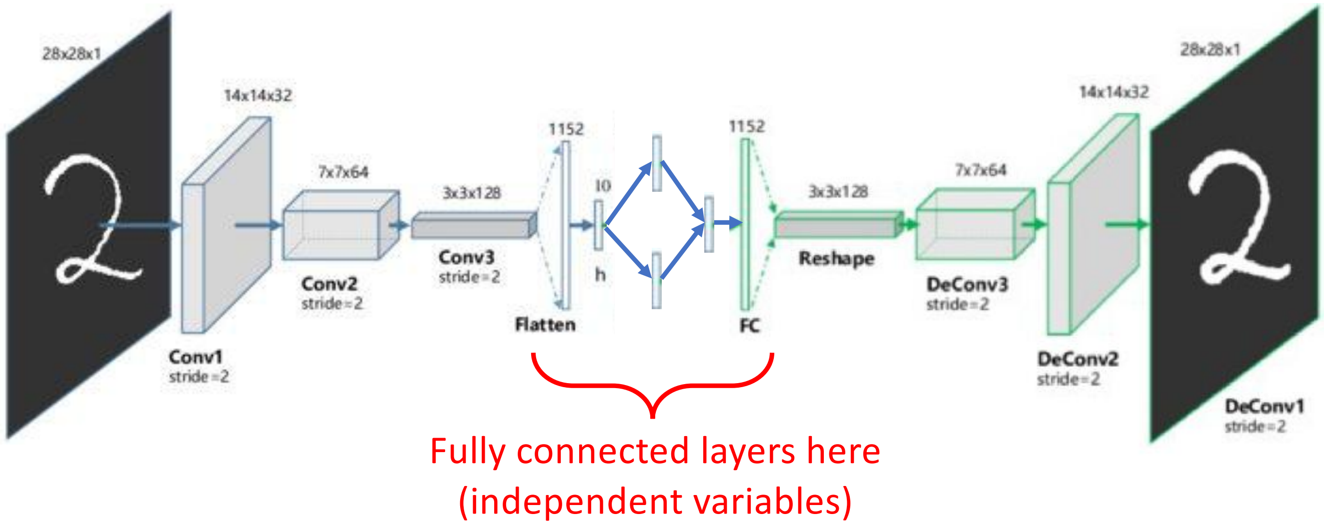

Image is modified from: Deep Clustering with Convolutional Autoencoder. NIPS 2017.

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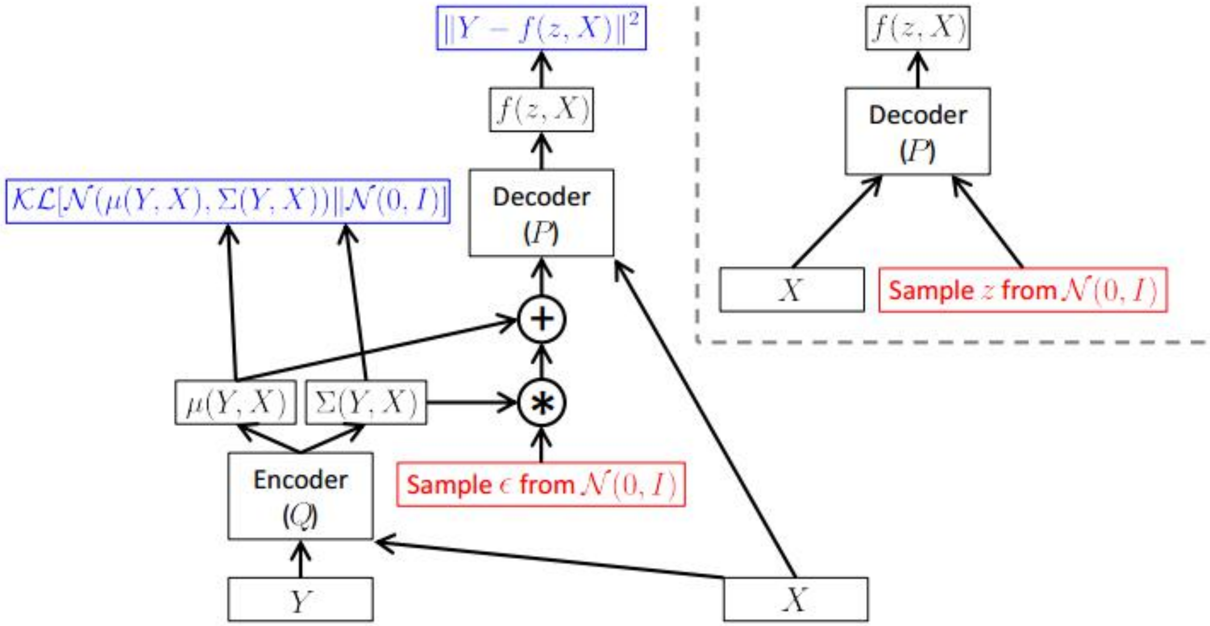
Conditional Variational Autoencoder

- **Train and inference with labelled data.**



Learning structured output representation using deep conditional generative models. NeurIPS 2015.

Recap: Variational Autoencoder

- **Recap: Setting up the objective**
  - Maximise P(X)
  - Set Q(z) to be an arbitrary distribution

$$\mathcal{D}\left[Q(z)\|P(z|X)\right] = E_{z\sim Q}\left[\log Q(z) - \log P(z|X)\right]$$

$$\mathcal{D}\left[Q(z)\|P(z|X)\right] = E_{z\sim Q}\left[\log Q(z) - \log P(X|z) - \log P(z)\right] + \log P(X)$$

$$\log P(X) - \mathcal{D}\left[Q(z)\|P(z|X)\right] = E_{z\sim Q}\left[\log P(X|z)\right] - \mathcal{D}\left[Q(z)\|P(z)\right]$$

$$\boxed{\log P(X) - \mathcal{D}\left[Q(z|X)\|P(z|X)\right] = E_{z\sim Q}\left[\log P(X|z)\right] - \mathcal{D}\left[Q(z|X)\|P(z)\right]}$$

Auto-Encoding Variational Bayes. Diederik P. Kingma, Max Welling. ICLR 2013

Recap: Variational Autoencoder

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- **Recap: Setting up the objective**

$$\log P(X) - \mathcal{D}\left[Q(z|X) \| P(z|X)\right] = E_{z\sim Q}\left[\log P(X|z)\right] - \mathcal{D}\left[Q(z|X) \| P(z)\right]$$

encoder ideal reconstruction KLD

Auto-Encoding Variational Bayes. Diederik P. Kingma, Max Welling. ICLR 2013

Conditional Variational Autoencoder

- **Setting up the objective with labels**
  - Maximise P(Y|X)
  - Set Q(z) to be an arbitrary distribution

$$\mathcal{D}\left[Q(z|Y,X)\|P(z|Y,X)\right] = E_{z\sim Q(\cdot|Y,X)}\left[\log Q(z|Y,X) - \log P(z|Y,X)\right]$$

$$\mathcal{D}\left[Q(z|Y,X)\|P(z|Y,X)\right] = \\ E_{z\sim Q(\cdot|Y,X)}\left[\log Q(z|Y,X) - \log P(Y|z,X) - \log P(z|X)\right] + \log P(Y|X)$$

$$\log P(Y|X) - \mathcal{D}\left[Q(z|Y,X)\|P(z|Y,X)\right] = \\ E_{z\sim Q(\cdot|Y,X)}\left[\log P(Y|z,X)\right] - \mathcal{D}\left[Q(z|Y,X)\|P(z|X)\right]$$

Learning structured output representation using deep conditional generative models. NeurIPS 2015.

Conditional Variational Autoencoder

- **Setting up the objective**

encoder ideal

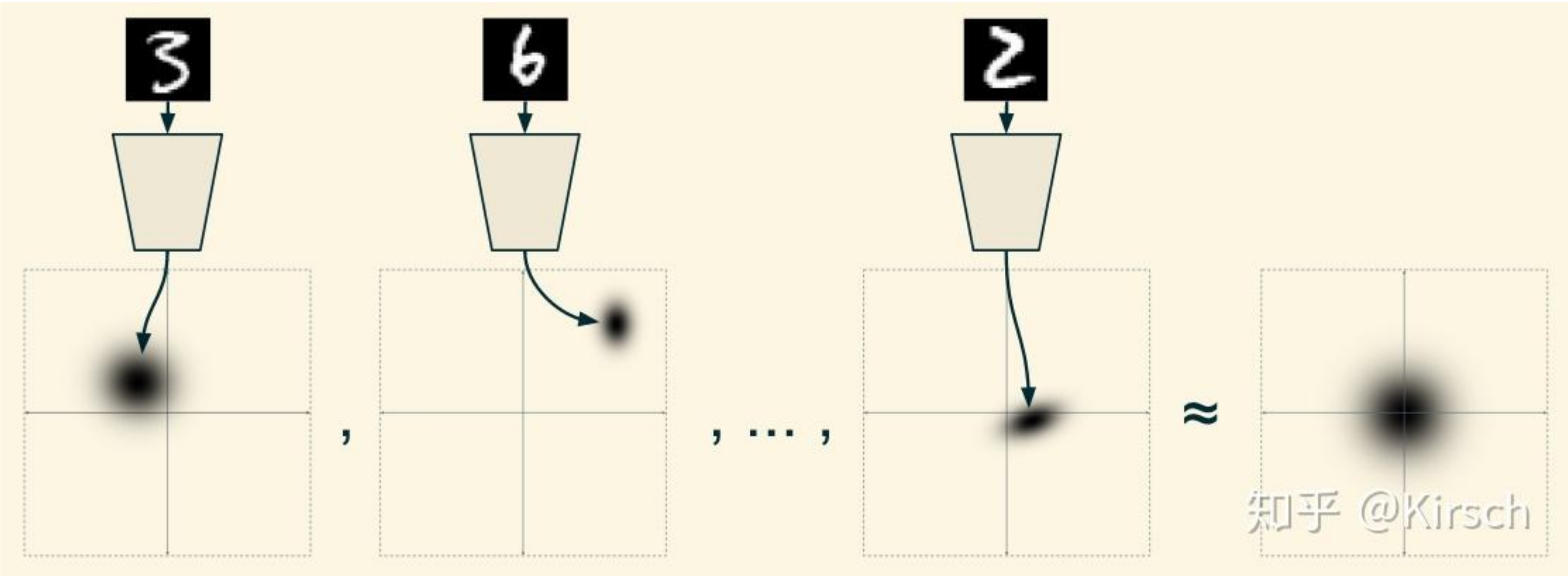
$$\log P(Y|X) - \mathcal{D}\left[Q(z|Y,X) \| P(z|Y,X)\right] = E_{z\sim Q(\cdot|Y,X)}\left[\log P(Y|z,X)\right] - \mathcal{D}\left[Q(z|Y,X) \| P(z|X)\right]$$

reconstruction KLD

Learning structured output representation using deep conditional generative models. NeurIPS 2015.

Conditional Variational Autoencoder

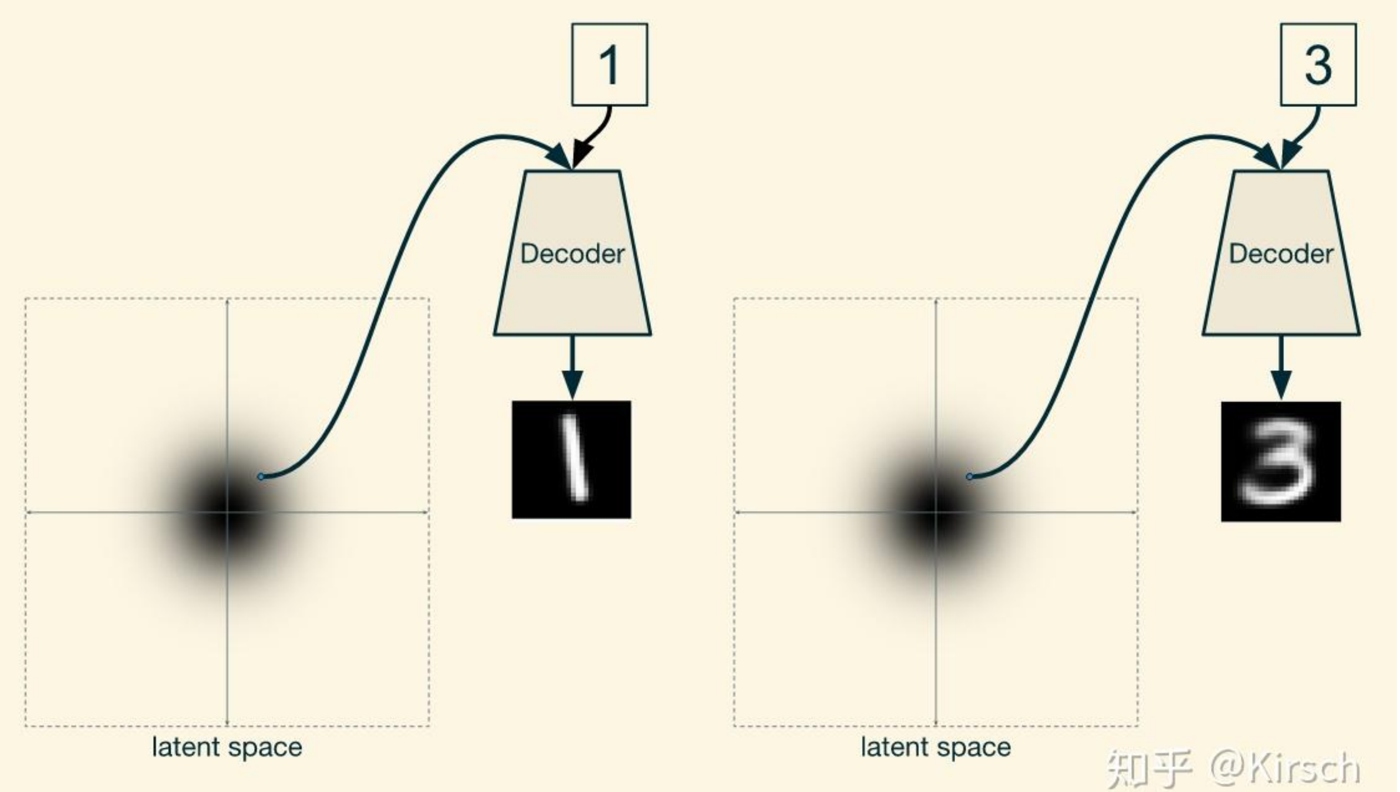
- **Train and inference without labelled data i.e., vanilla VAE**



Learning structured output representation using deep conditional generative models. NeurIPS 2015.

Conditional Variational Autoencoder

- **Train and inference with labelled data.**

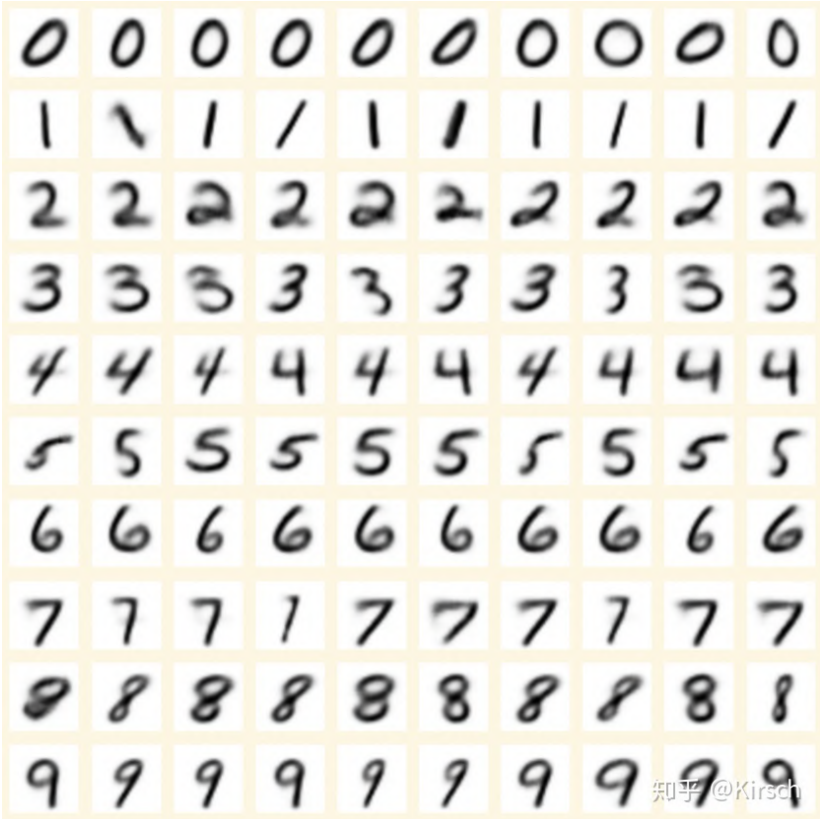


A variational autoencoder generating images according to given labels

Learning structured output representation using deep conditional generative models. NeurIPS 2015.

Conditional Variational Autoencoder

- **Train and inference with labelled data.**



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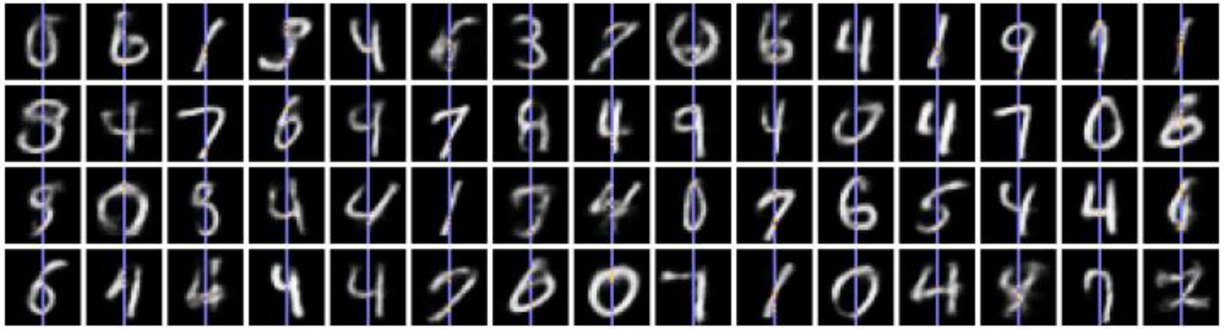
Conditional Variational Autoencoder

- **Train and inference with labeled data.**



(a) CVAE

(b) Regressor

Learning structured output representation using deep conditional generative models. NeurIPS 2015.

VAE variants

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Representation learning

Hierarchical representation learning

Temporal representation learning

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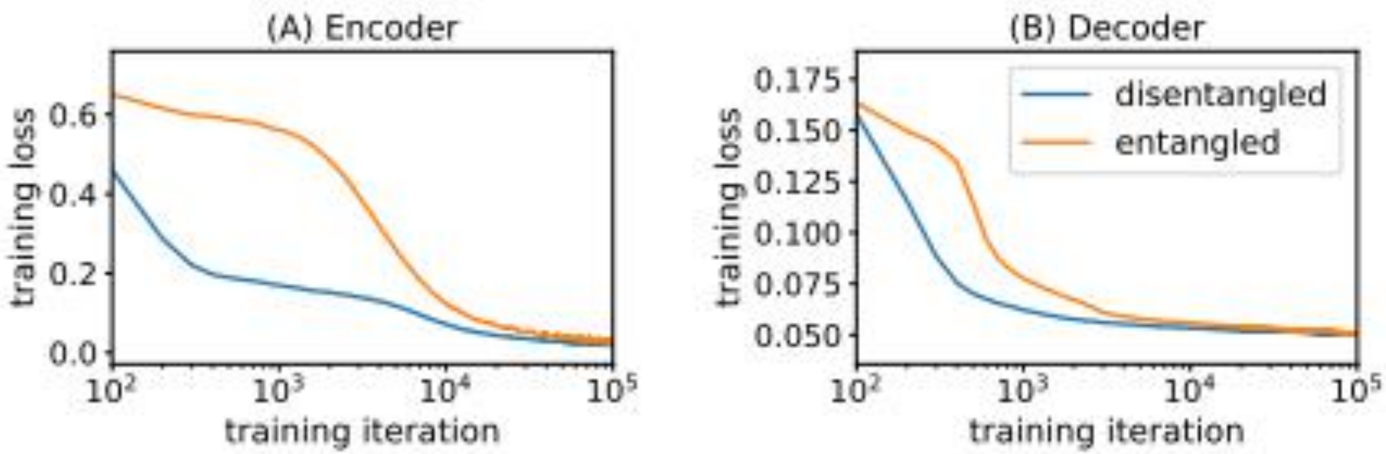
Before we start

- **Disentangled / Factorised representation**
  - Each variable in the inferred latent representation is only sensitive to one single generative factor and relatively invariant to other factors
  - Good interpretability and easy generalization to a variety of tasks

β-VAE: Learning Basic Visual Concepts with a Constrained Variational Framework. Irina Higgins, Loic Matthey, Arka Pal, Christopher Burgess, Xavier Glorot, Matthew Botvinick, Shakir Mohamed, and Alexander Lerchner. ICLR 2017.

Before we start

- **Unsupervised hierarchical representation learning**



Rethinking Style and Content Disentanglement in Variational Autoencoders. ICLR 2018 Workshops.

β-VAE

- **Unsupervised representation learning**
  - Augment the original VAE framework with a single hyper-parameter β that modulates the learning constraints
  - Impose a limit on the capacity of the latent information channel

β-VAE: Learning Basic Visual Concepts with a Constrained Variational Framework. Irina Higgins, Loic Matthey, Arka Pal, Christopher Burgess, Xavier Glorot, Matthew Botvinick, Shakir Mohamed, and Alexander Lerchner. ICLR 2017.

β-VAE

$$\max_{\phi,\theta} \mathbb{E}_{\mathbf{x}\sim\mathcal{D}}[\mathbb{E}_{\mathbf{z}\sim q_\phi(\mathbf{z}|\mathbf{x})} \log p_\theta(\mathbf{x}|\mathbf{z})]$$

$$\text{subject to } D_{\mathrm{KL}}(q_\phi(\mathbf{z}|\mathbf{x})\|p_\theta(\mathbf{z})) < \delta$$

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β-VAE

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$$\begin{aligned}\mathcal{F}(\theta,\phi,\beta) &= \mathbb{E}_{\mathbf{z}\sim q_\phi(\mathbf{z}|\mathbf{x})} \log p_\theta(\mathbf{x}|\mathbf{z}) - \beta(D_{\mathrm{KL}}(q_\phi(\mathbf{z}|\mathbf{x})||p_\theta(\mathbf{z})) - \delta) \\ &= \mathbb{E}_{\mathbf{z}\sim q_\phi(\mathbf{z}|\mathbf{x})} \log p_\theta(\mathbf{x}|\mathbf{z}) - \beta D_{\mathrm{KL}}(q_\phi(\mathbf{z}|\mathbf{x})||p_\theta(\mathbf{z})) + \beta\delta \\ &\geq \mathbb{E}_{\mathbf{z}\sim q_\phi(\mathbf{z}|\mathbf{x})} \log p_\theta(\mathbf{x}|\mathbf{z}) - \beta D_{\mathrm{KL}}(q_\phi(\mathbf{z}|\mathbf{x})||p_\theta(\mathbf{z})) \qquad \text{; Because } \beta,\delta \geq 0\end{aligned}$$

β-VAE: Learning Basic Visual Concepts with a Constrained Variational Framework. Irina Higgins, Loic Matthey, Arka Pal, Christopher Burgess, Xavier Glorot, Matthew Botvinick, Shakir Mohamed, and Alexander Lerchner. ICLR 2017.

β-VAE

$$L_{\mathrm{BETA}}(\phi,\beta) = -\mathbb{E}_{\mathbf{z}\sim q_\phi(\mathbf{z}|\mathbf{x})} \log p_\theta(\mathbf{x}|\mathbf{z}) + \beta D_{\mathrm{KL}}\left(q_\phi(\mathbf{z}|\mathbf{x}) \| p_\theta(\mathbf{z})\right)$$

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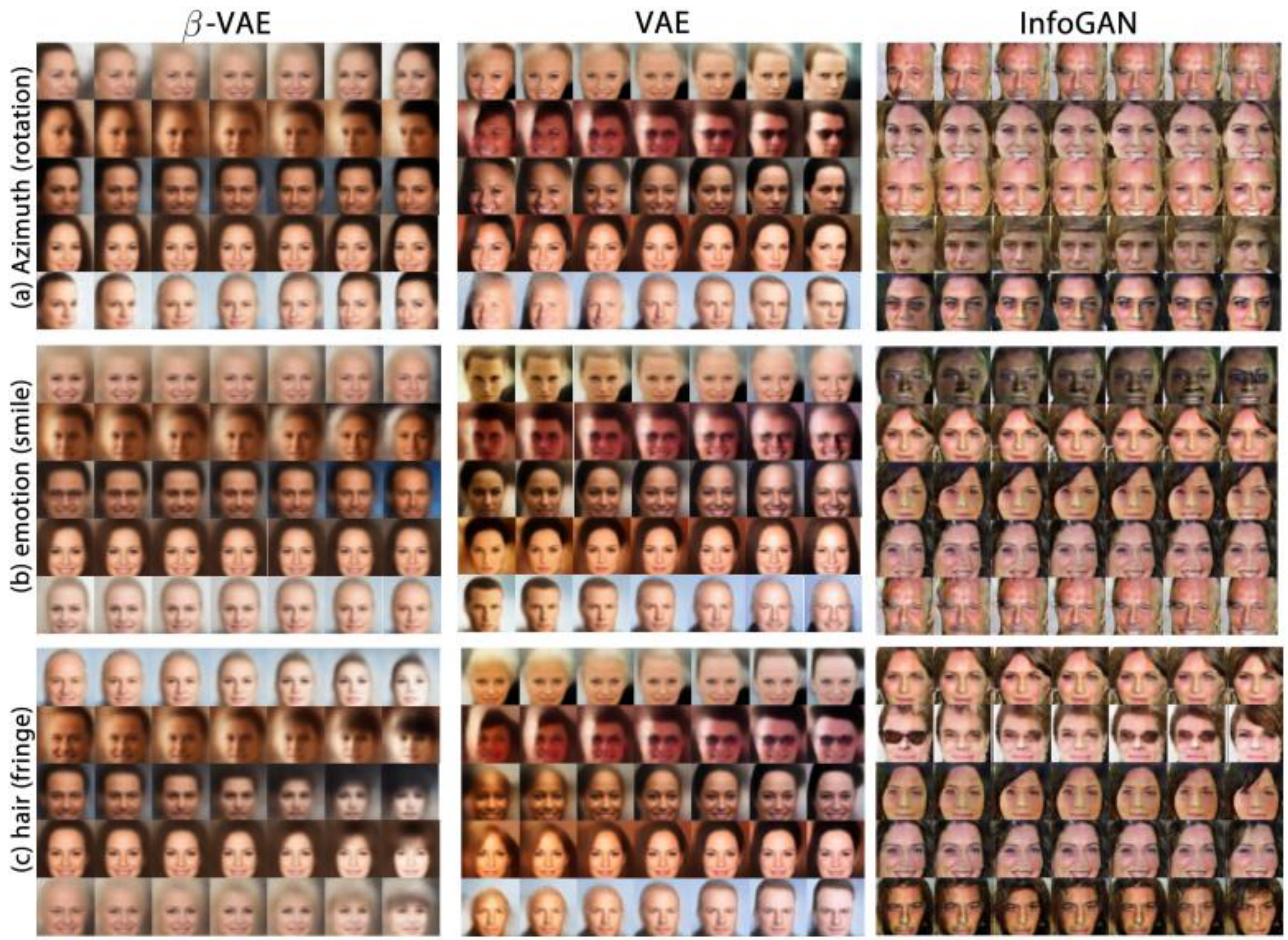
β-VAE



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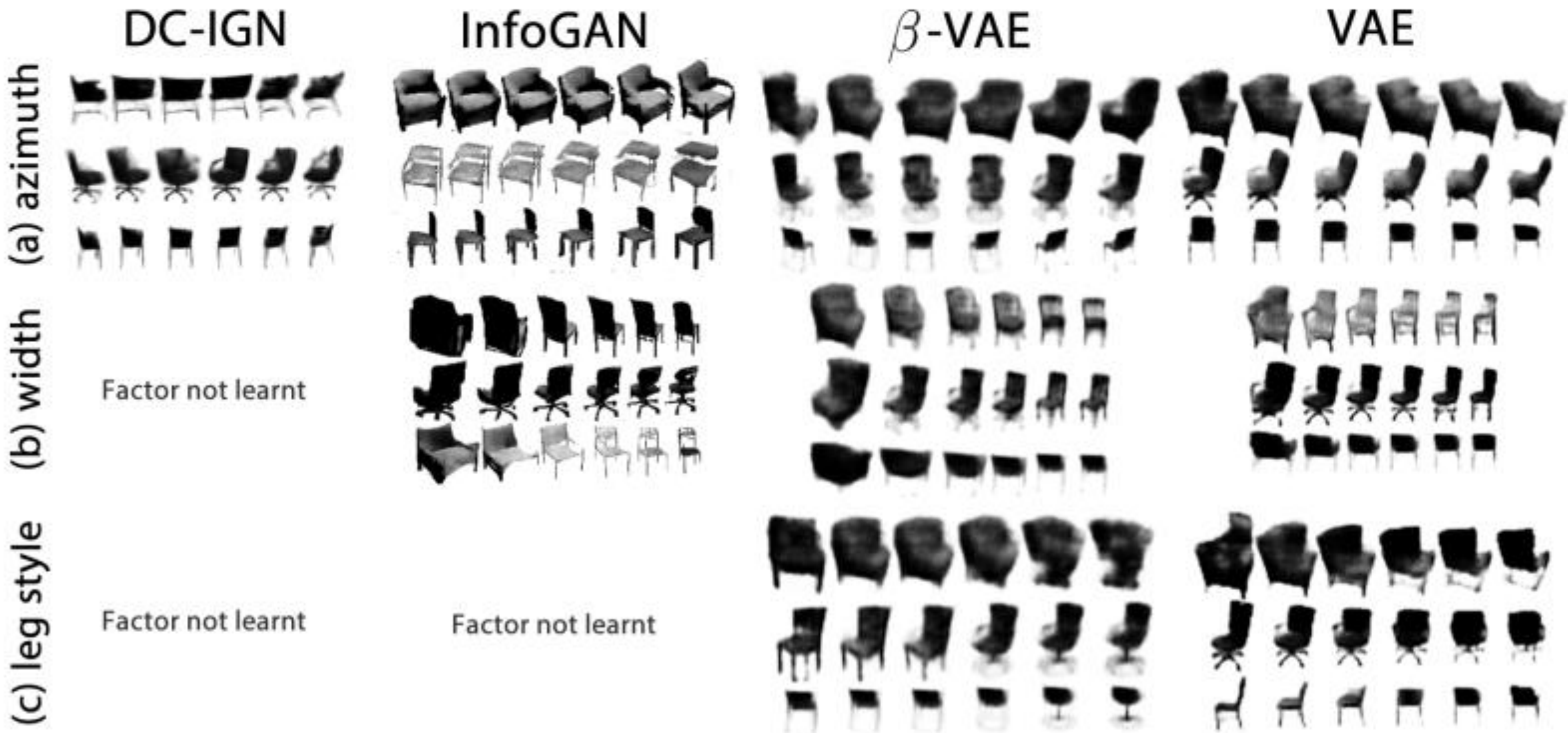

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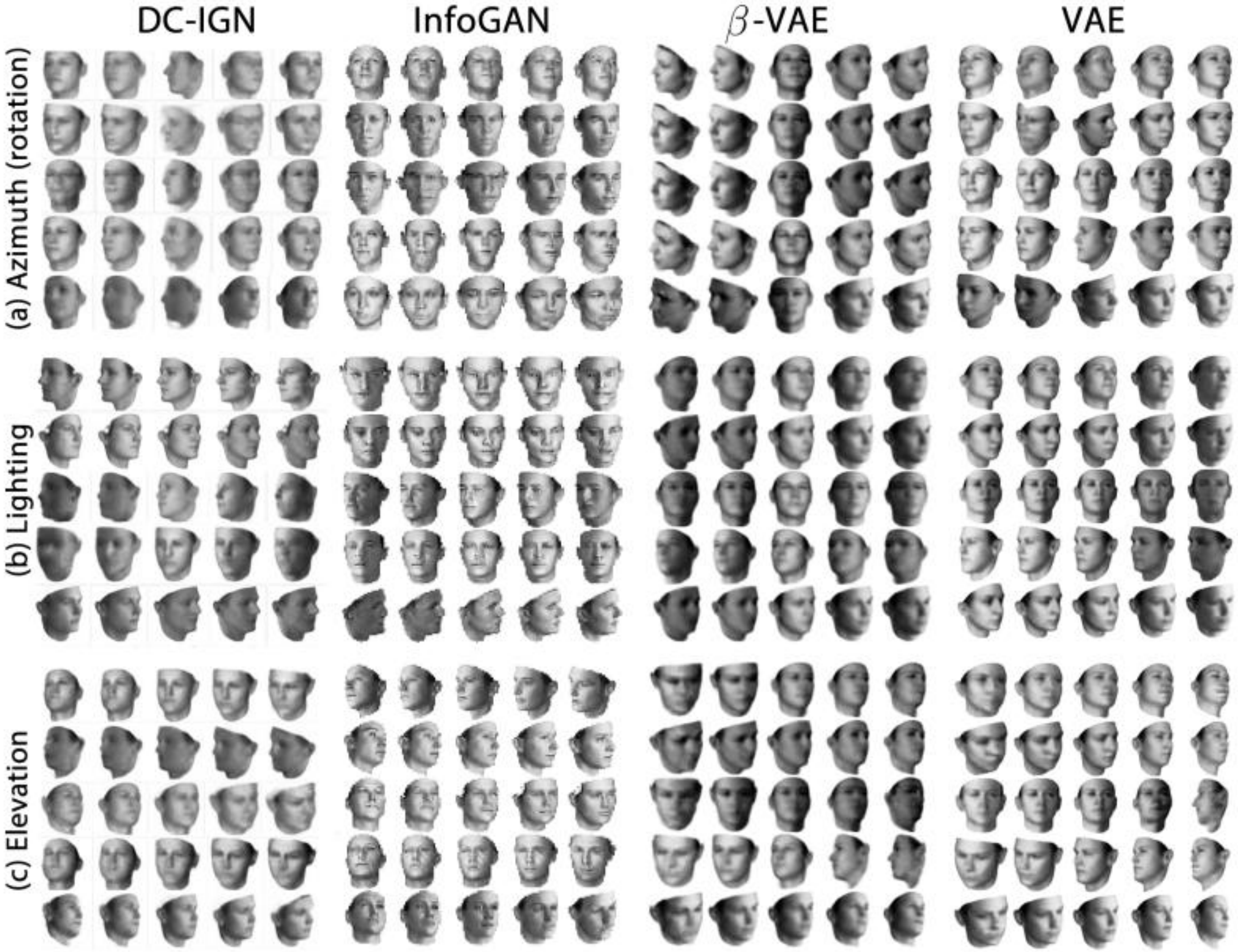

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β-VAE

- **Discussion: It is really unsupervised?**
  - It is unsupervised/self-supervised learning, because it does not need any label data
  - It is not fully unsupervised learning, it works because of the inductive bias of the neural network model, the hierarchical design introduces prior knowledge about the data

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VAE variants

Representation learning

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Hierarchical representation learning

Temporal representation learning

IWAE（Importance Weighted Autoencoder）

- **Optimise a tighter lower bound than VAE**
  - VAE just optimises a lower bound of log P(X)

$$\log P(X) - \mathcal{D}\left[Q(z|X) \| P(z|X)\right] = E_{z\sim Q}\left[\log P(X|z)\right] - \mathcal{D}\left[Q(z|X) \| P(z)\right]$$

encoder ideal reconstruction KLD

ELBO

Importance Weighted Autoencoders. ICLR 2016.

IWAE

- **Optimise a tighter lower bound than VAE**

$$\log p(x) = \log \int p(x,z)dz = \log \int \frac{p(x,z)}{q(z|x)} q(z|x)dz = \log E_{q(z|x)}[\frac{p(x,z)}{q(z|x)}]$$

$$\log E_{q(z|x)}[\frac{p(x,z)}{q(z|x)}] = \log E_{z_1,z_2,\ldots,z_k \sim q(z|x)}[\frac{1}{k}\sum_{i=1}^{k} \frac{p(x,z_i)}{q(z_i|x)}]$$

$$L_k(x) = E_{z_1,z_2,\ldots,z_k \sim q(z|x)}[\log \frac{1}{k}\sum_{i=1}^{k} \frac{p(x,z_i)}{q(z_i|x)}] \leq \log E_{z_1,z_2,\ldots,z_k \sim q(z|x)}[\frac{1}{k}\sum_{i=1}^{k} \frac{p(x,z_i)}{q(z_i|x)}] = \boxed{\log p(x)}$$

Importance Weighted Autoencoders. ICLR 2016.

IWAE

$$ELBO(\theta) = \mathbf{E}_q[\log p(x, z)] - \mathbf{E}_q[\log q_\theta(z \mid x)]$$

VAE 的loss： $E_{z \sim q(z|x)}[\log \frac{p(x,z)}{q(z|x)}]$

而IWAE的loss： $E_{z_1, z_2, \ldots, z_k \sim q(z|x)}[\log \frac{1}{k} \sum_{i=1}^{k} \frac{p(x, z_i)}{q(z_i|x)}]$

Importance Weighted Autoencoders. ICLR 2016.

IWAE

- **Why “Importance weighted”**

$$\nabla_\theta \; E_{z_1, z_2, \ldots, z_k \sim q(z|x,\theta)} [\log \frac{1}{k} \sum_{i=1}^{k} \frac{p(x, z_i|\theta)}{q(z_i|x,\theta)}] = E_{z_1, z_2, \ldots, z_k \sim q(z|x,\theta)} [\nabla_\theta \; \log \frac{1}{k} \sum_{i=1}^{k} w_i]$$

where $w_i = \frac{p(x, z_i|\theta)}{q(z_i|x,\theta)}$

VAE: $\frac{1}{k} \sum_{i=1}^{k} \nabla_\theta \log w_i$

IWAE: $\sum_{i=1}^{k} \tilde{w}_i \nabla_\theta \; \log w_i$

Importance Weighted Autoencoders. ICLR 2016.

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Temporal representation learning
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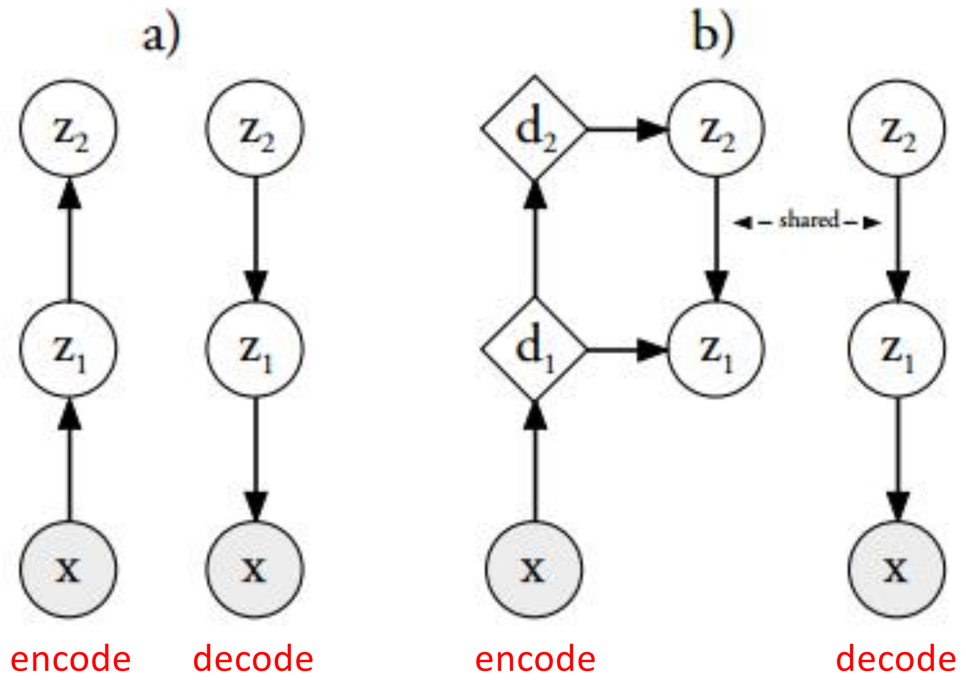
Ladder VAE

- **To learn hierarchical latent representation**
- **Deep models with several layers of dependent stochastic variables are difficult to train**
  - Limiting the improvements obtained using these highly expressive models

LVAE: Ladder Variational Autoencoder. Casper Kaae Sønderby, Tapani Raiko, Lars Maaløe, Søren Kaae Sønderby, and Ole Winther. NIPS 2016.

Ladder VAE



Hierarchical VAE　　Ladder VAE

LVAE: Ladder Variational Autoencoder. Casper Kaae Sønderby, Tapani Raiko, Lars Maaløe, Søren Kaae Sønderby, and Ole Winther. NIPS 2016.

Ladder VAE

$$\mathcal{L}(\theta, \phi; \mathbf{x})_{WU} = -\beta KL(q_\phi(z|x)||p_\theta(\mathbf{z})) + E_{q_\phi(z|x)}\left[\log p_\theta(\mathbf{x}|\mathbf{z})\right]$$

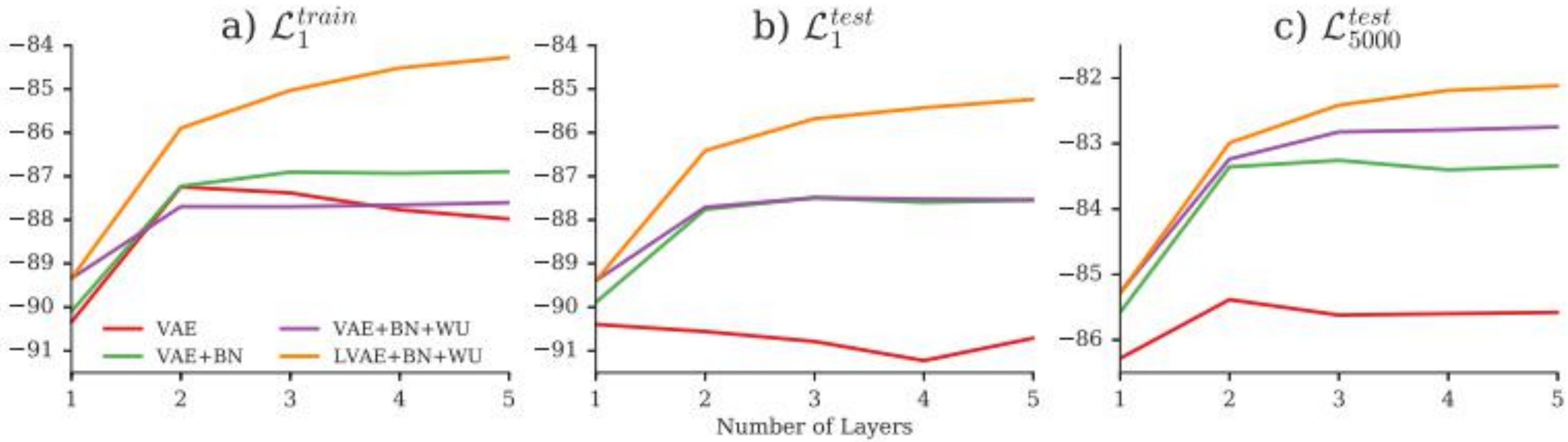


Figure 3: MNIST log-likelihood values for VAEs and the LVAE model with different number of latent layers, Batch-normalization (*BN*) and Warm-up (*WU*). a) Train log-likelihood, b) test log-likelihood and c) test log-likelihood with 5000 importance samples.

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Ladder VAE

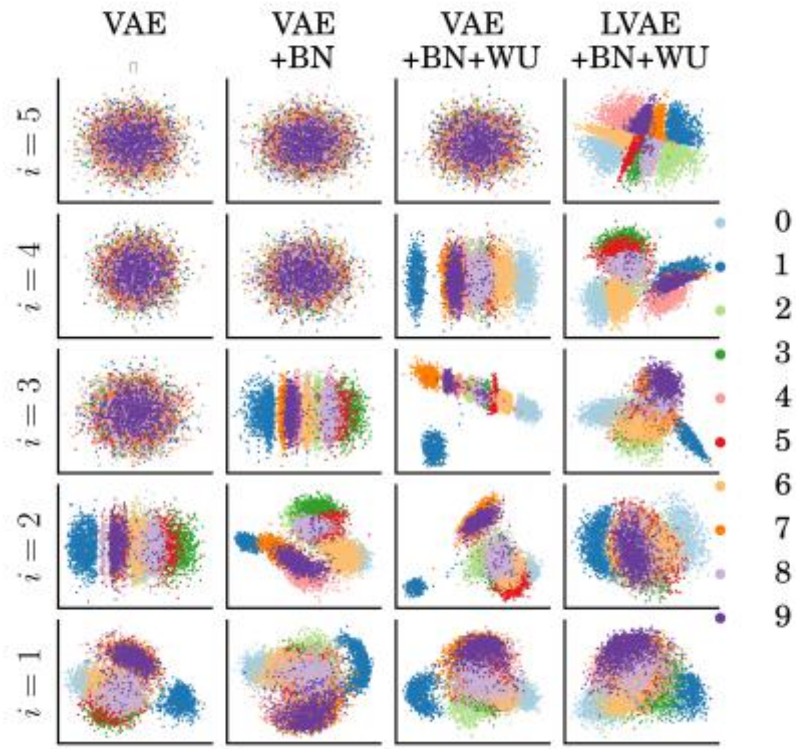
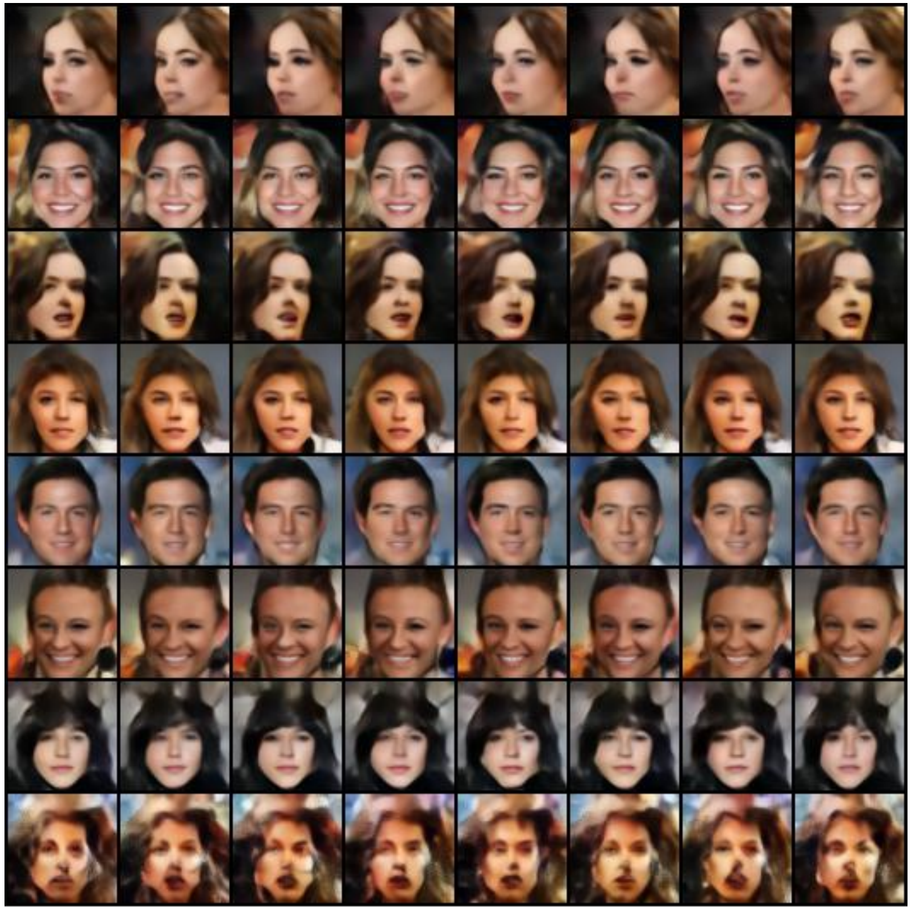


Figure 6: PCA-plots of samples from $q(z_i|z_{i-1})$ for 5-layer VAE and LVAE models trained on MNIST. Color-coded according to true class label

LVAE: Ladder Variational Autoencoder. Casper Kaae Sønderby, Tapani Raiko, Lars Maaløe, Søren Kaae Sønderby, and Ole Winther. NIPS 2016.

Ladder VAE



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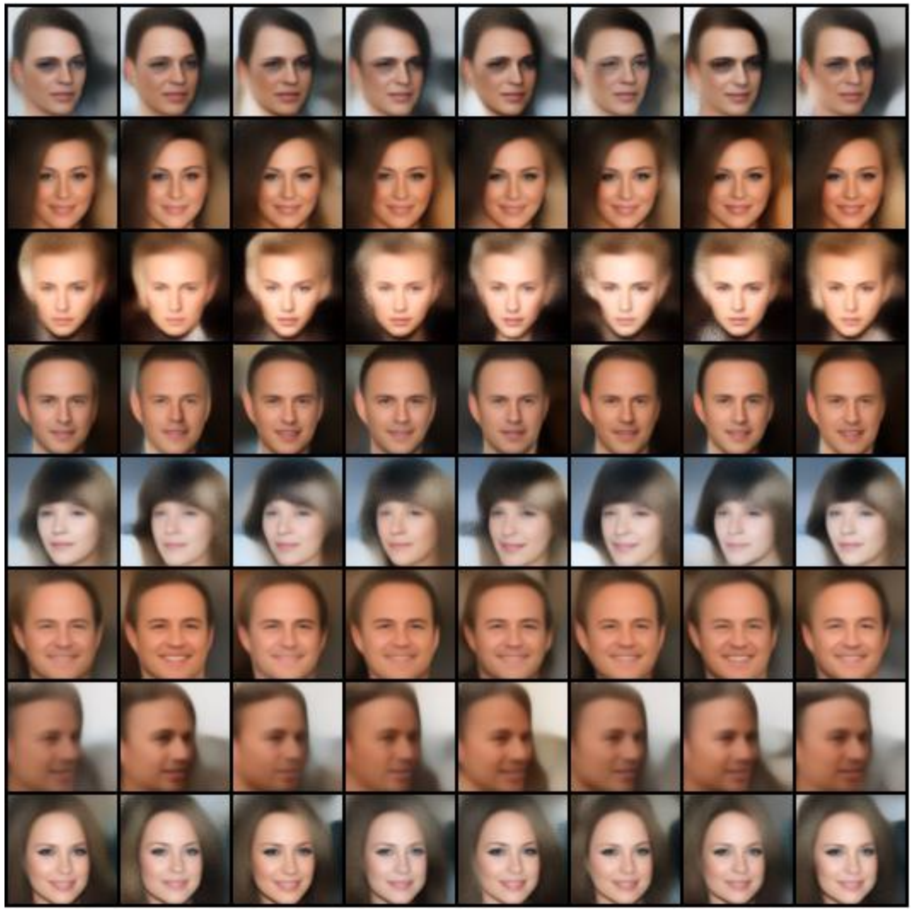
Ladder VAE



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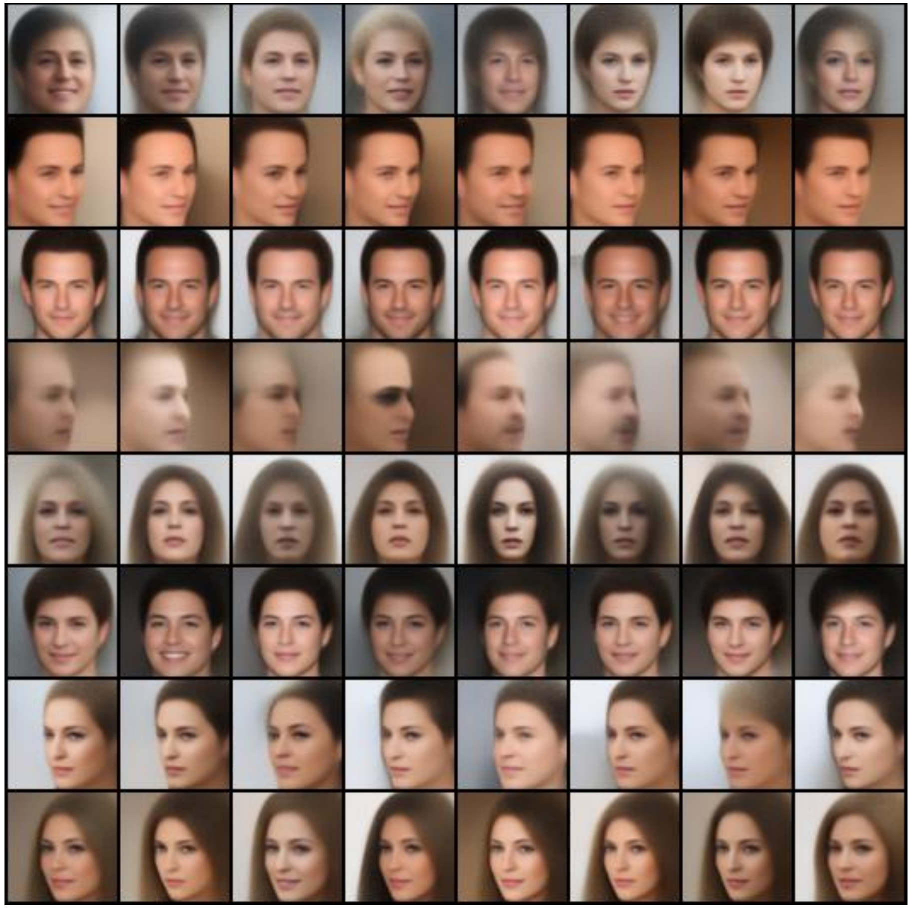

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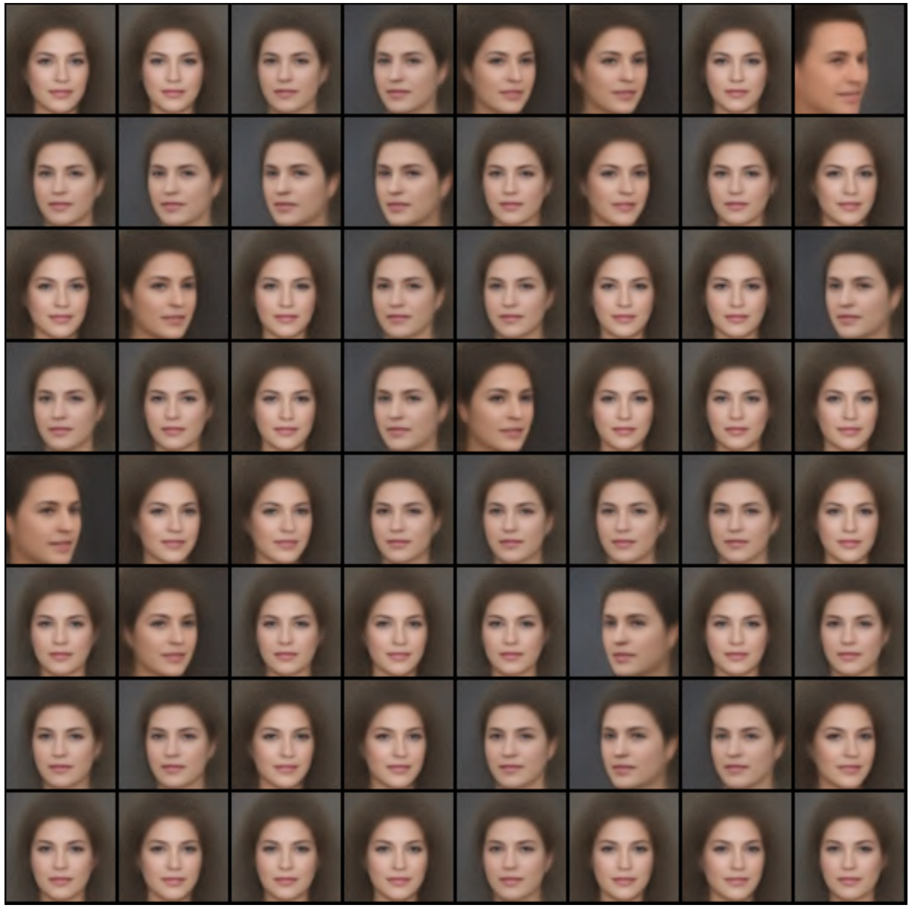

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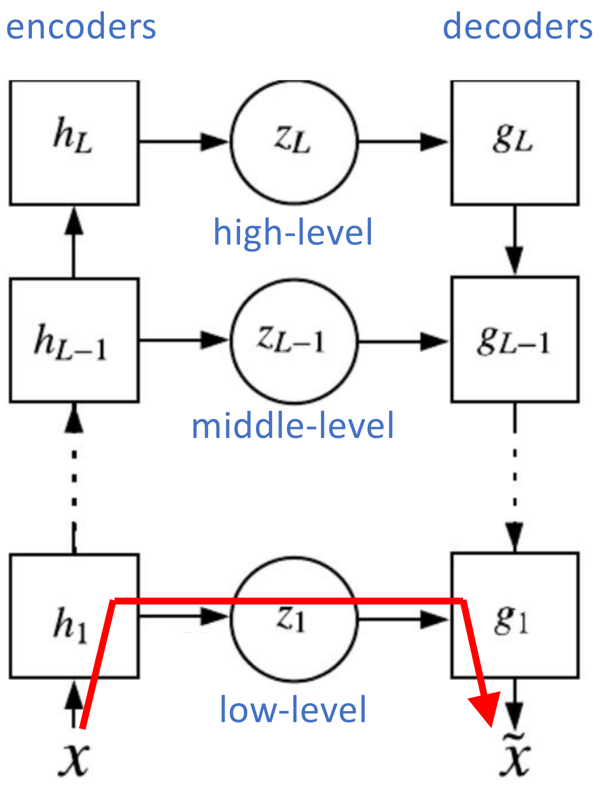
Progressive + Fade-in VAE

- **Discussion**

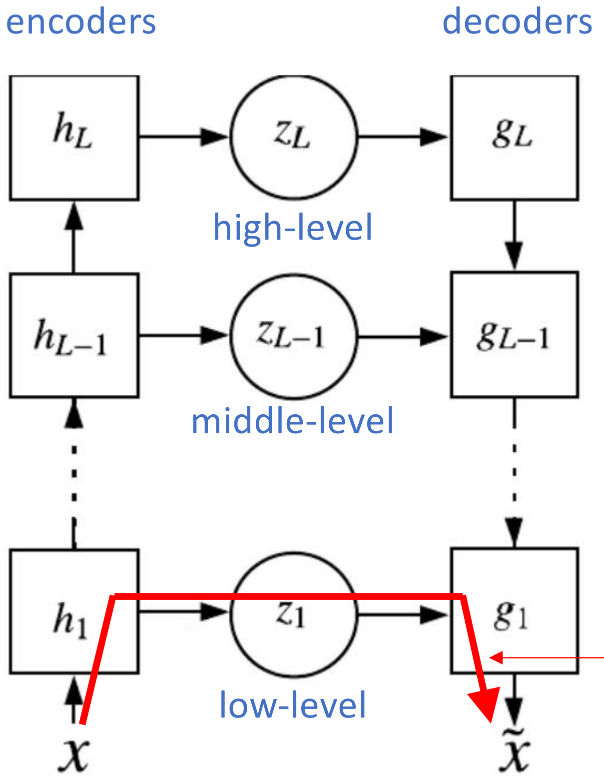


Can we directly train a hierarchical VAE with ladder structure like that?

Progressive Learning and Disentanglement of Hierarchical Representations. ICLR 2020.

Progressive + Fade-in VAE

- **Discussion**



$$
\begin{aligned}
\mathrm{E}_{q(x)}[KL(q(z|x)||p(z))] &= \int\int q(x)q(z|x)log\frac{q(z|x)}{p(z)}dxdz \\
&= \int\int q(x,z)log\frac{q(z|x)q(x)q(z)}{p(z)q(x)p(z)}dxdz \\
&= \int\int [q(x,z)log\frac{q(x,z)}{q(x)q(z)} + q(x,z)log\frac{q(z)}{p(z)}]dxdz \\
&= MI_{q(x,z)}(x,z) + \int\int q(x,z)log\frac{q(z)}{p(z)}dxdz \\
&= MI_{q(x,z)}(x,z) + \int q(z)log\frac{q(z)}{p(z)}dz \\
&= \boxed{MI_{q(x,z)}(x,z)} + KL(q(z)||p(z))
\end{aligned}
$$

Information **SHORTCUT** problem

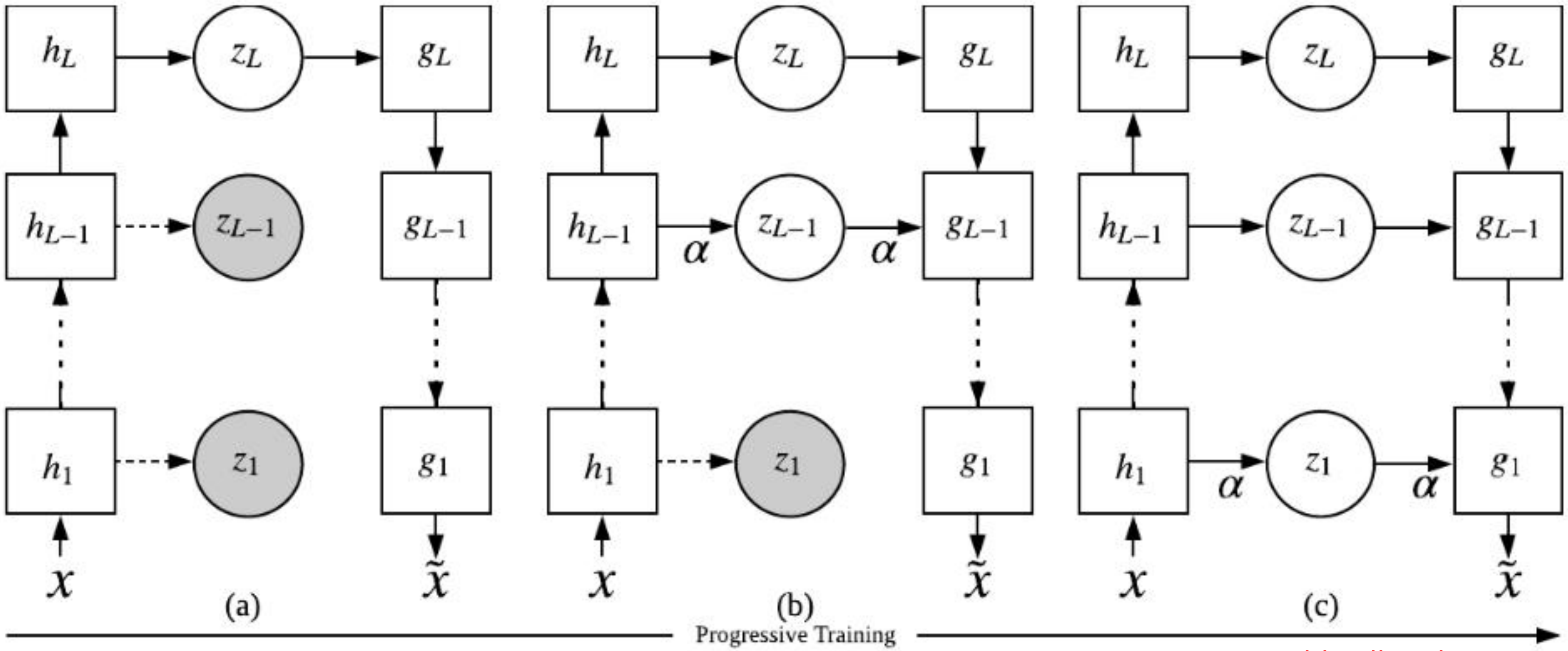
all information go through the low-level path,
other paths are ignored.
model is lazy…

Progressive Learning and Disentanglement of Hierarchical Representations. ICLR 2020.

Progressive + Fade-in VAE

- **Progressive + Fade-in**

α increase from 0 to 1 gradually



Stage 1: enable high-level path

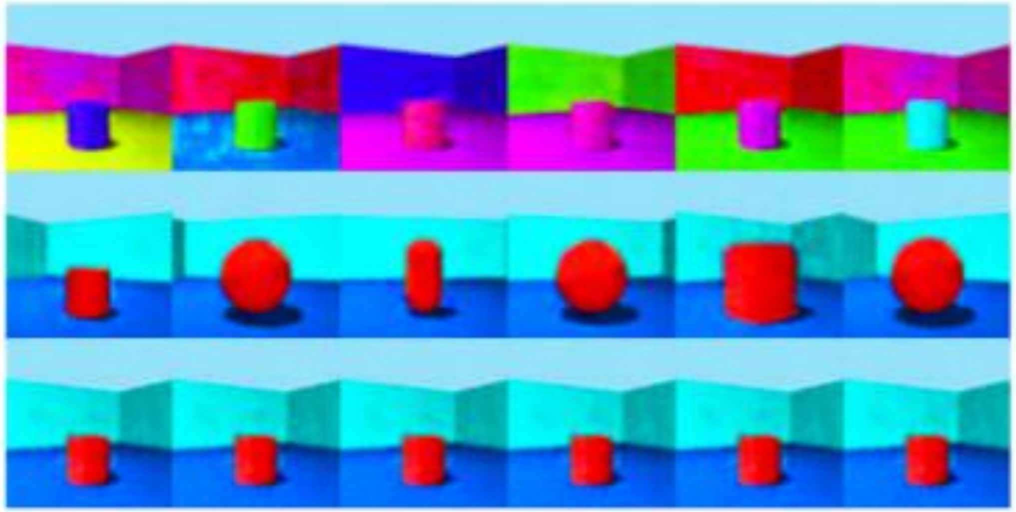
Stage 2: enable high-level and middle paths

Stage 3: enable all paths …

Progressive Learning and Disentanglement of Hierarchical Representations. ICLR 2020.

Progressive + Fade-in VAE

- **Results**



z_3 High-level: background and foreground colors

z_2 Middle-level: shape

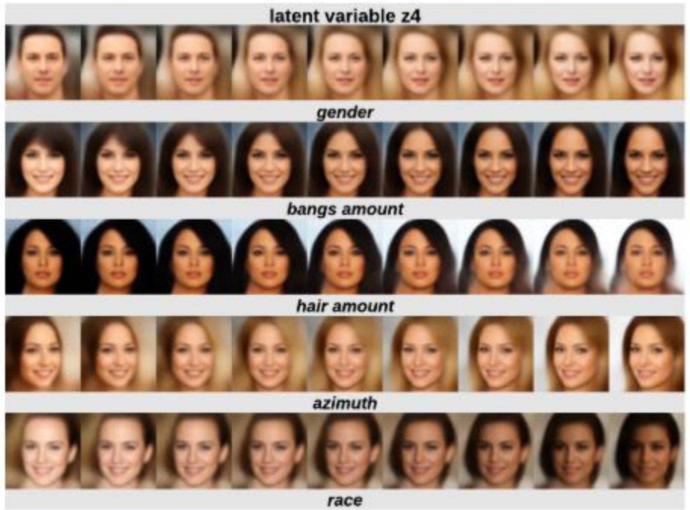
z_1 Low-level: …

Progressive Learning and Disentanglement of Hierarchical Representations. ICLR 2020.

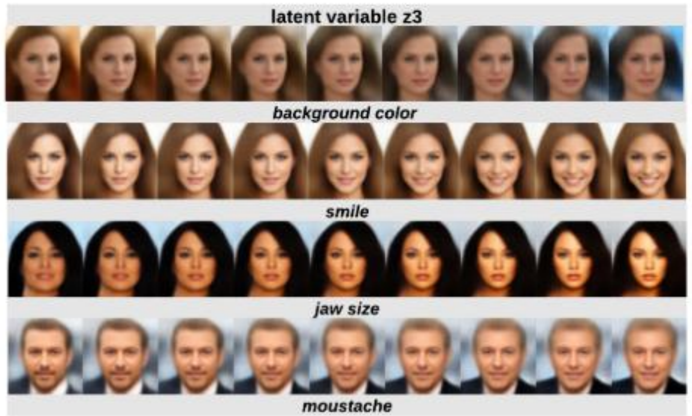
Progressive + Fade-in VAE

- **Results**

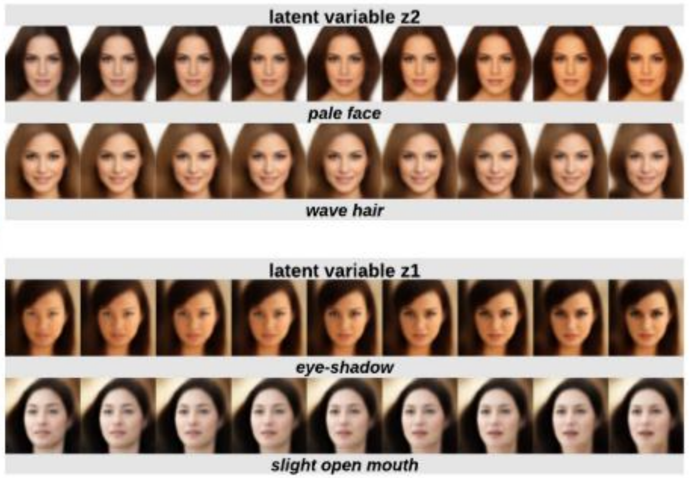
High-level



Middle-level



Low-level



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Other variants:
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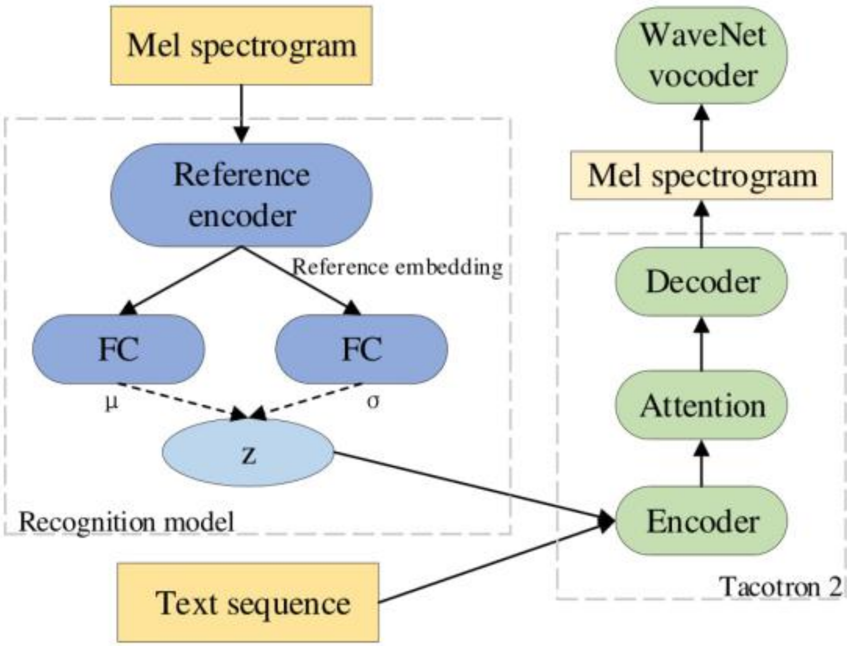
- Conditional VAE

VAE in speech

- **Learning latent representations for style control and transfer in end-to-end speech synthesis**
- **RNN as encoder**



Learning latent representations for style control and transfer in end-to-end speech synthesis. ICASSP 2019.

VAE variants

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- Convolutional VAE
- Conditional VAE

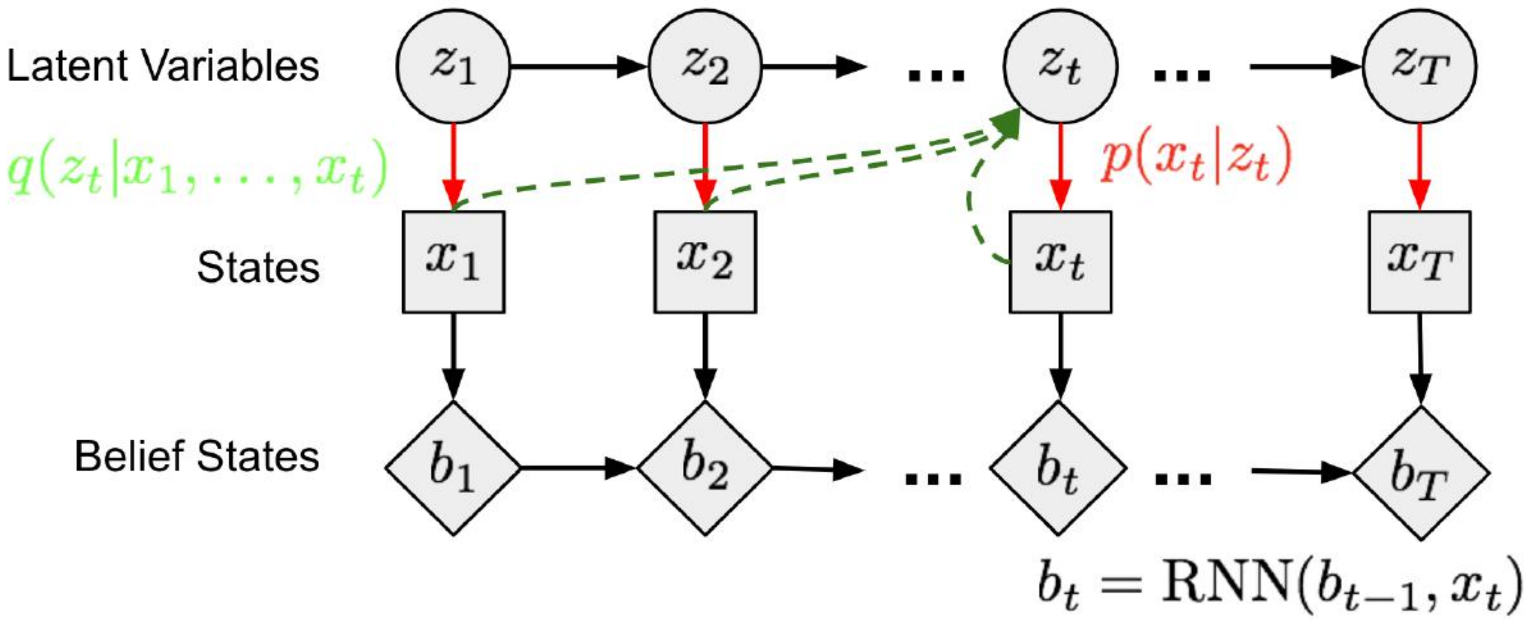
Representation learning
- β-VAE
- IWAE

Hierarchical representation learning
- Ladder VAE
- Progressive + Fade-in VAE

Temporal representation learning
- VAE in speech
- Temporal Difference VAE (TD-VAE)

TD-VAE

- **State-space model as a Markov Chain model**



Temporal Difference VAE. ICLR 2019.

TD-VAE

$$b_t = belief(x_1, \ldots, x_t) = belief(b_{t-1}, x_t) \qquad b_t = \mathrm{RNN}(b_{t-1}, x_t)$$

$$p(x_{t+1}, \ldots, x_T | x_1, \ldots, x_t) \approx p(x_{t+1}, \ldots, x_T | b_t)$$

Temporal Difference VAE. ICLR 2019.

TD-VAE

$$
\begin{aligned}
\log p(x) &\geq \log p(x) - D_{\mathrm{KL}}(q(z|x) \| p(z|x)) \\
&= \mathbb{E}_{z\sim q} \log p(x|z) - D_{\mathrm{KL}}(q(z|x) \| p(z)) \\
&= \mathbb{E}_{z\sim q} \log p(x|z) - \mathbb{E}_{z\sim q} \log \frac{q(z|x)}{p(z)} \\
&= \mathbb{E}_{z\sim q}[\log p(x|z) - \log q(z|x) + \log p(z)] \\
&= \mathbb{E}_{z\sim q}[\log p(x,z) - \log q(z|x)] \\
\log p(x) &\geq \mathbb{E}_{z\sim q}[\log p(x,z) - \log q(z|x)]
\end{aligned}
$$

Temporal Difference VAE. ICLR 2019.

TD-VAE

$$
\begin{aligned}
&\log p(x_t|x_{<t}) \\
&\geq \mathbb{E}_{(z_{t-1},z_t)\sim q}[\log p(x_t, z_{t-1}, z_t|x_{<t}) - \log q(z_{t-1}, z_t|x_{\leq t})] \\
&\geq \mathbb{E}_{(z_{t-1},z_t)\sim q}[\log p(x_t|z_{t-1}, z_t, x_{<t}) + \log p(z_{t-1}, z_t|x_{<t}) - \log q(z_{t-1}, z_t|x_{\leq t})] \\
&\geq \mathbb{E}_{(z_{t-1},z_t)\sim q}[\log p(x_t|z_t) + \log p(z_{t-1}|x_{<t}) + \log p(z_t|z_{t-1}) - \log q(z_{t-1}, z_t|x_{\leq t})] \\
&\geq \mathbb{E}_{(z_{t-1},z_t)\sim q}[\log p(x_t|z_t) + \log p(z_{t-1}|x_{<t}) + \log p(z_t|z_{t-1}) - \log q(z_t|x_{\leq t}) - \log q(z_{t-1}|z_t, x_{\leq t})]
\end{aligned}
$$

Notice two things:

- The red terms can be ignored according to Markov assumptions.
- The blue term is expanded according to Markov assumptions.
- The green term is expanded to include an one-step prediction back to the past as a smoothing distribution.

Temporal Difference VAE. ICLR 2019.

TD-VAE

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$$\log p(x_t|x_{<t}) \geq \mathbb{E}_{(z_{t-1},z_t)\sim q}[\log p(x_t|z_t) + \log p(z_{t-1}|x_{<t}) + \log p(z_t|z_{t-1}) - \log q(z_t|x_{\leq t}) - \log q(z_{t-1}|z_t, x_{\leq t})]$$

Precisely, there are four types of distributions to learn:

1. $p_D(.)$ is the **decoder** distribution:
   - $p(x_t \mid z_t)$ is the encoder by the common definition;
   - $p(x_t \mid z_t) \to p_D(x_t \mid z_t)$;
2. $p_T(.)$ is the **transition** distribution:
   - $p(z_t \mid z_{t-1})$ captures the sequential dependency between latent variables;
   - $p(z_t \mid z_{t-1}) \to p_T(z_t \mid z_{t-1})$;
3. $p_B(.)$ is the **belief** distribution:
   - Both $p(z_{t-1} \mid x_{<t})$ and $q(z_t \mid x_{\leq t})$ can use the belief states to predict the latent variables;
   - $p(z_{t-1} \mid x_{<t}) \to p_B(z_{t-1} \mid b_{t-1})$;
   - $q(z_t \mid x_{\leq t}) \to p_B(z_t \mid b_t)$;
4. $p_S(.)$ is the **smoothing** distribution:
   - The back-to-past smoothing term $q(z_{t-1} \mid z_t, x_{\leq t})$ can be rewritten to be dependent of belief states too;
   - $q(z_{t-1} \mid z_t, x_{\leq t}) \to p_S(z_{t-1} \mid z_t, b_{t-1}, b_t)$;

Temporal Difference VAE. ICLR 2019.

TD-VAE

To incorporate the idea of jumpy prediction, the sequential ELBO has to not only work on $t, t+1$, but also two distant timestamp $t_1 < t_2$. Here is the final TD-VAE objective function to maximize:

$$J_{t_1,t_2} = \mathbb{E}[\log p_D(x_{t_2}|z_{t_2}) + \log p_B(z_{t_1}|b_{t_1}) + \log p_T(z_{t_2}|z_{t_1}) - \log p_B(z_{t_2}|b_{t_2}) - \log p_S(z_{t_1}|z_{t_2}, b_{t_1}, b_{t_2})]$$

Temporal Difference VAE. ICLR 2019.

Summary

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Full list:

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Thanks