Deep Learning
lecture 6
Variational Autoencoder

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Apr-7

Logistics

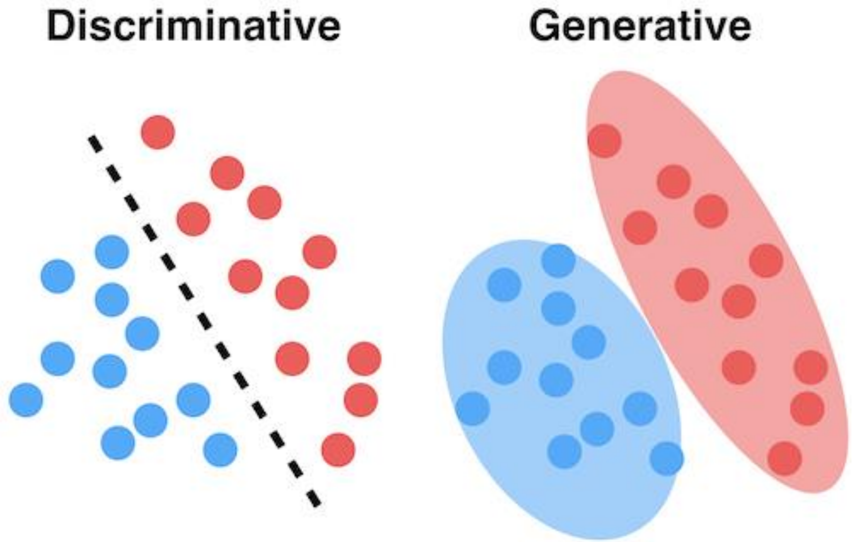
- Coding Project 2 grading is finished
  - Many submissions have run-time errors during evaluation!
  - Pay attention to format and evaluation!!!

- Coding Project 3 will be released tomorrow
  - Due in 3 weeks
  - Try to start early
- Don’t forget about your homework!
  - No late submission

Today’s Topic

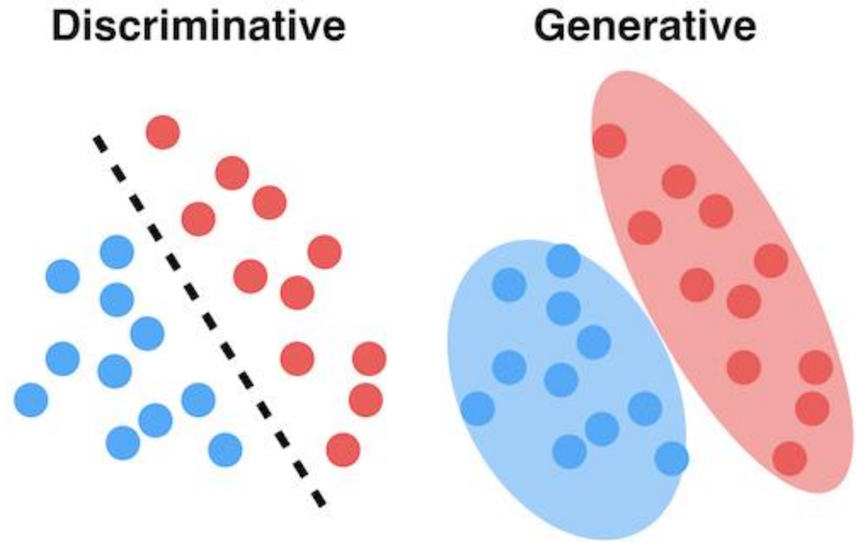
- Latent Variable Model
    - Variational inference
- Variational Autoencoder

Discriminative v.s. Generative (Recap)



- Discriminative model (lecture 2-3)
  - Feedforward networks
  - straightforward to learn
- Generative model
  - The problem itself is hard (need to model high-dimensional data distribution)
  - Inference is non-trivial (posterior distribution)

Discriminative v.s. Generative (Recap)



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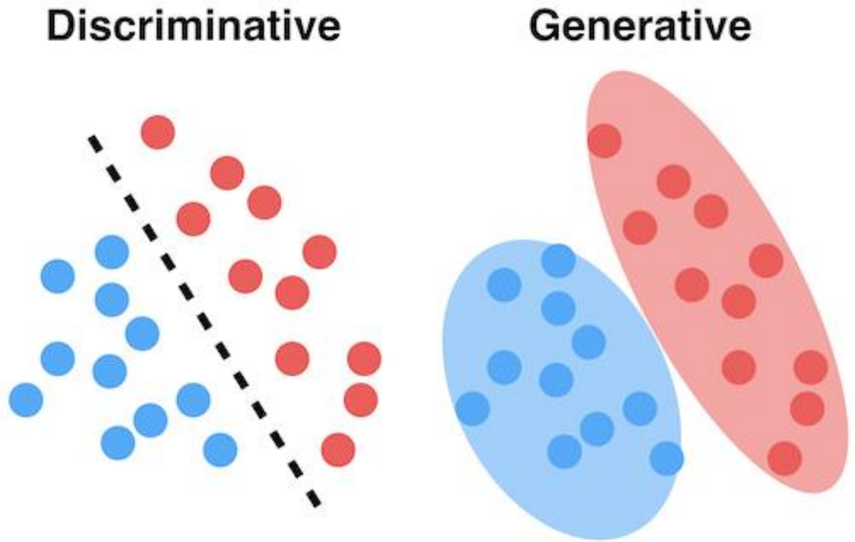
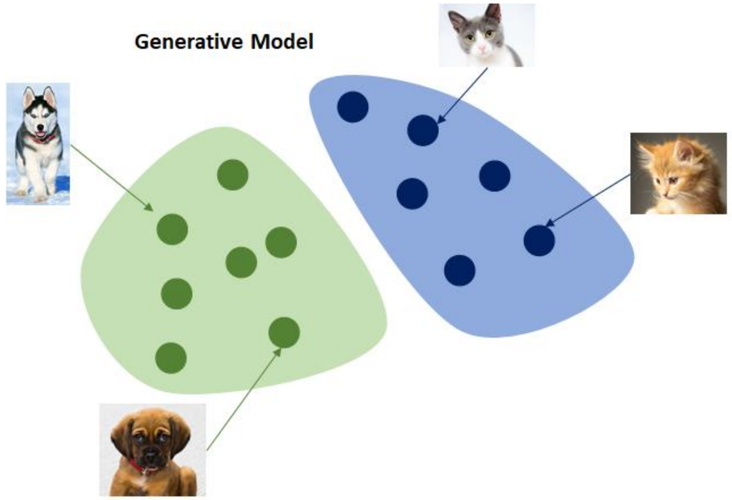
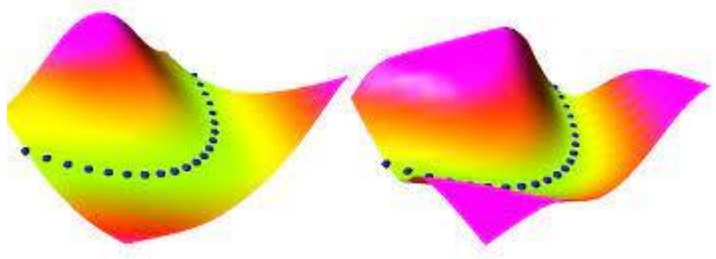


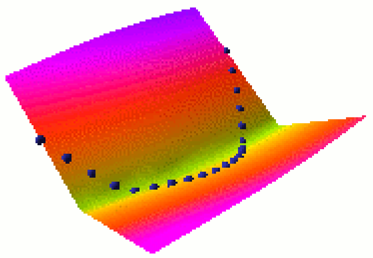
- Discriminative model (lecture 2-3)
  - Feedforward networks
  - straightforward to learn
  - Typically require labels (supervised learning)
- Generative model
  - The problem itself is hard (need to model high-dimensional data distribution)
  - Inference is non-trivial (posterior distribution
  - We have a probability distribution to draw samples!
    - Unsupervised by nature (directly learn $p(x)$)
    - Fill missing information (inpainting, learn complex latent structures)

Generative Model



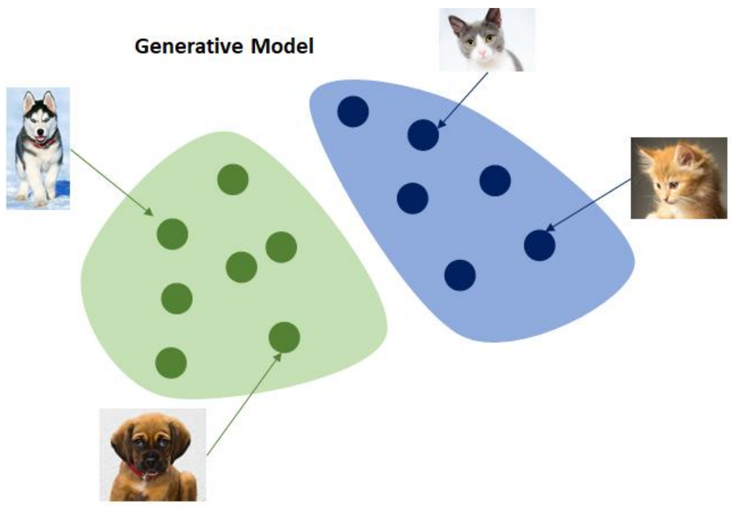
- Goal: learn $p(x;\theta)$
- What we have learned …
  - Energy-based model (lecture 4)
    - $p(x) = \frac{1}{Z}\exp(-E(x))$ (extremely flexible)
    - Sampling: MCMC
      - Gradients! (Stochastic Gradient MCMC)
    - Z: partition function (key challenge)
      - No closed-form density for $p(x)$ → NO MLE Learning!
    - Learning: Contrastive Divergence
      - Decrease $E(x)$ on data samples & increase $E(x')$ on non-data samples

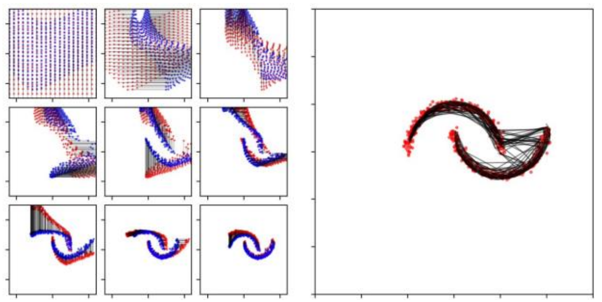


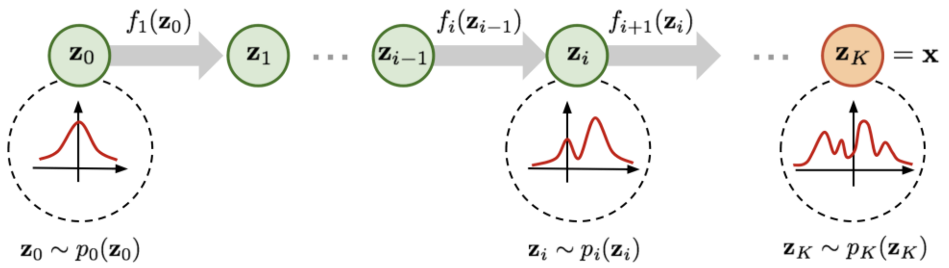


Generative Model

- Goal: learn $p(x;\theta)$
- What we have learned …
  - Energy-based model (lecture 4)
    - Most flexible! Hard to sample & learn!
  - Flow model (lecture 5)
    - $x = f(z;\theta)$ where $f(;\theta)$ is bijection, $z \sim N(0, I)$
      - z is also called latent representation of x
    - Sampling is straightforward!
    - MLE training is easy
      - $\log p(x) = \log p(z) - \sum_i \log\det|\partial f_i/\partial x|$
      - f_i needs to have a structured Jacobian





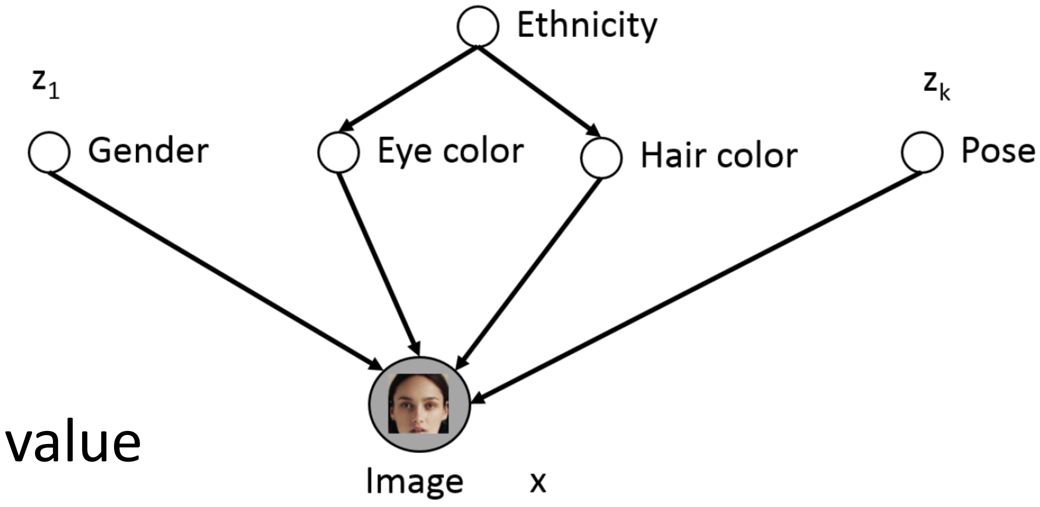


Generative Model

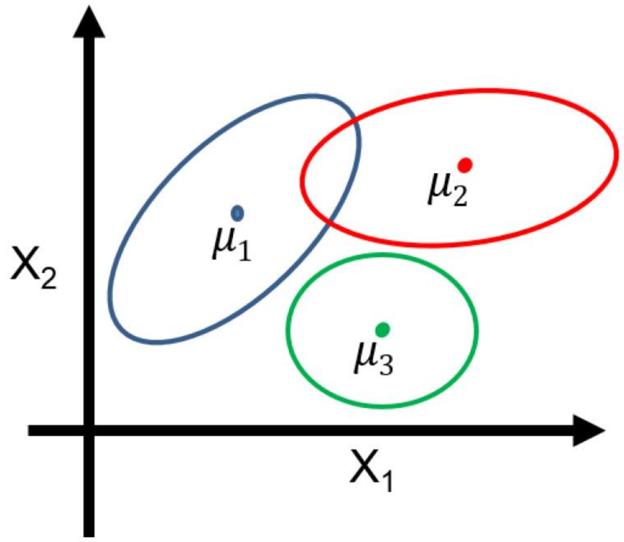
- Goal: learn $p(x;\theta)$
- What we have learned …
  - Energy-based model (lecture 4)
    - No explicit sampling → hard training and expensive generation
  - Flow Model (lecture 5)
    - $x = f(z)$: easy sampling and tractable likelihood
    - Most limited modeling capacity
      - **… because of the bijection constraint!**
- What if $x = f(z)$ is NOT a bijection?
  - Still easy generation!
  - What about MLE training? How to compute $p(x)$?

Latent Variable Model

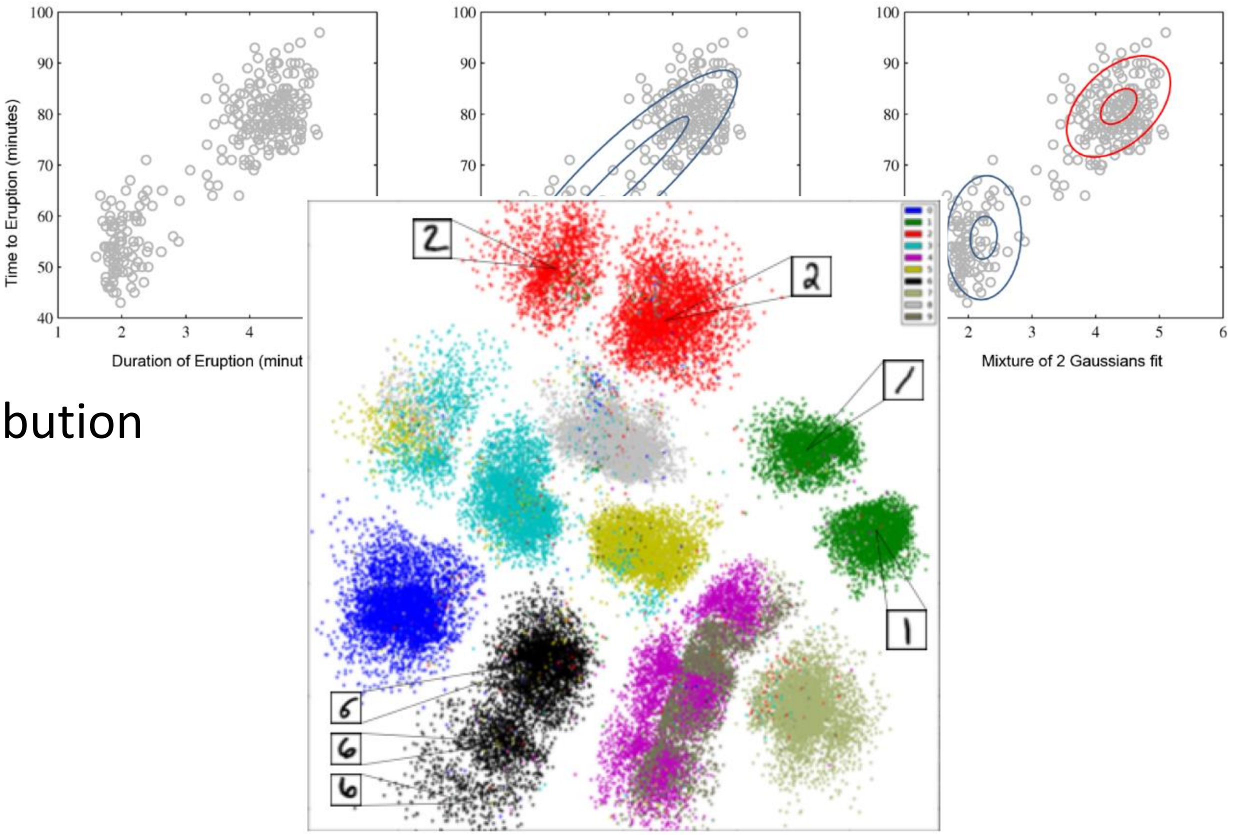
- A more general formulation: $p(x,z) = p(z)p(x|z)$
  - x data; z latent variable
  - When z is given, $p(x|z)$ is easy to compute
- Example
  - x: image (pixel values)
  - z: latent feature/factors
  - Only grey circle is observed
  - $p(z)$: prior distribution of factors
  - $p(x|z)$: a Gaussian/Categorical on each pixel value
    - $p(x|z) = N(\mu(z), \Sigma(z))$



Latent Variable Model



- $p(x,z) = p(z)p(x|z)$
  - x data; z latent variable
- Example: Gaussian Mixture Model
  - $z \sim \text{Categorical}(w_1, \dots, w_K)$
  - $x \sim N(\mu_z, \Sigma_z)$
  - Generative process
    - Pick a cluster z
    - Generate x according to the cluster distribution
  - Unsupervised learning
    - Unlabeled data
    - E.g. clustering of handwritten digits



Latent Variable Model: Training

- Learning the latent variable model
  - Joint probability: $p(x, z; \theta)$ for random variable X and Z
    - $p(x, z; \theta) = p(z; \theta)p(x|z; \theta)$
  - Dataset $D = \{x^{(i)}\}$ for X, variable Z is never observed
- Maximal Likelihood Learning

$$L(\theta) = \log \prod_{x \in D} p(x; \theta) = \sum_{x \in D} \log \sum_{z} p(x, z; \theta)$$

  - Marginal probability can be expensive to compute!
    - When z is continuous, the objective even becomes intractable

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  - Marginal probability can be expensive to compute!
    - When z is continuous, the objective even becomes intractable
- Goal: a fast approximation of the marginal probability
  - Remark: $L(\theta)$ is tractable when $p(x, z) \propto \exp(-E(x, z))$

Latent Variable Model: Training

- Goal: approximation of $\log \sum_z p(x, z; \theta)$
- Idea#1: Importance Sampling
  - Proposal distribution $q(z)$

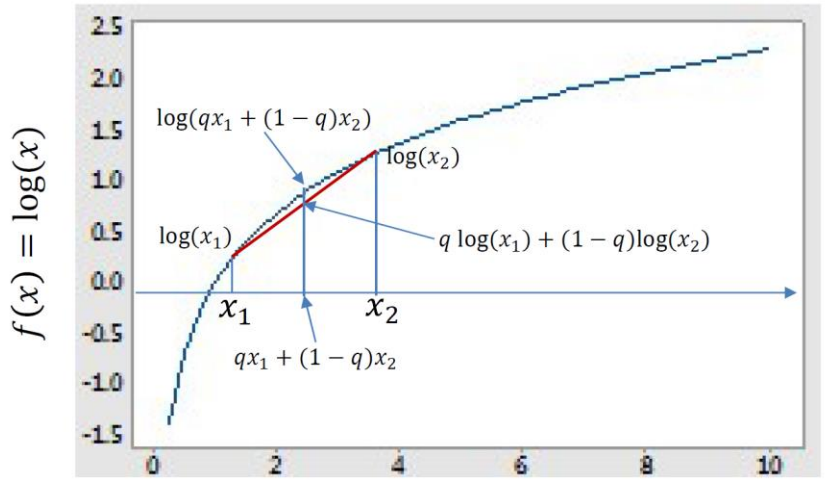
$$p(x) = \sum_z q(z) \cdot \frac{p(x, z; \theta)}{q(z)}$$

    - The probability can be approximated by drawing samples from $q(z)$
  - Learning objective $L(x; \theta)$

$$L(x; \theta) = \log \sum_z q(z) \cdot \frac{p(x, z; \theta)}{q(z)}$$

Latent Variable Model: Training

- Goal: approximation of $\log \sum_z q(z) \cdot \frac{p(x,z;\theta)}{q(z)}$
- Idea#2: concavity of $\log(\cdot)$
  - $\mathbf{log} \sum_z q(z) \cdot \frac{p(x,z;\theta)}{q(z)}$
  - For any $0 < x_1 \le x_2 \le 1$,
    - $\log(\alpha x_1 + (1-\alpha)x_2) \ge \alpha \log(x_1) + (1-\alpha)\log(x_2)$
  - More general, for any weights $\alpha_i > 0$ & $\sum_i \alpha_i = 1$,
    - $\log(\sum_i \alpha_i x_i) \ge \sum_i \alpha_i \log(x_i)$



Latent Variable Model: Training

- Goal: approximation of $\log \sum_z q(z) \cdot \frac{p(x,z;\theta)}{q(z)}$
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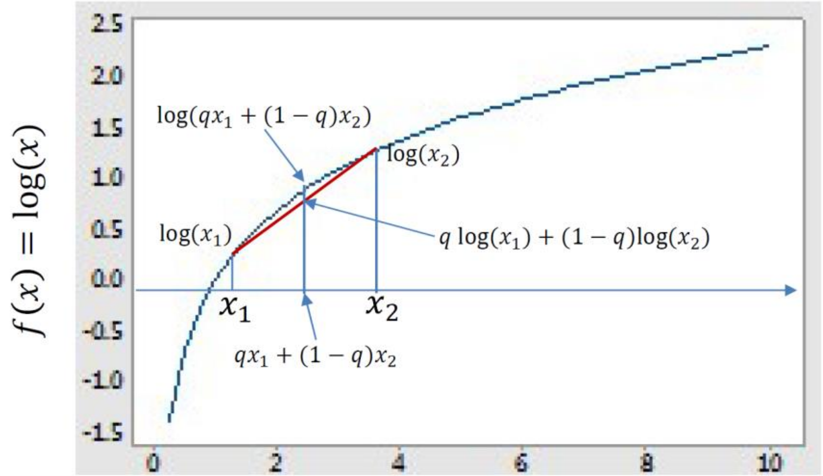


Latent Variable Model: Training

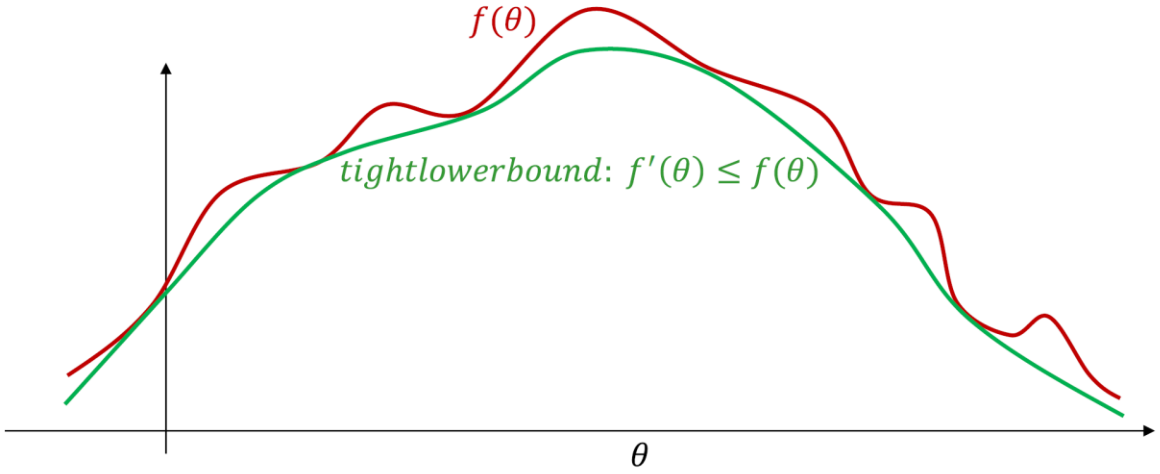
- Goal: approximate $\log \sum_z p(x, z; \theta)$
  - Ideas: importance sampling & concavity of $\log(\cdot)$
- Evidence Lower Bound (ELBO)

$$\log p(x; \theta) = \log \sum_z p(x, z; \theta) \geq \sum_z q(z) \log \frac{p(x, z; \theta)}{q(z)}$$

  - A tractable lower bound of the true objective
    - Easy to optimize
- When will the equality hold?
  - i.e., a tight lower bound
  - Sol: $q(z) \leftarrow p(z|x; \theta)$

Evidence Lower Bound

- ELBO becomes exact when $q(z) = p(z|x;\theta)$
  - $\sum_z q(z) \log \frac{p(x,z;\theta)}{q(z)} = \sum_z q(z) \log \frac{p(x,z;\theta)}{p(z|x;\theta)}$
  - $= \sum_z q(z) \log p(x;\theta)$
  - $= \log p(x;\theta)$
- We can optimize a tight lower bound by setting $q(z) = p(z|x;\theta)$
- An iterative process
  - Optimize $p(x,z;\theta)$ w.r.t. fixed $q(z)$
    - $J(\theta) = \sum_z q(z) \log \frac{p(x,z;\theta)}{q(z)}$
  - Set $q(z) \leftarrow p(z|x;\theta)$
  - Repeat



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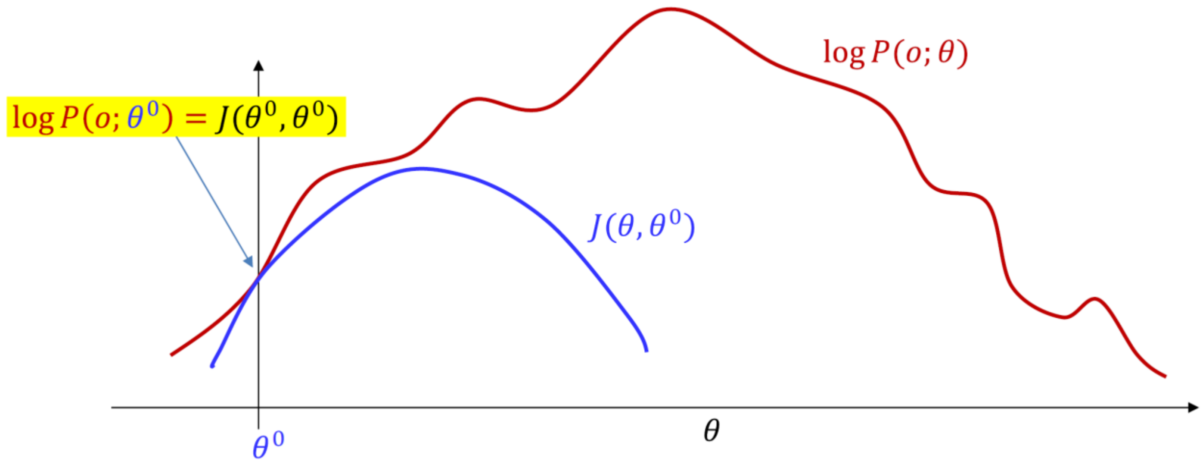

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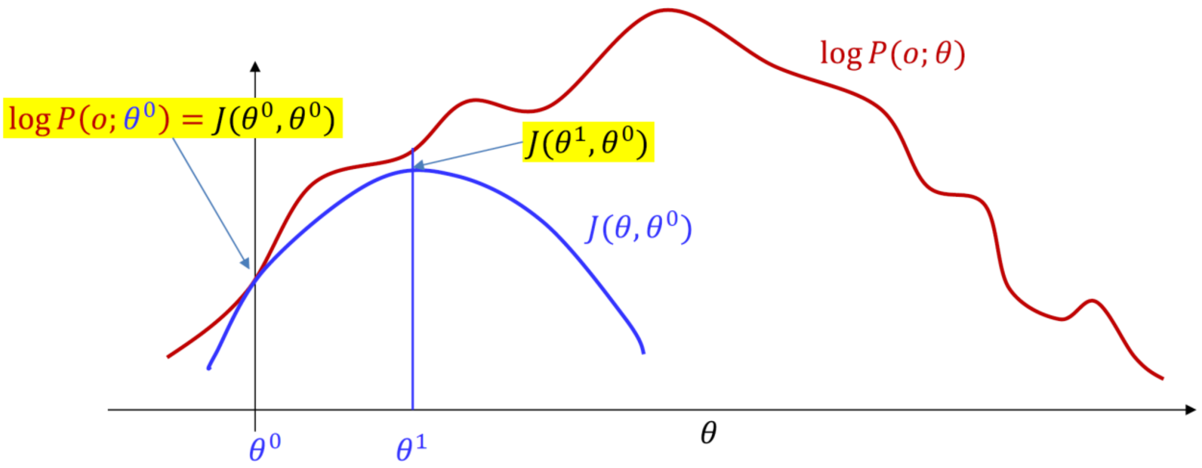

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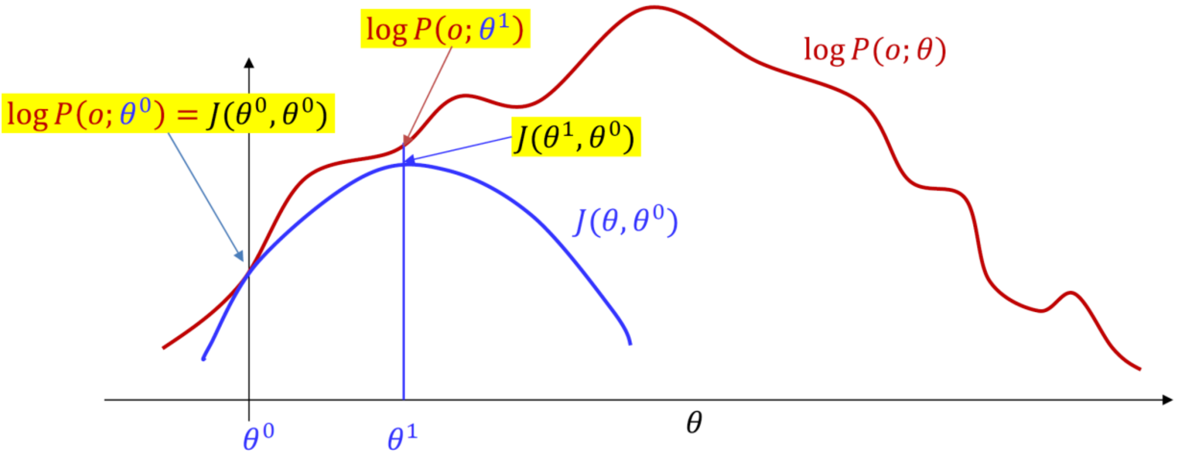
  - Repeat



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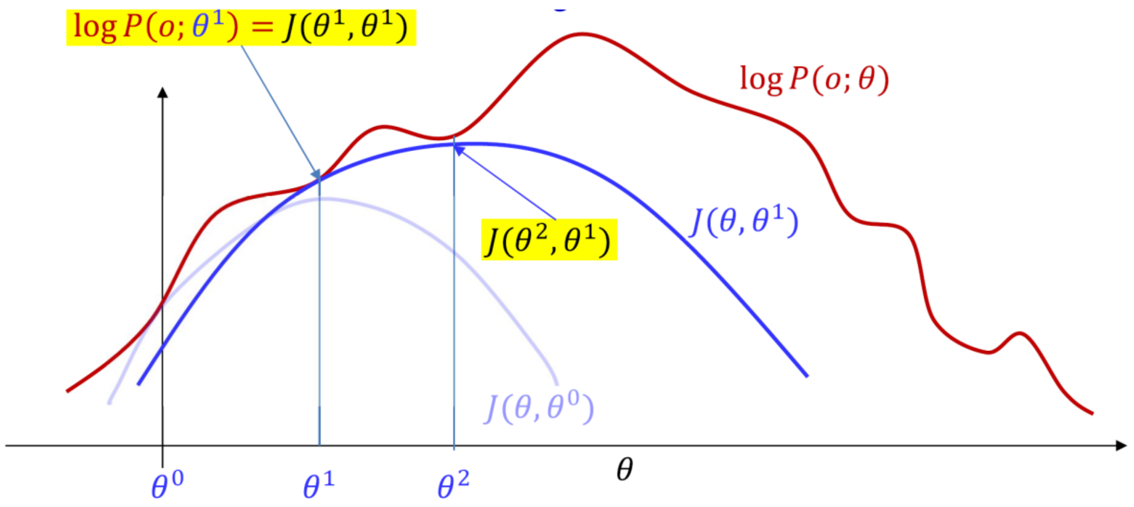
  - Repeat



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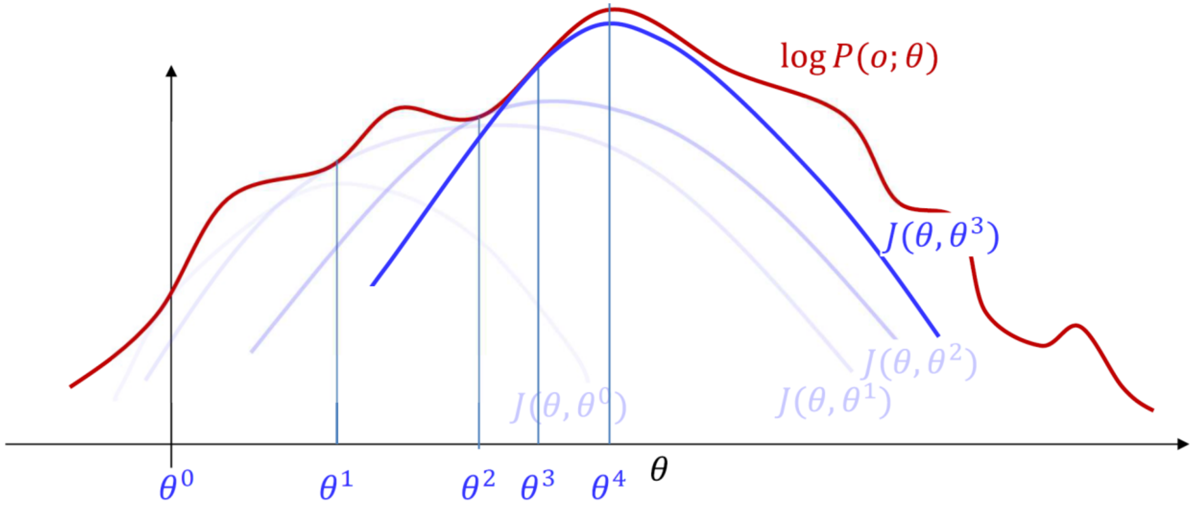
  - Set $q(z) \leftarrow p(z|x;\theta)$
  - Repeat
  - Converge to a local optimum



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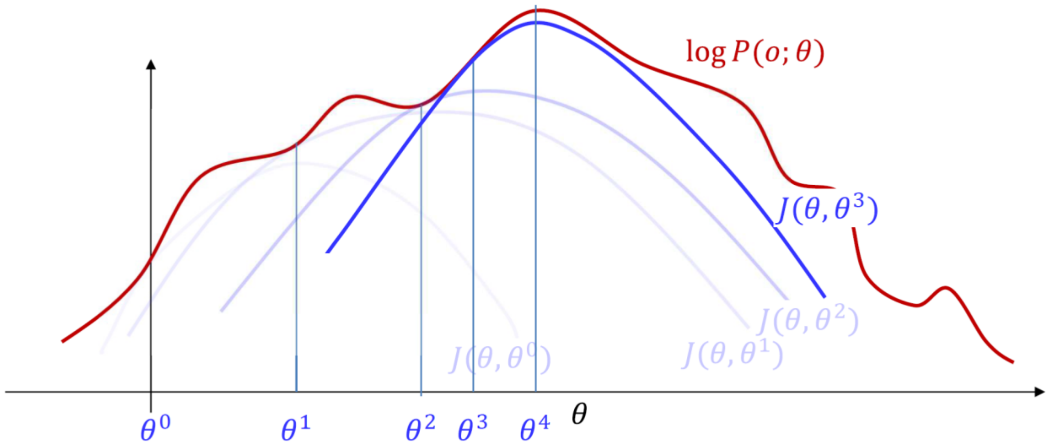
  - $= \log p(x;\theta)$
- We can optimize a tight lower bound by setting $q(z) = p(z|x;\theta)$
- An iterative process
  - Optimize $p(x,z;\theta)$ w.r.t. fixed $q(z)$ (M-step)
  - Set $q(z) \leftarrow p(z|x;\theta)$ (E-step)
  - ***An EM algorithm***
- How to set $q(z) \leftarrow p(z|x;\theta)$?



Variational Inference

- Goal: $q(z;\phi) \leftarrow p(z|x)$
  - Find a parameterized distribution $q(z;\phi)$ to approximate the true posterior
    - In our case, approximate $p(z|x;\theta)$ w.r.t. a fixed θ
  - Distance metric between $q(z;\phi)$ and $p(z|x)$
    - $KL(q||p) = \sum_z q(z) \log \frac{q(z)}{p(z)}$
- Variational Inference: $\min_{\phi} KL(q||p)$

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- Variational Inference: $\min_{\phi} KL(q||p)$
  - Remark: pay attention to the order of KL (reverse KL)!
  - Mean-field variational inference
    - A factored proposal: $q(z) = \prod_i q_i(z_i|x)$
    - By calculus of variation （变分法，泛函分析领域）
      $$\log q_i^\star(z_i|x) = \mathrm{E}_{z_{j\neq i}}[\log p(z,x)] + constant$$
    - Repeatedly update the distribution of $q_i(z_i)$ using the expectation of $p(z,x)$

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- Variational Inference: $\min_\phi KL(q||p)$
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  - $= \sum_z q(z;\phi) \log p(x) - \sum_z q(z;\phi) \log \frac{p(z,x)}{q(z;\phi)}$

Variational Inference

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  - $= \underbrace{\log p(x)}_{\text{Constant}} - \sum_z q(z;\phi) \log \frac{p(z,x)}{q(z;\phi)}$

Variational Inference

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  - $= \log p(x) - \sum_z q(z;\phi) \log \frac{p(z,x)}{q(z;\phi)}$
  - $L(\phi) = \sum_z q(z;\phi) \log \frac{p(z,x)}{q(z;\phi)}$

Evidence Lower Bound (ELBO)!!!

Also called variational lower bound in VI

Variational Inference

- Goal: $q(z;\phi) \leftarrow p(z|x)$
  - Find a parameterized distribution $q(z;\phi)$ to approximate the posterior
    - In our case, approximate $p(z|x;\theta)$ w.r.t. a fixed θ
  - Distance metric between $q(z;\phi)$ and $p(z|x)$
    - $KL(q||p) = \sum_z q(z) \log \frac{q(z)}{p(z)}$
- Variational Inference: $\min_{\phi} KL(q||p)$
  - $KL(q(z;\phi)||p(z|x)) = \sum_z q(z;\phi) \log \frac{q(z;\phi)}{p(z|x)} = \sum_z q(z;\phi) \log \frac{q(z;\phi)p(x)}{p(z,x)}$
  - $= \log p(x) - \sum_z q(z;\phi) \log \frac{p(z,x)}{q(z;\phi)}$
  - $L(\phi) = \sum_z q(z;\phi) \log \frac{p(z,x)}{q(z;\phi)}$

Variational Inference

- Goal: $q(z;\phi) \leftarrow p(z|x)$
  - Find a parameterized distribution $q(z;\phi)$ to approximate the posterior
    - In our case, approximate $p(z|x;\theta)$ w.r.t. a fixed θ
  - Distance metric between $q(z;\phi)$ and $p(z|x)$
    - $KL(q||p) = \sum_z q(z) \log \frac{q(z)}{p(z)}$
- Variational Inference: $\min_{\phi} KL(q||p)$
  - $\log p(x) = KL\big(q(z;\phi)||p(z|x)\big) + \sum_z q(z;\phi) \log \frac{p(z,x)}{q(z;\phi)}$
  - $=$ approximate error $+$ ELBO $\geq$ ELBO
  - $L(\phi) = \sum_z q(z;\phi) \log \frac{p(z,x)}{q(z;\phi)}$

Variational Inference (Explained)

- General Formulation of Bayesian Inference
  - Dataset $D = \{x\}$
  - Model $p(x; \theta)$ with parameter θ
  - Goal $p(\theta|x)$
    - Remark: optimization learns a single θ^* while BI learns a distribution
- Variational Inference as a Mean of Approximate Bayesian Inference
  - Use $q(\theta; \phi)$ to approximate $p(\theta|x)$
  - VI Objective: $KL(q||p) = C + ELBO$
  - Interpretation: VI objective is a *lower bound* of $\log p(x)$

$$\log p(x; \theta) = \textcolor{blue}{approximation\ error} + \textcolor{red}{ELBO}$$

- VAE naturally inherits all the nice mathematical properties of VI ☺
  - Further read: black-box variational inference https://arxiv.org/abs/1401.0118

Latent Variable Model: Training

- Latent Variable Model: $p(z, x) = p(z)p(x|z)$
  - MLE objective: $p(x; \theta) = \sum_z p(z, x; \theta)$
- ELBO: $p(x; \theta) \geq \sum_z q(z) \log \frac{p(x,z;\theta)}{q(z)} = L(\theta; q)$
  - Iterative learning: (1) optimize θ and (2) $q(z) \leftarrow p(z|x; \theta)$

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  - Approximate $p(z|x;\theta)$ by a tractable distribution $q(z;\phi)$

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$$L(\phi;\theta) = \sum_z q(z;\phi) \log \frac{p(z,x;\theta)}{q(z;\phi)}$$

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$$L(\phi;\theta) = \sum_z q(z;\phi) \log \frac{p(z,x;\theta)}{q(z;\phi)}$$

Use VI to learn a separate $q(z;\phi)$ for each possible x?

Latent Variable Model: Training

- Latent Variable Model: $p(z,x) = p(z)p(x|z)$
  - MLE objective: $p(x;\theta) = \sum_z p(z,x;\theta)$
- ELBO: $p(x;\theta) \geq \sum_z q(z) \log \frac{p(z,x;\theta)}{q(z)} = L(\theta;q)$
  - Iterative learning: (1) optimize θ and (2) $q(z) \leftarrow p(z|x;\theta)$
- Amortized Variational Inference
  - Approximate $p(z|x;\theta)$ by a conditional tractable distribution $q(z|x;\phi)$

$$L(\phi;\theta) = \sum_z q(z|x;\phi) \log \frac{p(z,x;\theta)}{q(z|x;\phi)}$$

  - A universal approximation q for any x and $p(z|x)$

Latent Variable Model: Training

- Latent Variable Model: $p(z, x) = p(z)p(x|z)$
  - MLE objective: $p(x; \theta) = \sum_z p(z, x; \theta)$
- ELBO: $p(x; \theta) \geq \sum_z q(z) \log \frac{p(x,z;\theta)}{q(z)} = L(\theta; q)$
  - Iterative learning: (1) optimize θ and (2) $q(z) \leftarrow p(z|x; \theta)$
- Amortized Variational Inference
  - Approximate $p(z|x; \theta)$ by a conditional tractable distribution $q(z|x; \phi)$

$$L(\phi; \theta) = \sum_z q(z|x; \phi) \log \frac{p(z, x; \theta)}{q(z|x; \phi)}$$

- Joint Learning $J(\theta, \phi; x)$

$$J(\theta, \phi; x) = \sum_z q(z|x; \phi) \log \frac{p(z, x; \theta)}{q(z|x; \phi)}$$

Latent Variable Model: Training

- Learning objective $J(\theta, \phi; x)$
  - $J(\theta, \phi; x) = \sum_z q(z|x;\phi)(\log p(z, x; \theta) - \log q(z|x;\phi))$

Latent Variable Model: Training

- Learning objective $J(\theta, \phi; x)$
  - $J(\theta, \phi; x) = \sum_z q(z|x; \phi)(\log p(z, x; \theta) - \log q(z|x; \phi))$
  - $\quad\quad\quad\quad\quad = \sum_z q(z|x; \phi)(\log p(x|z; \theta) - \log q(z|x; \phi) + \log p(z; \theta))$

Latent Variable Model: Training

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  - $= \sum_z q(z|x;\phi) \log p(x|z;\theta) - \sum_z q(z|x;\phi) \log \frac{q(z|x;\phi)}{p(z;\theta)}$
  - $= E_{z \sim q(z|x;\phi)}[\log p(x|z;\theta)] - KL(q(z|x;\phi)||p(z;\theta))$

Expectation of log likelihood (reconstruction) KL divergence

- Design of $p(z, x; \theta)$ and $q(z|x;\phi)$
  - Principle: easy to compute!
  - Gaussian prior: $p(z) \sim N(0, I)$
  - Gaussian likelihood: $p(x_{ij}|z;\theta) \sim N\left(f_{ij}(z;\theta), 1\right)$
  - Isomorphic Gaussian: $q(z|x;\phi) \sim N\left(\mu(x;\phi), \mathrm{diag}\left(\exp\left(\sigma(x;\phi)\right)\right)\right)$

Latent Variable Model: Training

- Learning objective $J(\theta, \phi; x)$
  - $J(\theta, \phi; x) = \sum_z q(z|x; \phi)(\log p(z, x; \theta) - \log q(z|x; \phi))$
  - $= \sum_z q(z|x; \phi)(\log p(x|z; \theta) - \log q(z|x; \phi) + \log p(z; \theta))$
  - $= \sum_z q(z|x; \phi) \log p(x|z; \theta) - \sum_z q(z|x; \phi) \log \frac{q(z|x; \phi)}{p(z;\theta)}$
  - $= E_{z \sim q(z|x;\phi)}[\log p(x|z; \theta)] - KL(q(z|x; \phi)||p(z; \theta))$

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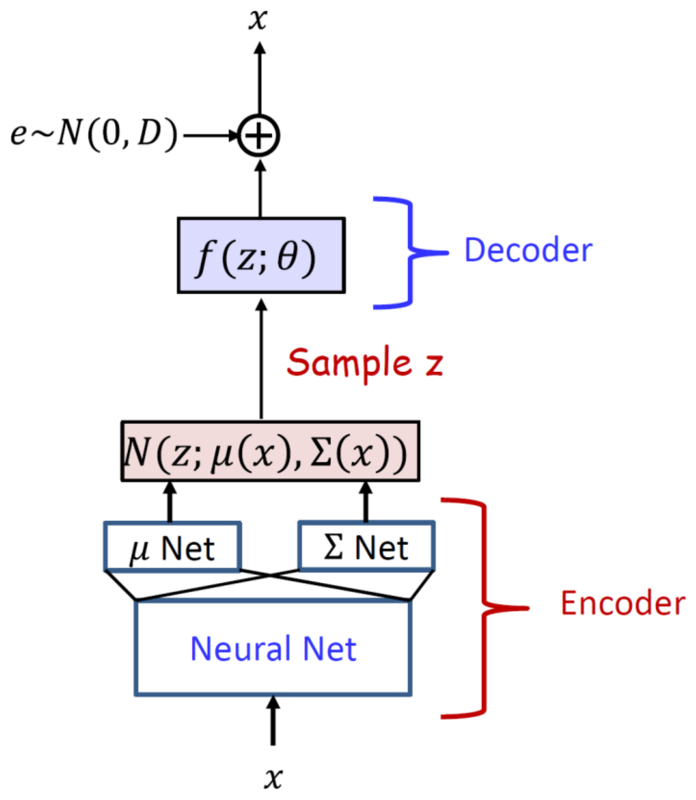
  - Isomorphic Gaussian: $q(z|x; \phi) \sim N\left(\mu(x; \phi), \text{diag}(\exp(\sigma(x; \phi)))\right)$

Neural networks!

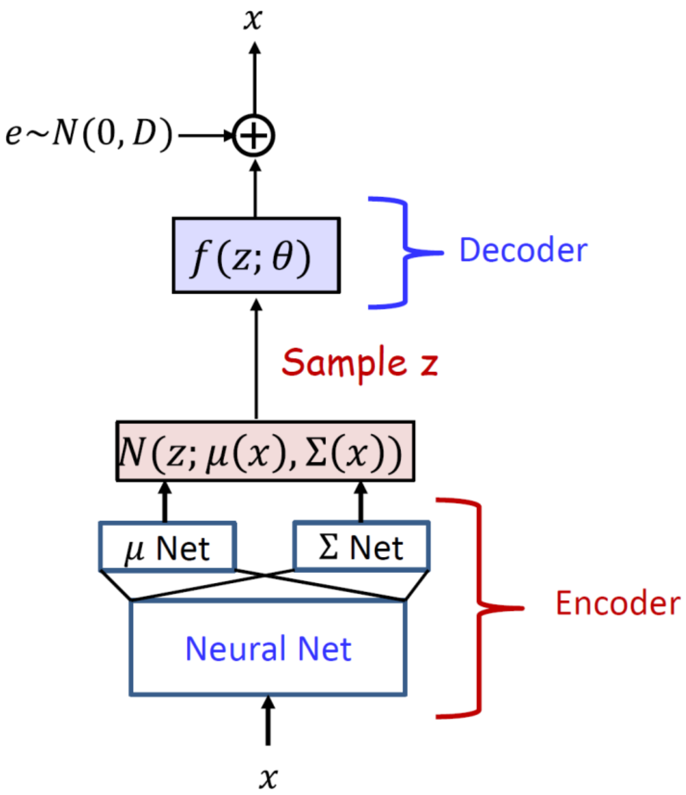
Variational Autoencoder

- VAE Architecture
  - Isomorphic Gaussian: $q(z|x;\phi)\sim N\left(\mu(x;\phi), \mathrm{diag}\left(\exp\left(\sigma(x;\phi)\right)\right)\right)$
  - Gaussian prior: $p(z)\sim N(0,I)$
  - Gaussian likelihood: $p(x|z;\theta)\sim N(f(z;\theta),I)$
- Autoencoder $x \to z \to x$
  - Unsupervised learning (data to data, z never observed)
  - Encoder $q(z|x;\phi)$: $x \to z$
  - Decoder $p(x|z;\theta)$: $z \to x$
  - Remark
    - $p(x|z)$ is the actual generative model
    - $q(z|x)$ is only the proposal
      - but optimized to approximate $p(z|x)$



Variational Autoencoder

- Training via jointly optimizing ELBO
  - $J(\phi, \theta; x) = \mathrm{E}_{z \sim q(z|x;\phi)}[\log p(x|z;\theta)] - KL(q(z|x;\phi)||p(z))$
  - Two terms: likelihood term & KL term

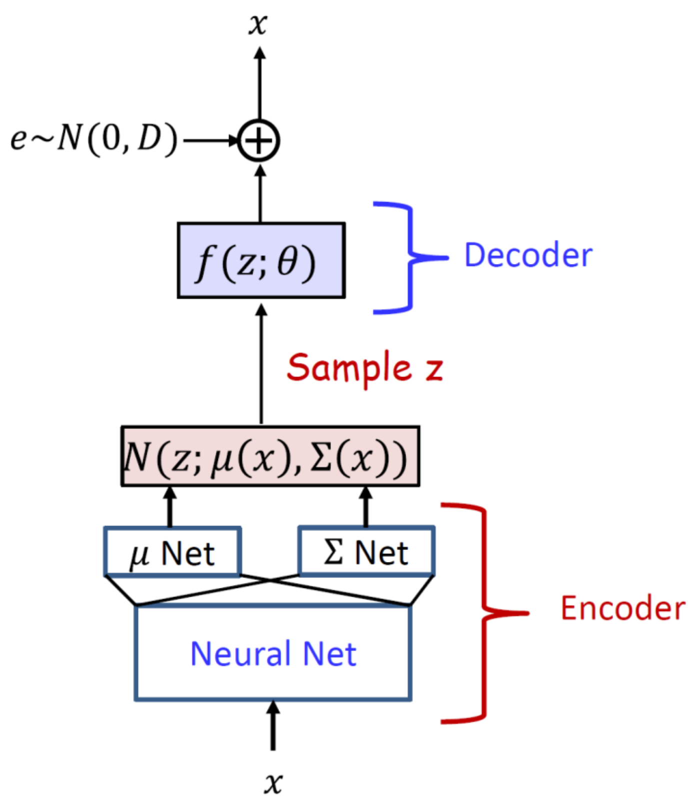


Variational Autoencoder

- Training via jointly optimizing ELBO
  - $J(\phi, \theta; x) = \mathrm{E}_{z \sim q(z|x;\phi)}[\log p(x|z;\theta)] - KL(q(z|x;\phi)||p(z))$
- KL penalty
  - $q(z|x;\phi) \sim N\left(\mu(x;\phi), \mathrm{diag}\left(\exp\left(\sigma(x;\phi)\right)\right)\right)$
  - $p(z) \sim N(0, I)$
  - Closed-form!

$$D_{\mathrm{KL}}(\mathcal{N}_0 \| \mathcal{N}_1) = \frac{1}{2}\left\{\mathrm{tr}\left(\boldsymbol{\Sigma}_1^{-1}\boldsymbol{\Sigma}_0\right) + (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)^{\mathrm{T}}\boldsymbol{\Sigma}_1^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0) - k + \ln\frac{|\boldsymbol{\Sigma}_1|}{|\boldsymbol{\Sigma}_0|}\right\}$$

- Implement it in your coding project ☺

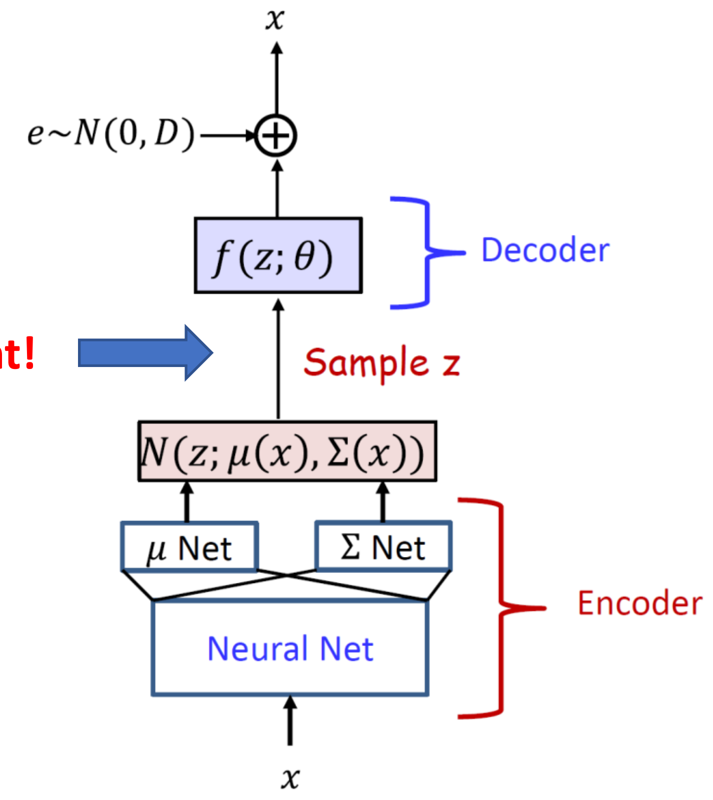


Variational Autoencoder

- Training via jointly optimizing ELBO
  - $J(\phi, \theta; x) = \mathrm{E}_{z \sim q(z|x;\phi)}[\log p(x|z;\theta)] - KL(q(z|x;\phi)||p(z))$
- Likelihood term (reconstruction loss)
  - Monte-Carlo estimate!
    - Draw samples from $q(z|x;\phi)$
    - Compute gradient of θ: $L(\theta) \propto \sum_z |x - f(z;\theta)|^2$
      - $x \sim N(f(z;\theta); I)$
      - $p(x) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2}|x - f(z;\theta)|^2\right)$
    - How to get **the gradient of $\boldsymbol{\phi}$** through $q(z;\phi)$??

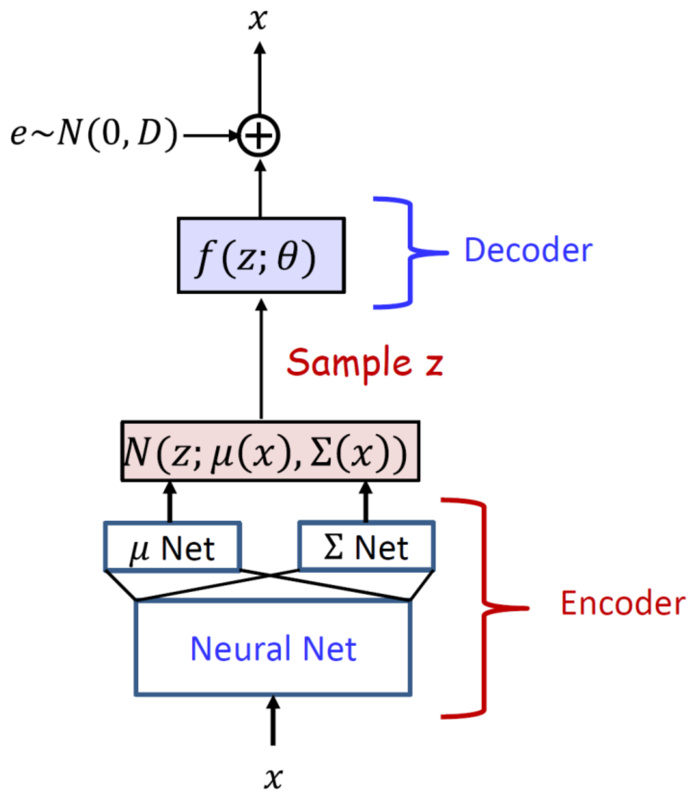
$$L(\phi) = E_{z \sim \boldsymbol{q(z;\phi)}}[\log p(x|z)]$$

No gradient!



Variational Autoencoder

- Training via jointly optimizing ELBO
  - $J(\phi, \theta; x) = \mathrm{E}_{z\sim q(z|x;\phi)}[\log p(x|z;\theta)] - KL(q(z|x;\phi)||p(z))$
- Likelihood term (reconstruction loss)
  - Monte-Carlo estimate!
    - Draw samples from $q(z|x;\phi)$
    - Compute gradient of θ: $L(\theta) \propto \sum_z |x - f(z;\theta)|^2$
  - Re-parameterization trick
    - Recap in autoregressive flow
      - $z\sim N(\mu, \sigma^2) \quad \Leftrightarrow \quad z = \mu + \sigma\cdot\epsilon,\ \epsilon\sim N(0,1)$
    - $L(\phi) \propto \mathrm{E}_{z\sim q(z|\phi)}[|f(z) - x|^2]$
    - $\qquad \propto \mathrm{E}_{\epsilon\sim N(0,I)}[|f(\mu(x;\phi) + \sigma(x;\phi)\cdot\epsilon) - x|^2]$
      - Monte-Carlo estimate for $\nabla L(\phi)$!
      - 1 sample for ϵ is sufficient for stable training



Variational Autoencoder

- Variational Autoencoder (VAE)
  - Encoder $q(z|x;\phi)$
  - Decoder $p(x|z;\theta)$
  - End-to-end unsupervised learning ($x \rightarrow z \sim q(z|x) \rightarrow x$)

    $J(\phi,\theta;x) = \mathrm{E}_{\epsilon\sim N(0,I)}[\log p(x|\mu(x;\phi)+\sigma(x;\phi)\cdot\epsilon;\theta)] - KL(q(z;\phi)||p(z))$
  - By Kingma & Welling, ICLR 2013 (34k citation)

Auto-Encoding Variational Bayes

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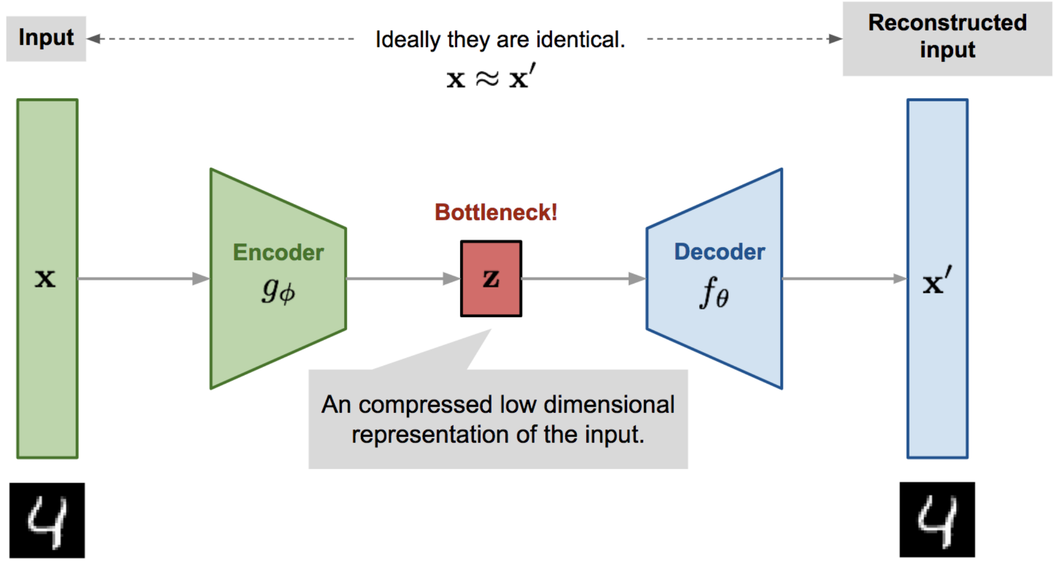
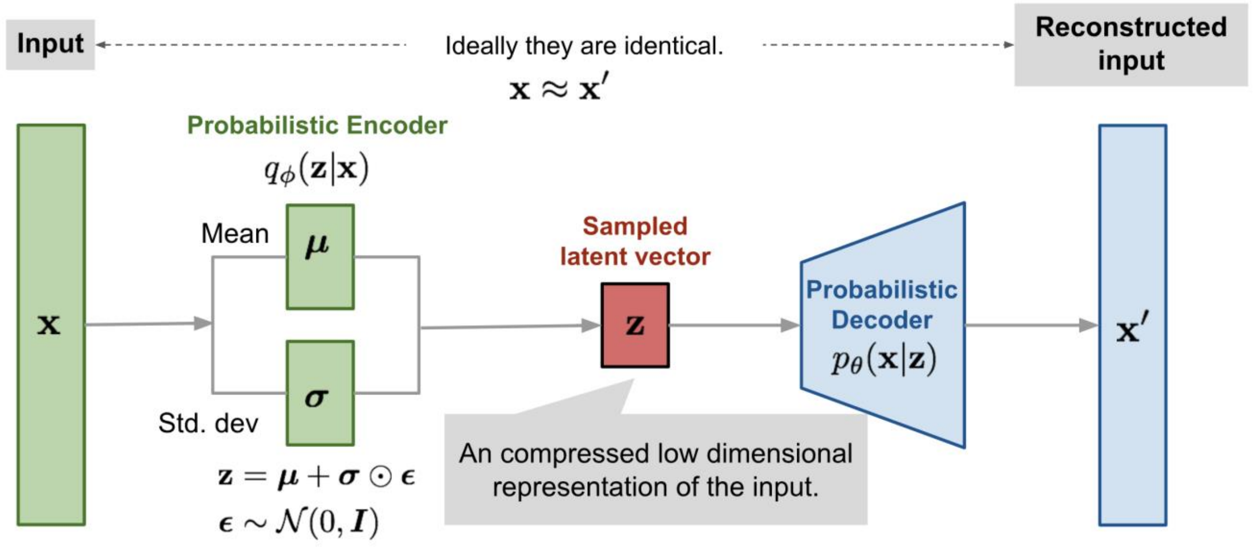
VAE v.s. Standard AE

- Autoencoder
  - A classical unsupervised learning method for representation learning
- VAE: a simple generative extension of AE
  - Generative model: AE + Gaussian noise on z
  - KL penalty: L2 constraint on the latent vector z



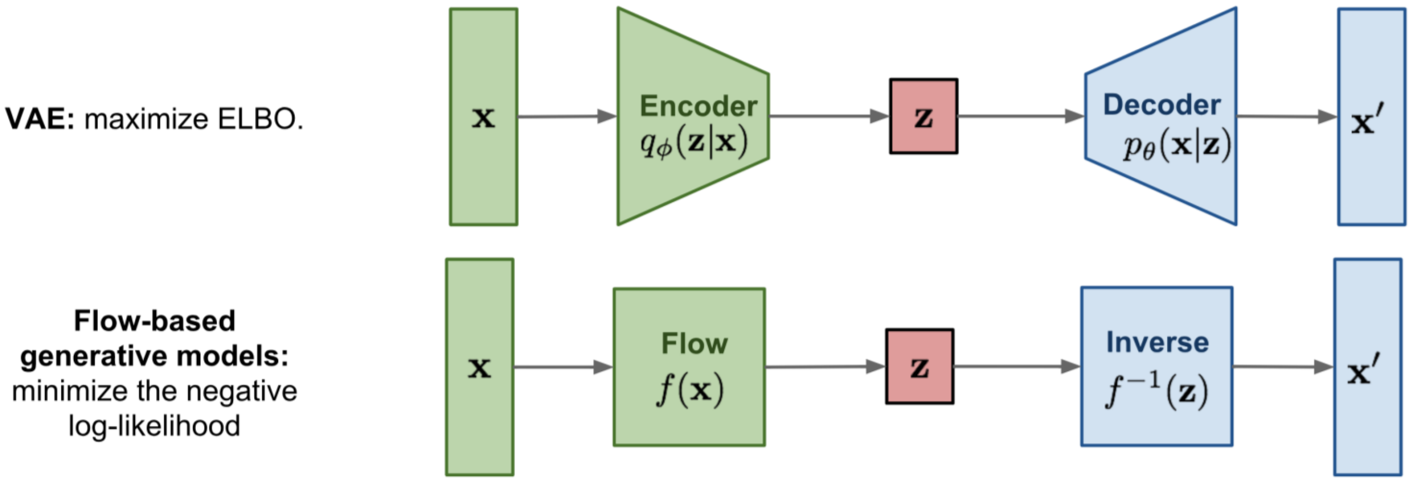
AE



VAE

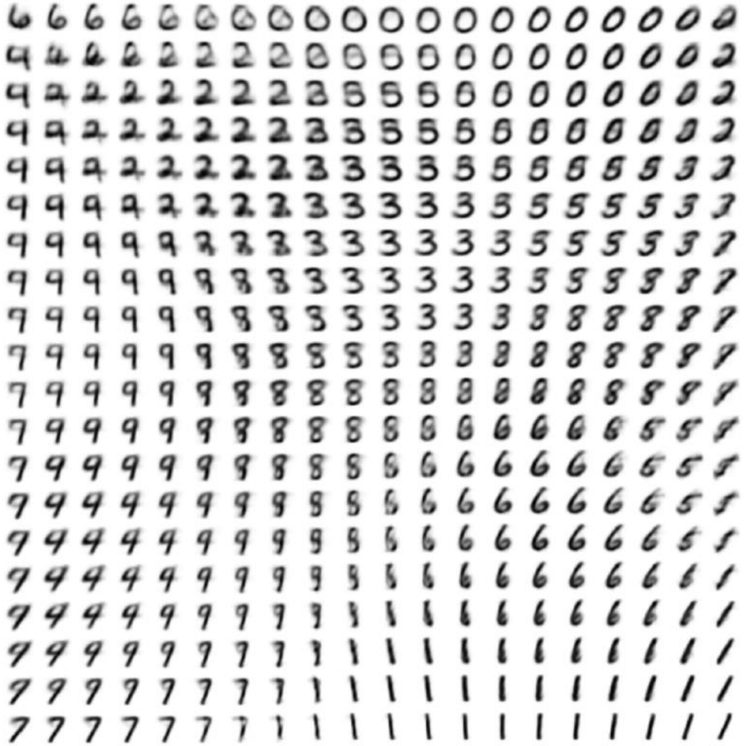
VAE v.s. Flow Model

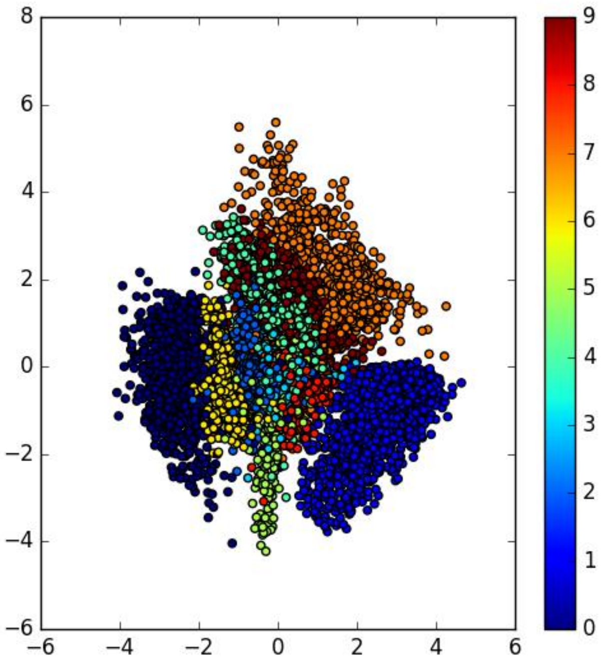
- Both model has a latent representation z
- Flow model
  - Encoder: inference mapping; decoder: generation mapping
  - Exact inference but no dimension reduction!
- VAE
  - Approximate inference
  - Dimension reduction
  - Flexible architecture



Variational Autoencoder

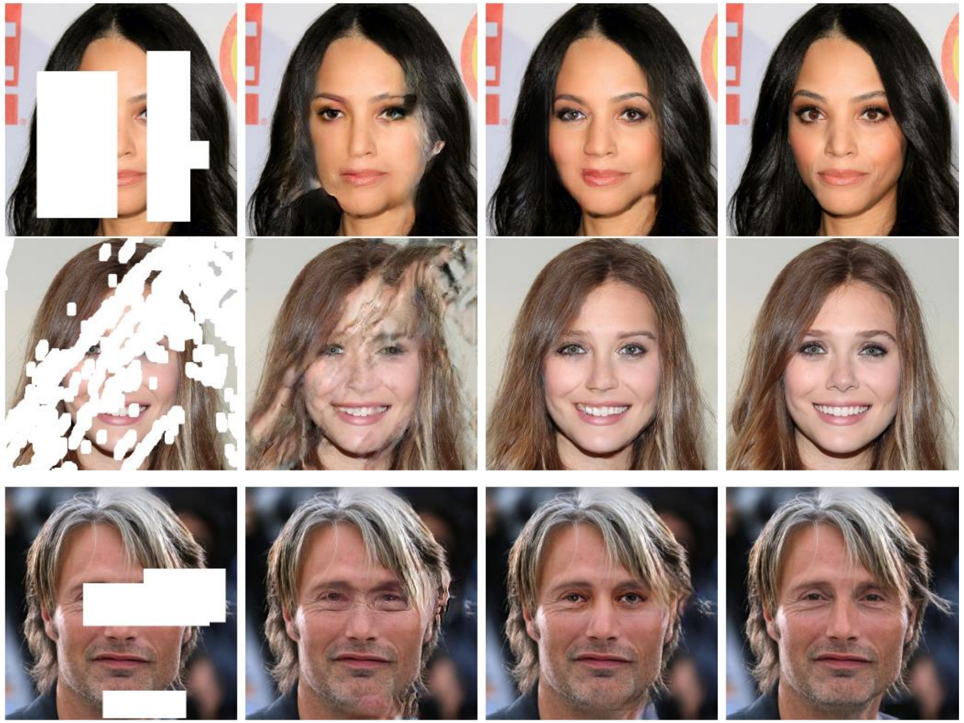
- Interpretable latent space
  - By interpolating z, we can observe how the generated samples vary
  - Automatic clustering in the (low-dimensional) latent space

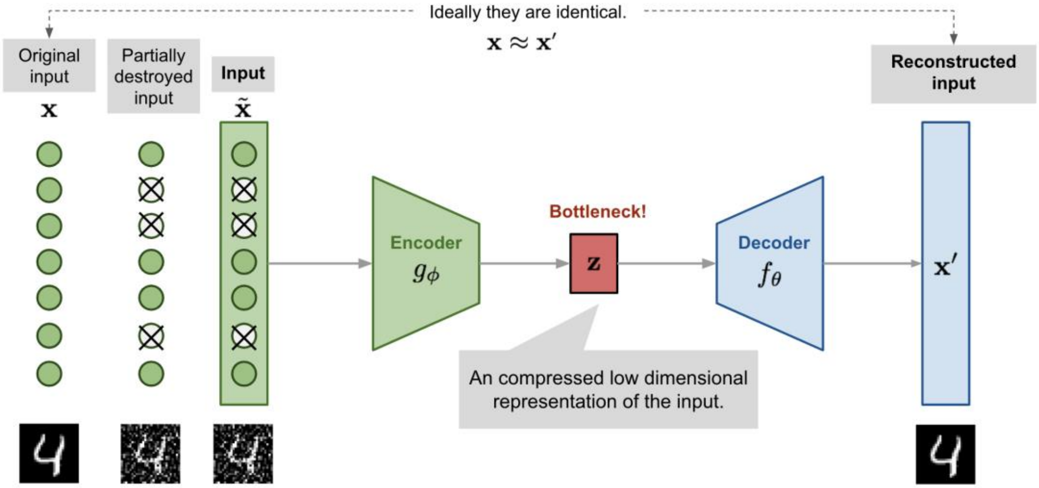




Inpainting with VAE

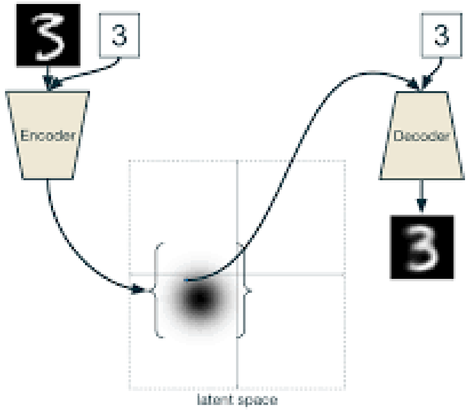
- Inference the mixing pixels?
  - Fully observable training data $D = \{x^{(i)}\}$
  - Standard VAE: $q(z|x)$ & $p(x|z)$
  - Corrupted data: $\bar{x} = x \odot mask$
  - Goal: $q(z|\bar{x}) \approx q(z|x)$
    - We do not need to change the generator $p(x|z)$
- Randomized mask in training!
  - $x \odot mask \rightarrow z \rightarrow x$
  - Better encoder architecture
    - Masked convolution
    - Idea: convolution only on unmasked pixels
    - Image Inpainting for Irregular Holes Using Partial Convolutions (ECCV 2018)



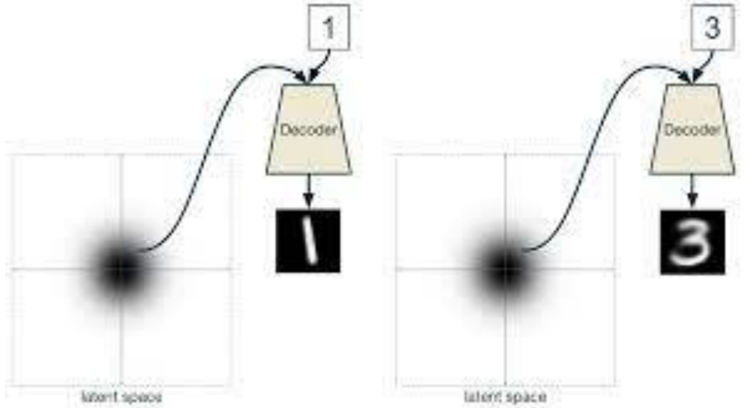


Conditioned VAE

- Include label in VAE
  - $D = \{(x^{(i)}, y^{(i)})\}$
  - Encoder: $q(z|x, y; \phi)$
  - Decoder: $p(x|y, z; \theta)$
  - Conditioned generation!



conditioned VAE

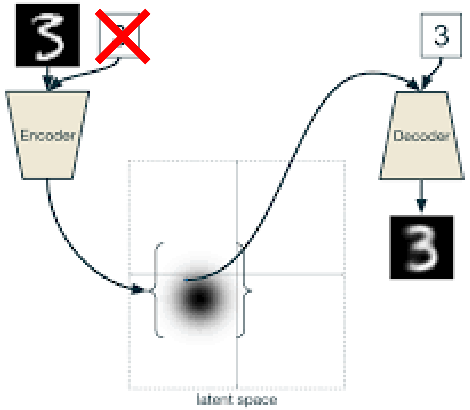


conditioned generation

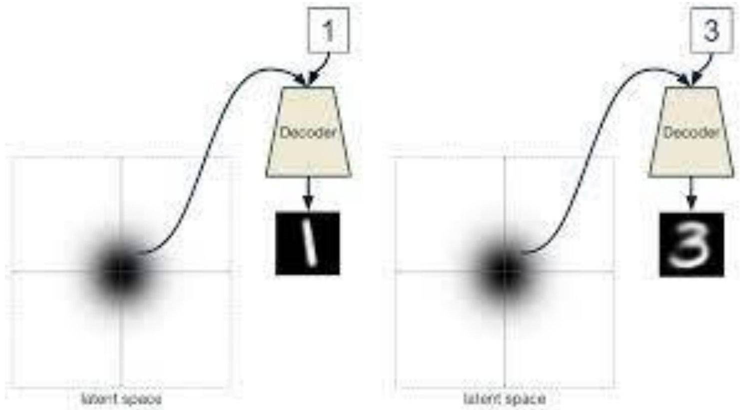
- What if we have both labeled data and unlabeled data?

Conditioned VAE

- Semi-supervised learning
  - $D_l = \{(x^{(i)}, y^{(i)})\}$
  - $D_u = \{(x^{(i)})\}$
  - Decoder: $p(x|y, z; \theta)$
  - Encoder?
    - $q(z, y|x; \phi)$
    - In practice: $q(z, y|x; \phi) = q(z|x; \phi) \cdot q(y|x; \phi)$



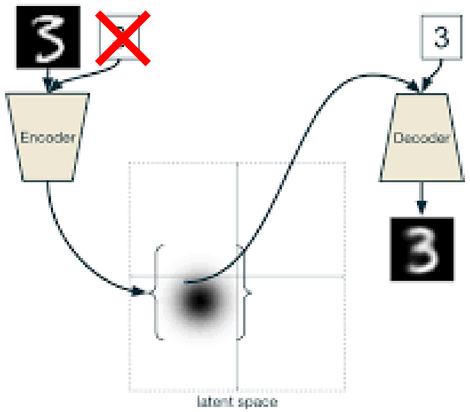
conditioned VAE



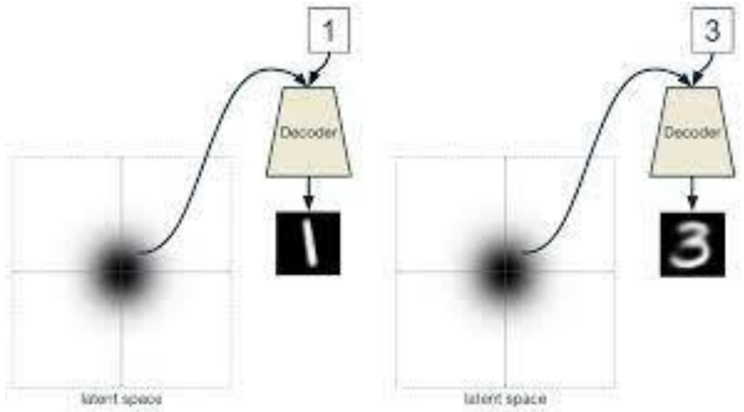
conditioned generation

Conditioned VAE

- Semi-supervised learning
  - $D_l = \{(x^{(i)}, y^{(i)})\}$
  - $D_u = \{(x^{(i)})\}$
  - Decoder: $p(x|y,z;\theta)$
  - Encoder: $q(z,y|x;\phi)$
- Training
  - Easy on supervised data
    - Cross-entropy loss on $q(y|x;\phi)$ on labeled data
  - What about unlabeled data?



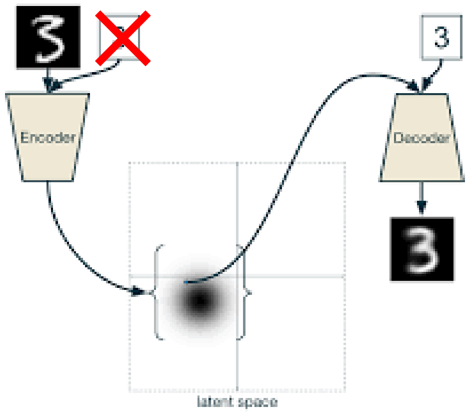
conditioned VAE



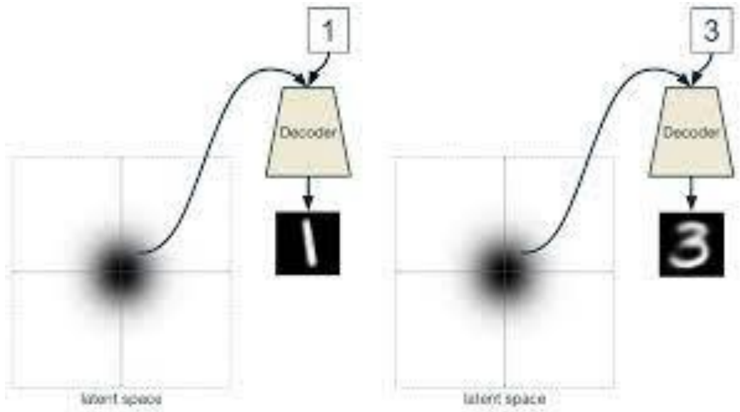
conditioned generation

Conditioned VAE

- Semi-supervised learning
  - $D_l = \{(x^{(i)}, y^{(i)})\}$
  - $D_u = \{(x^{(i)})\}$
  - Decoder: $p(x|y, z; \theta)$
  - Encoder: $q(z, y|x; \phi)$



conditioned VAE

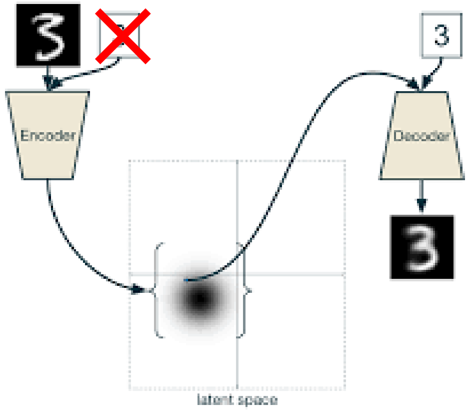


conditioned generation

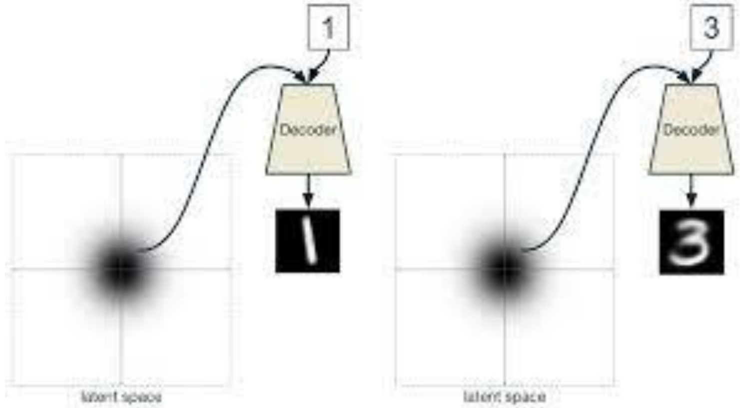
- Training on D_u
  - Loss = reconstruction + KL penalty
  - KL penalty: $KL(q(z)||p(z)) + KL(q(y)||p(y))$ ($p(y)$~uniform)
  - Reconstruction loss: $L = E_{z,y \sim q(z,y)}[\log p(x|z, y; \theta)]$

Conditioned VAE

- Semi-supervised learning
  - $D_l = \{(x^{(i)}, y^{(i)})\}$
  - $D_u = \{(x^{(i)})\}$
  - Decoder: $p(x|y,z;\theta)$
  - Encoder: $q(z,y|x;\phi)$
- Training on D_u
  - Loss = reconstruction + KL penalty
  - KL penalty: $KL(q(z)||p(z)) + KL(q(y)||p(y))$ $(p(y) \sim \text{uniform})$
  - Reconstruction loss: $L = E_{\epsilon \sim N(0,I), y \sim q(y)}[\log p(x|\mu(x) + \sigma(x) \cdot \epsilon, y; \theta)]$
    - Reparameterization trick for z



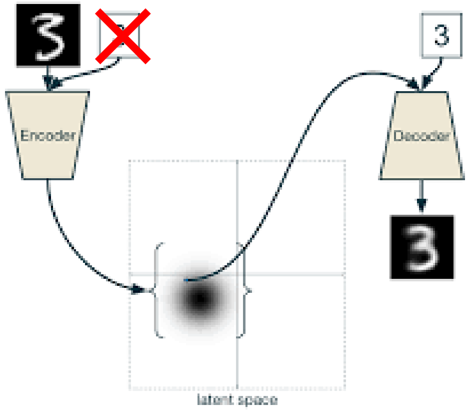
conditioned VAE



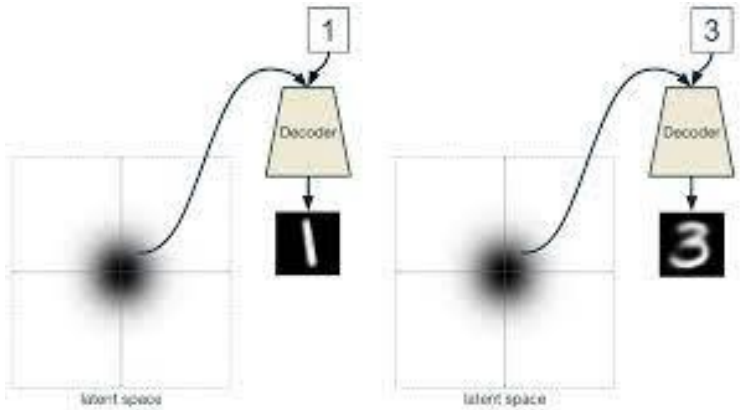
conditioned generation

Conditioned VAE

- Semi-supervised learning
  - $D_l = \{(x^{(i)}, y^{(i)})\}$
  - $D_u = \{(x^{(i)})\}$
  - Decoder: $p(x|y, z; \theta)$
  - Encoder: $q(z, y|x; \phi)$



conditioned VAE



conditioned generation

- Training on D_u
  - Loss = reconstruction + KL penalty
  - KL penalty: $KL(q(z)||p(z)) + KL(q(y)||p(y))$ ($p(y)$~uniform)
  - Reconstruction loss: $L = E_{\epsilon\sim N(0,I), y\sim q(y)}[\log p(x|\mu(x) + \sigma(x)\cdot\epsilon, y; \theta)]$
    - Reparameterization trick for z
    - What about y ?
      - …. although we do have tricks in lecture 11 :P

Conditioned VAE

- Semi-supervised learning
  - $D_l = \{(x^{(i)}, y^{(i)})\}$
  - $D_u = \{(x^{(i)})\}$
  - Decoder: $p(x|y, z; \theta)$
  - Encoder: $q(z, y|x; \phi)$
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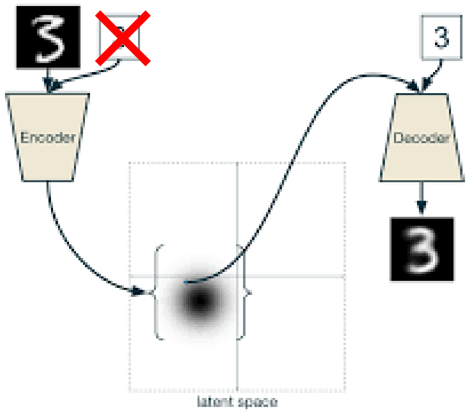
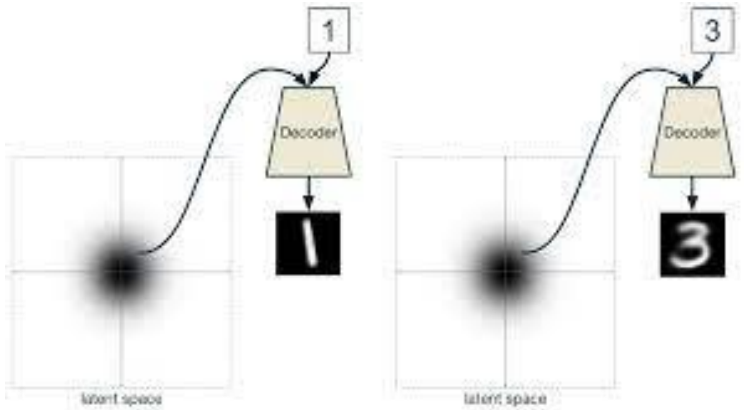
  - Loss = reconstruction + KL penalty
  - KL penalty: $KL(q(z)||p(z)) + KL(q(y)||p(y))$ $(p(y) \sim \text{uniform})$
  - Reconstruction loss: $L = E_{\epsilon \sim N(0,I), y \sim q(y)}[\log p(x|\mu(x) + \sigma(x) \cdot \epsilon, y; \theta)]$
    - Reparameterization trick for z
    - **We only have a few labels! Expand the expectation!**



conditioned VAE



conditioned generation

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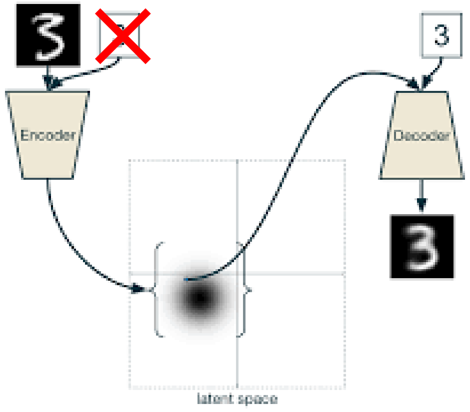
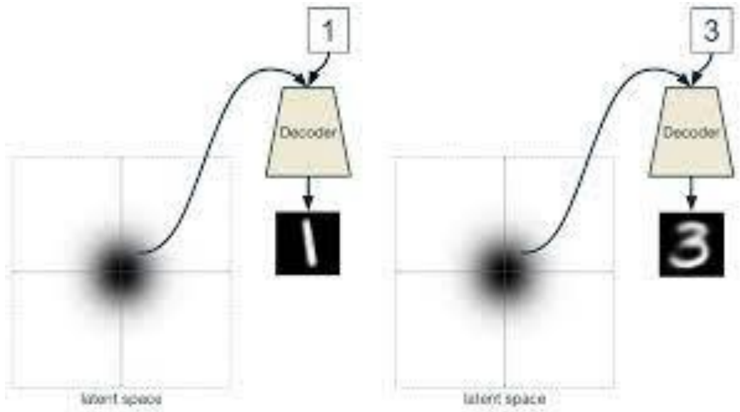


conditioned VAE



conditioned generation

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  - Loss = reconstruction + KL penalty
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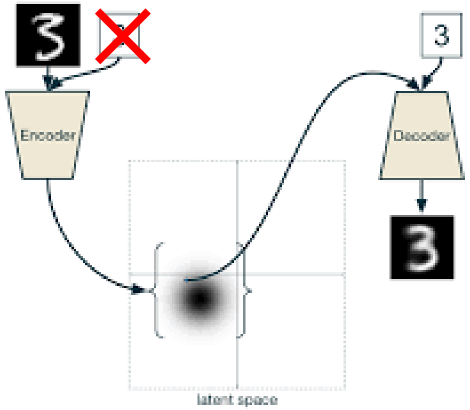
  - Reconstruction loss:
    - $L = E_{\epsilon \sim N(0,I), y \sim q(y)}[\log p(x|\mu(x) + \sigma(x) \cdot \epsilon, y; \theta)]$
    - $= E_{\epsilon \sim N(0,I)}[\sum_c q(y = c) \cdot \log p(x|\mu(x) + \sigma(x) \cdot \epsilon, y; \theta)]$

Conditioned VAE

- Semi-supervised learning
  - $D_l = \{(x^{(i)}, y^{(i)})\}$
  - $D_u = \{(x^{(i)})\}$
  - Decoder: $p(x|y, z; \theta)$
  - Encoder: $q(z, y|x; \phi)$
- Training on the entire dataset D
  - Supervised loss L^l
    - Cross entropy for $q(y)$; VAE loss for $q(z)$& $p(x|z, y)$
  - Unsupervised loss L^u
    - Expanded likelihood over y for reconstruction loss
  - Combined loss: $J(\theta, \phi) = L^l + \beta L^u$
    - Leverage massive unlabeled data!



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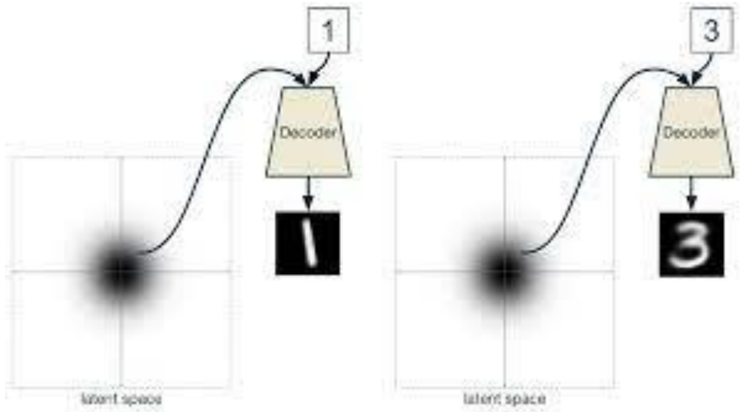

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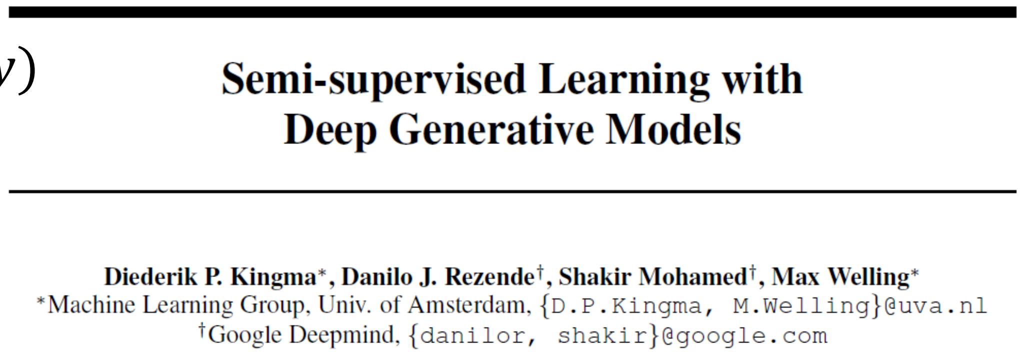

Semi-supervised Learning with Deep Generative Models

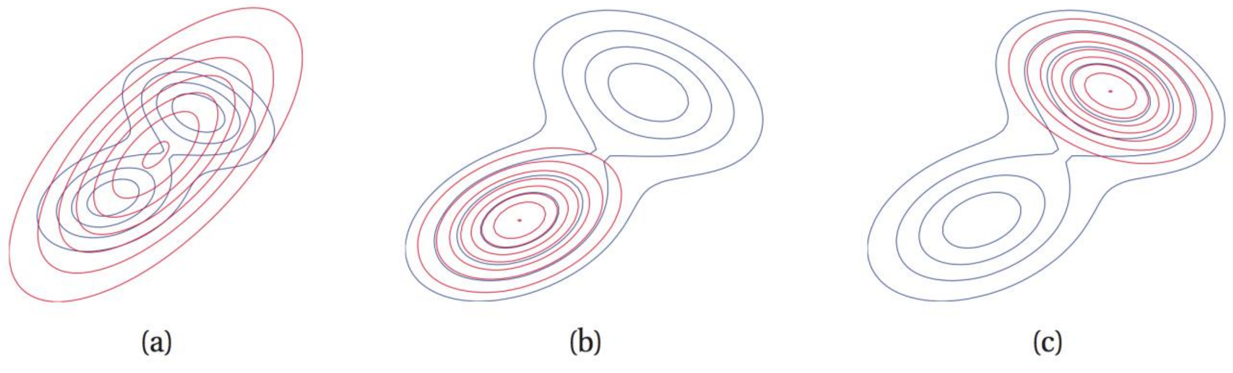
Diederik P. Kingma*, Danilo J. Rezende†, Shakir Mohamed†, Max Welling*
*Machine Learning Group, Univ. of Amsterdam, {D.P.Kingma, M.Welling}@uva.nl
†Google Deepmind, {danilor, shakir}@google.com

Variational Autoencoder: Summary

- Pros
  - Flexible architecture & stable training
- Cons
  - Approximate inference

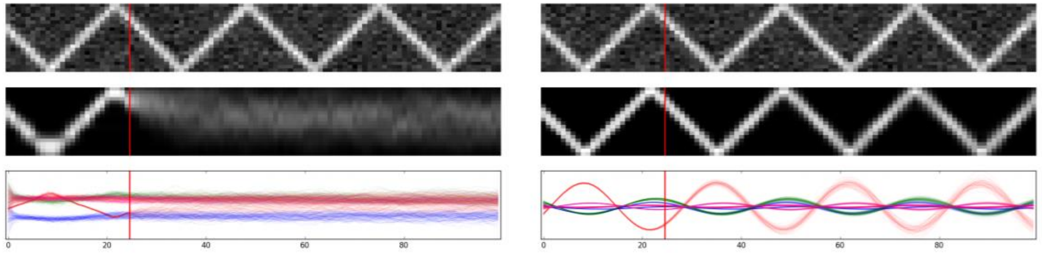
Variational Autoencoder: Summary

- Pros
  - Flexible architecture & stable training
- Cons
  - Approximate inference
    - Intrinsic issue of KL divergence in VI
      - KL is asymmetric
        - VI: $KL(q||p) = \sum_z q(z) \log \frac{q(z)}{p(z)}$
      - $KL(q||p)$: reverse (exclusive) KL
      - $KL(p||q)$: forward (inclusive) KL
      - The mode collapse issue
        - Use forward KL?
        - Further reading of interest
        - https://arxiv.org/abs/2202.01841



Variational Autoencoder:

- Pros
  - Flexible architecture & stable training
- Cons
  - Approximate inference
    - Intrinsic issue of KL divergence in VI
    - Assumed density of $q(z|x)$ & $p(z)$
      - $p(z) \sim N(0, I)$ for computation reason
        - We can have a more powerful prior (later in lecture 10)
        - E.g., structured VAE; VQ-VAE-2
      - $q(z|x) \sim N(\mu(x), \Sigma(x))$
        - What if $p(z|x)$ is multi-modal?
        - We need a more powerful proposal distribution
          - E.g., flow models as $q(z)$



(a) Predictions after 200 training epochs. (b) Predictions after 1100 training epochs.

Structured VAE

https://arxiv.org/abs/1603.06277

h_{top} $h_{\text{top}}, h_{\text{middle}}$ $h_{\text{top}}, h_{\text{middle}}, h_{\text{bottom}}$ Original

VQ-VAE-2

https://arxiv.org/abs/1906.00446

Variational Inference with Normalizing Flows

Danilo Jimenez Rezende DANILOR@GOOGLE.COM
Shakir Mohamed SHAKIR@GOOGLE.COM
Google DeepMind, London

https://arxiv.org/abs/1505.05770

Variational Autoencoder: Summary

- Pros
  - Flexible architecture & stable training
- Cons
  - Approximate inference
    - Intrinsic issue of KL divergence
    - Assumed density of $q(z)$ & $p(z)$
    - Variance due to single-step sampling
      - Importance-weighted autoencoder (Burda, Grosse & Ruslan, ICLR16)
        - https://arxiv.org/abs/1509.00519
      - Use more than one samples from $q(z|x)$ for a tighter lower-bound

Variational Autoencoder: Summary

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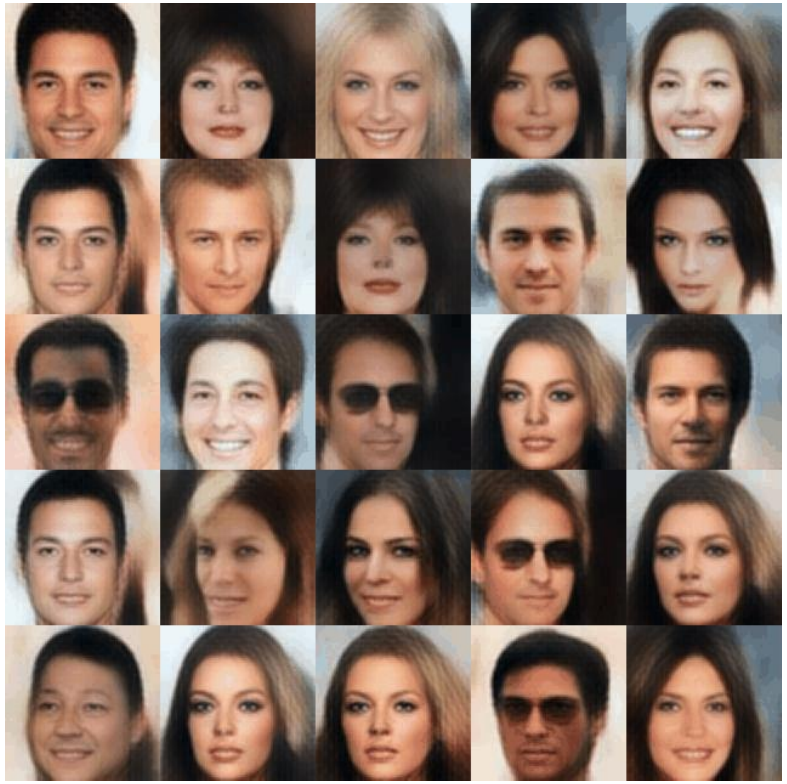
  - Approximate inference
    - Intrinsic issue of KL divergence
    - Assumed density of $q(z)$ & $p(z)$
    - Variance due to single-step sampling
    - MLE as the reconstruction loss
      - $p(x|z;\theta) = N(f(z;\theta), I)$
      - Blurry samples!
        - Improve the decoder architecture
        - Balancing the KL penalty and reconstruction loss
        - Gaussian latent to discrete latent (in lecture 11)
        - Change the loss! (next lecture ☺)



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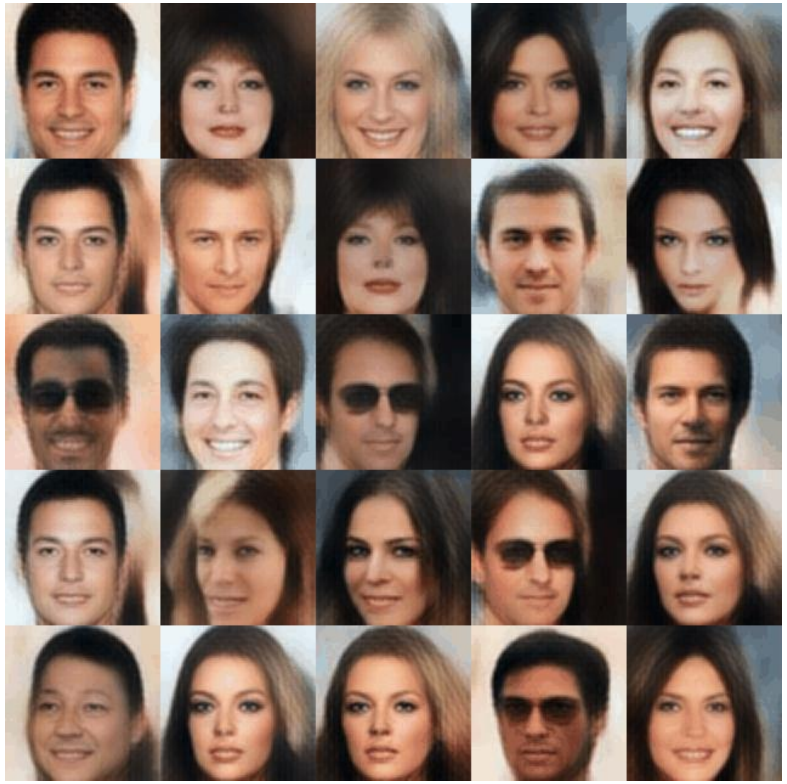


VAE Variants

- VAE Objective (ELBO)

$$J(\theta, \phi; x) = \underbrace{E_{z\sim q(z|x;\phi)}[\log p(x|z;\theta)]}_{\text{Reconstruction}} - \underbrace{KL(q(z|x;\phi)||p(z;\theta))}_{\text{KL penalty}}$$

VAE Variants

- β-VAE (Higgins et. al, DeepMind, ICLR 2017)

$$J(\theta, \phi; x) = E_{z \sim q(z|x;\phi)}[\log p(x|z;\theta)] - \boldsymbol{\beta}\, KL(q(z|x;\phi)||p(z;\theta))$$

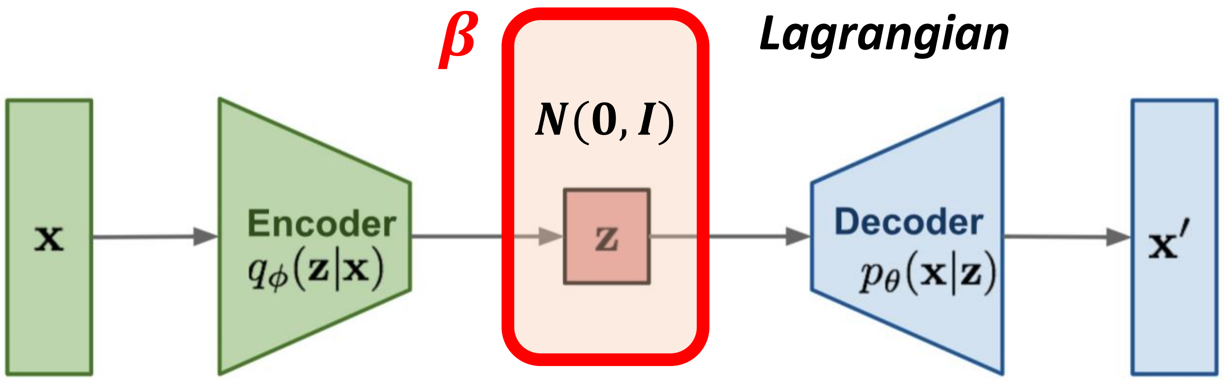
Reconstruction

KL penalty

- Interpretation

$$\max_{\theta,\phi} E_{x \sim D}\left[E_{z \sim q(z|x;\phi)}[\log p(x|z;\theta)]\right]$$

$$\text{subject to } KL(q(z|x;\phi)||p(z)) < \epsilon$$



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$$J(\theta, \phi; x) = E_{z\sim q(z|x;\phi)}[\log p(x|z;\theta)] - \boldsymbol{\beta}\, KL(q(z|x;\phi)||p(z;\theta))$$

Reconstruction KL penalty

- Special cases
  - $\beta = 0$: standard AE
  - $\beta = 1$: standard VAE
  - $\beta > 1$: force the latent space closer to isomorphic Gaussian
    - Insight: each dimension of z are forced to be independent
    - Disentangle factors!

VAE Variants

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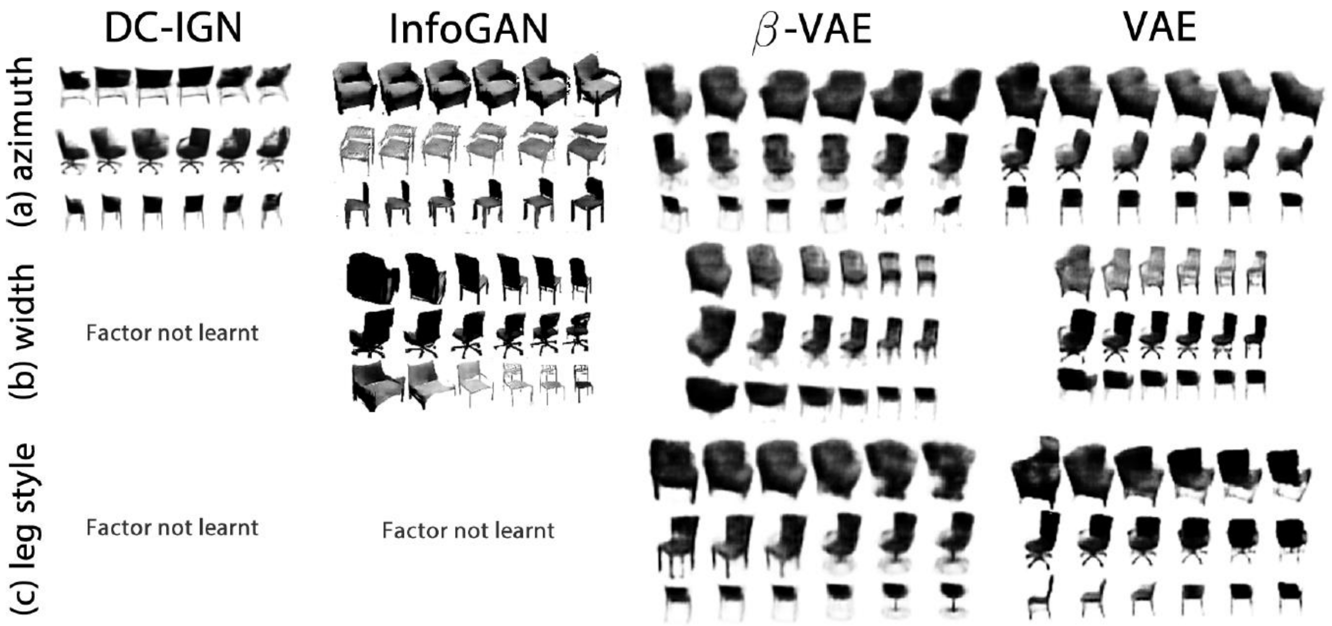
$$J(\theta, \phi; x) = E_{z \sim q(z|x;\phi)}[\log p(x|z;\theta)] - \boldsymbol{\beta}\, KL(q(z|x;\phi)||p(z;\theta))$$

Reconstruction KL penalty

- Learned factors in z



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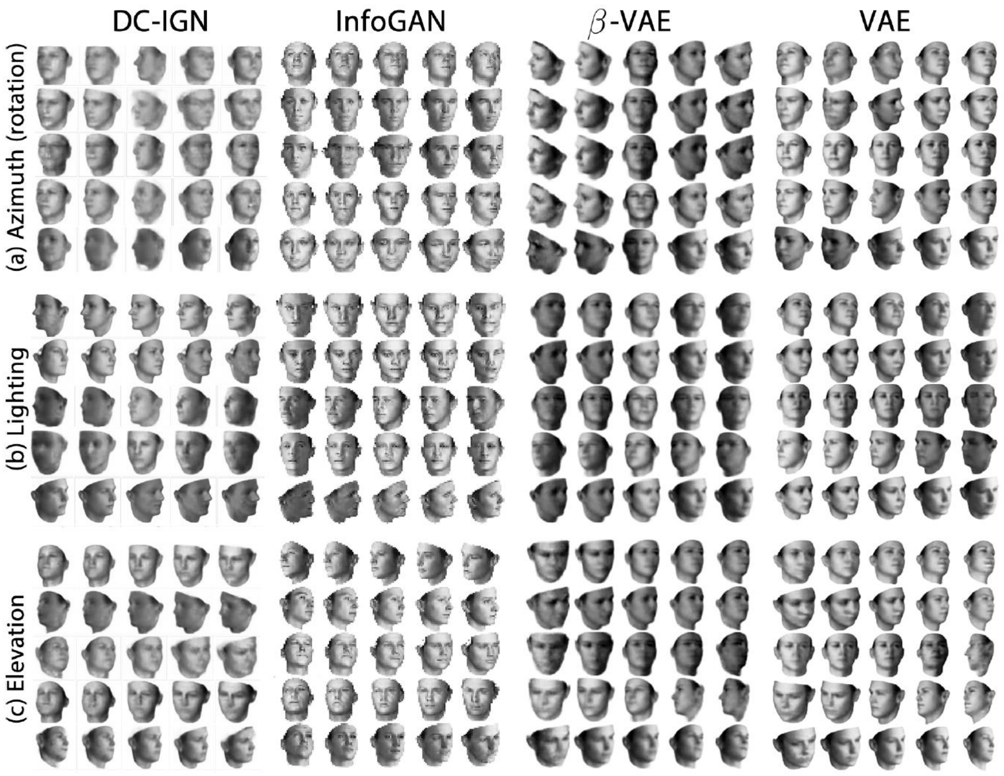
Reconstruction KL penalty

- Learned factors in z



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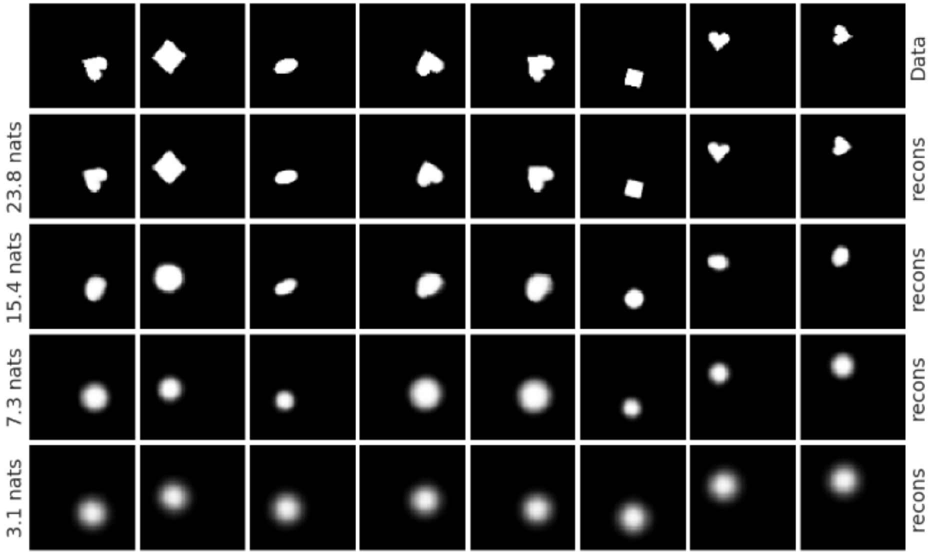
$$J(\theta,\phi;x) = \underbrace{E_{z\sim q(z|x;\phi)}[\log p(x|z;\theta)]}_{\text{Reconstruction}} - \boldsymbol{\beta}\, \underbrace{KL(q(z|x;\phi)||p(z;\theta))}_{\text{KL penalty}}$$

- Learned factors in z
  - Trade-off between reconstruction and disentangle features!

$KL(q||N(0,I))$



β can be critical!

VAE Variants

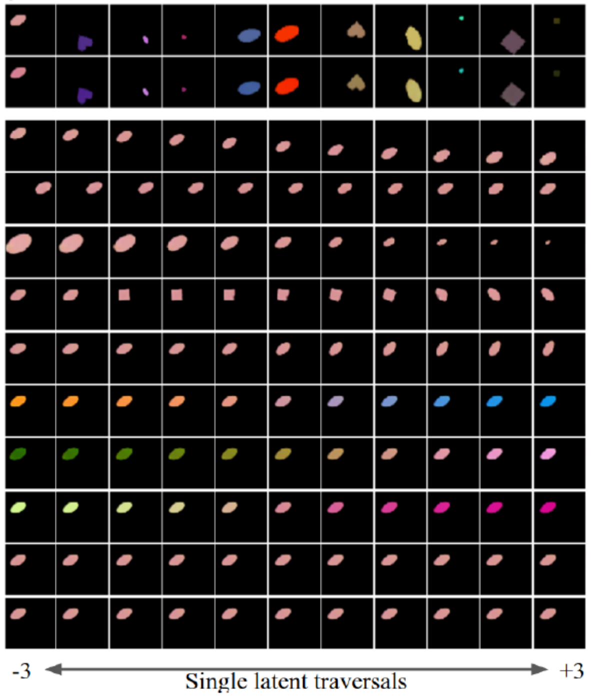
- Understanding disentangling in β-VAE (DeepMind, NIPS 2017)

$$J(\theta,\phi;x) = E_{z\sim q(z|x;\phi)}[\log p(x|z;\theta)] - \boldsymbol{\beta} \, |KL(q(z|x;\phi)||p(z;\theta)) - \boldsymbol{C}|$$

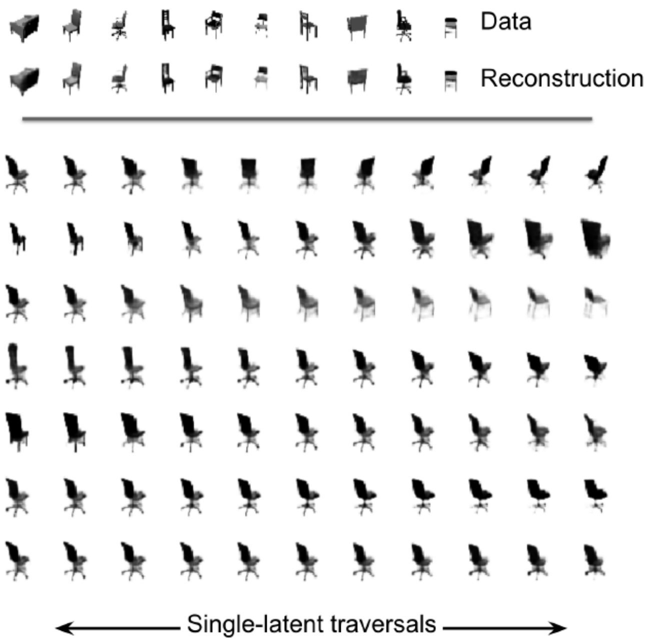
Reconstruction KL penalty **Controlled capacity**

- Learned factors in z
  - Gradually *increase* C!

(a) Coloured dSprites



(b) 3D Chairs



VAE Variants

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$$J(\theta, \phi; x) = \underbrace{E_{z \sim q(z|x;\phi)}[\log p(x|z;\theta)]}_{\text{Reconstruction}} - \boldsymbol{\beta}\, \underbrace{KL(q(z|x;\phi)||p(z;\theta))}_{\text{KL penalty}}$$

- Learned factors in z
  - A popular (unsupervised) approach for pretraining features
- No free lunch!
  - Challenging Common Assumptions in the Unsupervised Learning of Disentangled Representations, (Google Brain, ICML2019)
  - Disentangle features are fundamentally **impossible** without supervision or model inductive bias
    - Inductive bias or supervision is important (structured model)
    - Empirical successes can be highly random …
      - **Tune your model hard!**

Summary

- Generative Model
  - Learn a probability distribution $p(x;\theta)$
  - Energy-based model: $p(x) = \frac{1}{Z}\exp(-E(x;\theta))$
  - Flow model: $x = f(z;\theta)$ (f is a bijection)
  - Latent variable model: $p(x,z) = p(x|z)p(z)$
- Variational Autoencoder
  - A computation-efficient design of $p(x,z)$
    - Isomorphic Gaussian wherever possible
  - Variational inference for efficient and stable learning
    - ELBO & reparameterization trick
  - Flexible framework with nice mathematical property
    - But may suffer from blurry outputs… (next lecture!)

Lunch Time