Lecture 13: Deep Generative Models II: AE & VAE

Lan Xu SIST, ShanghaiTech Fall, 2024



Outline

- Representation learning
 - AutoEncoder
- Variational Autoencoders (VAEs)
 - □ VAE objective
 - Reparametrization trick
 - Connection to Auto-Encoders

Acknowledgement: Feifei Li et al's cs231n notes



Recall EM GMM

MLE: maximizing the log-likelihood

$$\ell(\theta) = \sum_{i=1}^{n} \log p(x^{(i)}; \theta)$$

ELBO: Evidence Lower Bound

$$\begin{split} \log p(\mathbf{x}) &= \log \int_z p(\mathbf{x}, z) \\ &= \log \int_z p(\mathbf{x}, z) \frac{q(\mathbf{z})}{q(\mathbf{z})} \\ &= \log (E_q[\frac{p(\mathbf{x}, \mathbf{z})}{q(\mathbf{z})}]) \\ &= \log (E_q[\log p(\mathbf{x}, \mathbf{z})] - E_q[\log q(\mathbf{z})] - E_q[\log p(\mathbf{z}, \mathbf{x})] + \log p(\mathbf{x}) \\ &= \log p(\mathbf{x}) - (E_q[\log p(\mathbf{z}, \mathbf{x})] - E_q[\log q(\mathbf{z})]) \\ &\geq E_q[\log p(\mathbf{x}, \mathbf{z})] - E_q[\log q(\mathbf{z})] \end{split}$$



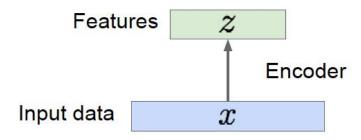
= ELBO

$$egin{aligned} EBLO &= E_q[\log p(\mathbf{x}, \mathbf{z})] - E_q[\log q(\mathbf{z})] \ &= E_q[\log rac{p(\mathbf{x}, \mathbf{z})}{p(\mathbf{z})}] - E_q[\log rac{q(\mathbf{z})}{p(\mathbf{z})}] \ &= E_q[\log p(\mathbf{x}|\mathbf{z})] - KL(q(\mathbf{z})||p(\mathbf{z})) \end{aligned}$$



Feature representation learning

Unsupervised approach for learning a lower-dimensional feature representation from unlabeled training data

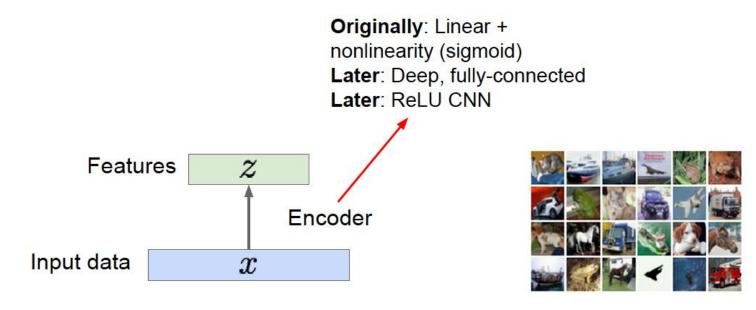






Feature representation learning

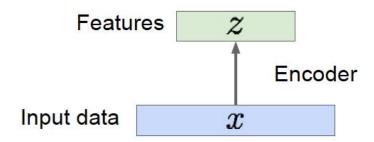
Unsupervised approach for learning a lower-dimensional feature representation from unlabeled training data





Feature representation learning

How to learn this feature representation?



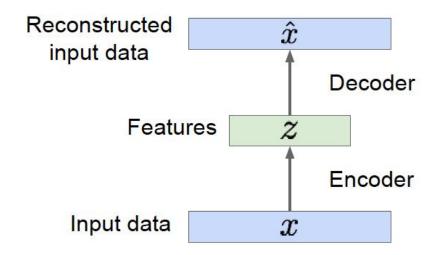


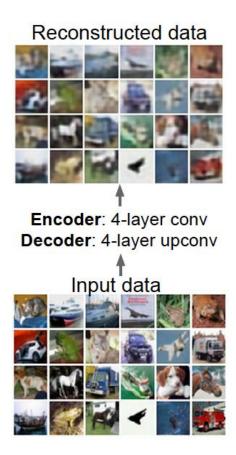


Feature representation learning

How to learn this feature representation?

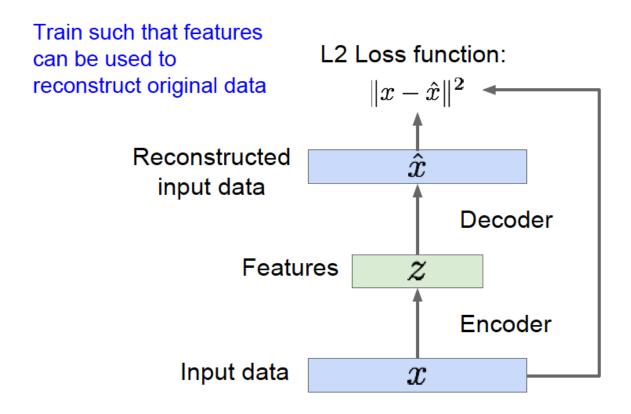
Train such that features can be used to reconstruct original data "Autoencoding" - encoding itself





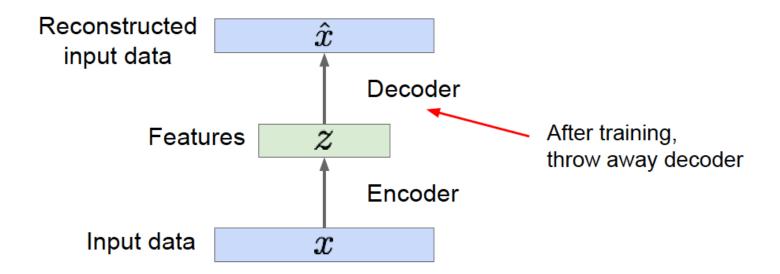


Feature representation learning



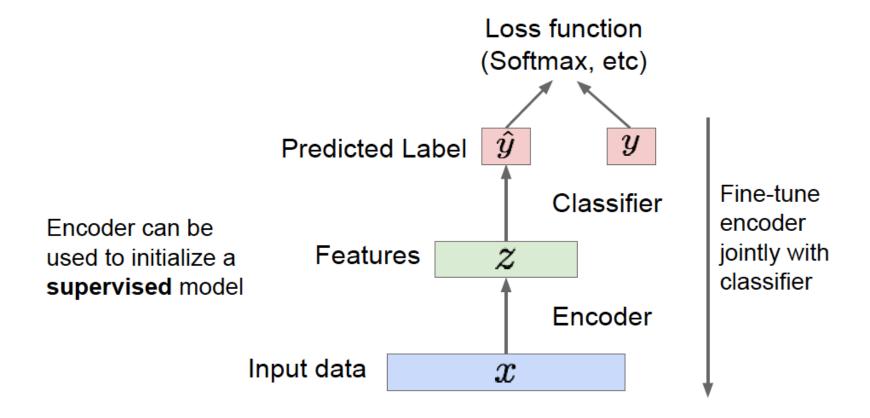


Feature representation learning

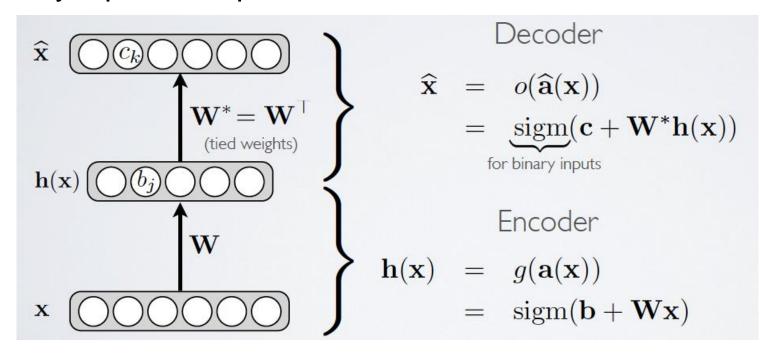




- Feature representation learning
- But not probabilistic: no way to sample new data



Binary input example



$$l(f(\mathbf{x})) = -\sum_{k} (x_k \log(\widehat{x}_k) + (1 - x_k) \log(1 - \widehat{x}_k))$$

- cross-entropy (more precisely: sum of Bernoulli cross-entropies)



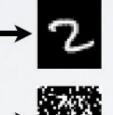
Regularization

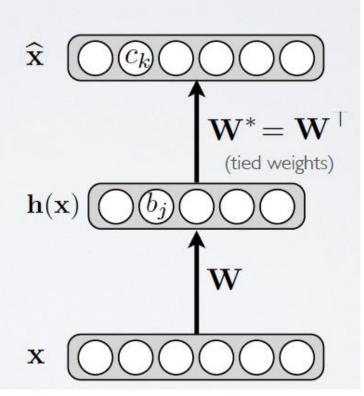
- Regularized autoencoders: add regularization term that encourages the model to have other properties
 - Sparsity of the representation (sparse autoencoder)
 - Robustness to noise or to the missing inputs (denoising autoencoder)
 - Smallness of the derivative of the representation (contracitve autoencoder)

Regularization

Undercomplete representation

- Hidden layer is undercomplete if smaller than the input layer
 - hidden layer "compresses" the input
 - will compress well only for the training distribution
- Hidden units will be
 - good features for the training distribution
 - but bad for other types of input



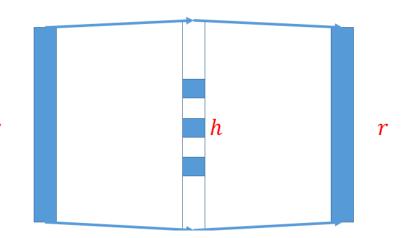


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Regularization

$$L_R = L(x, g(f(x))) + R(h)$$

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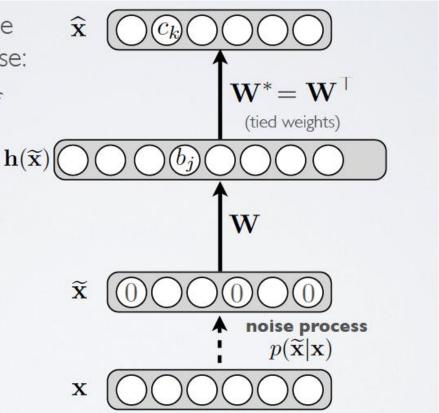
- Sparse autoencoder
 - Constrain the code to have sparsity
 - □ Training: minimize a loss function

$$L_R = L(x, g(f(x))) + \lambda |h|_1$$

Regularization

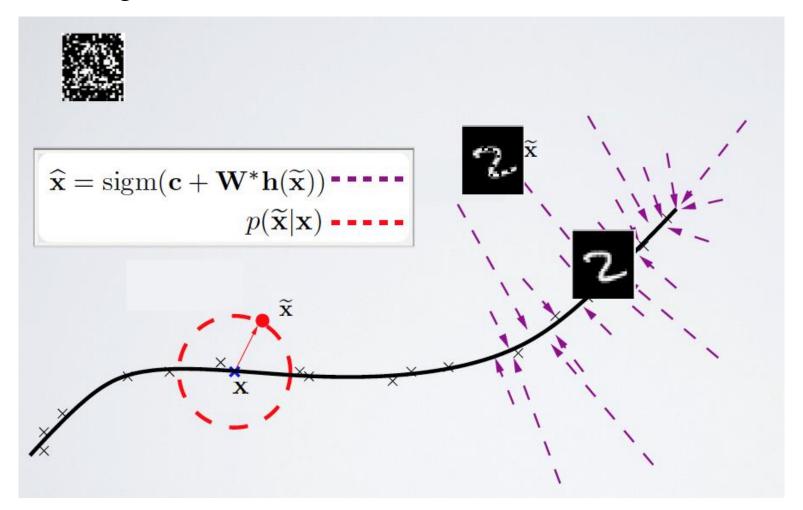
Denoising autoencoder

- Idea: representation should be robust to introduction of noise:
 - random assignment of subset of inputs to 0, with probability u
 - Gaussian additive noise
- Reconstruction $\widehat{\mathbf{x}}$ computed from the corrupted input $\widetilde{\mathbf{x}}$
- Loss function compares $\widehat{\mathbf{x}}$ reconstruction with the
 - noiseless input X



Regularization

Denoising autoencoder





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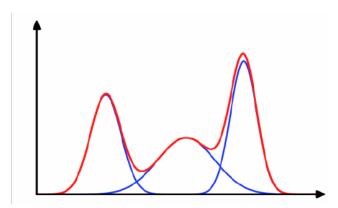
Latent variable model

- Data generation process
 - \square Latent variable \boldsymbol{z} $p(\boldsymbol{z}) = \text{something simple}$
 - \square A mapping from the latent space to observation $oldsymbol{x}$

$$p(x) = \int p(x, z) dz$$
 where $p(\boldsymbol{x}, \boldsymbol{z}) = p(\boldsymbol{x} \mid \boldsymbol{z})p(\boldsymbol{z})$

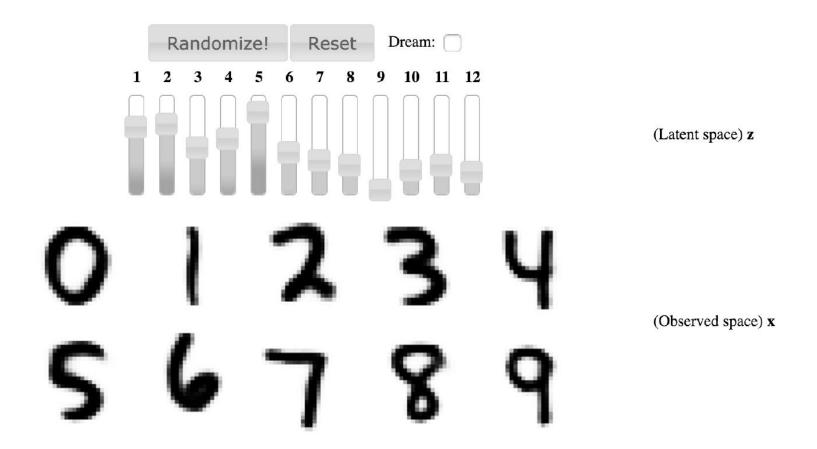
For example, a Gaussian mixture model

$$p_{\theta}(x) = \sum_{k=1}^{K} p_{\theta}(z=k) p_{\theta}(x|z=k)$$



An example

Generating hand-written digits

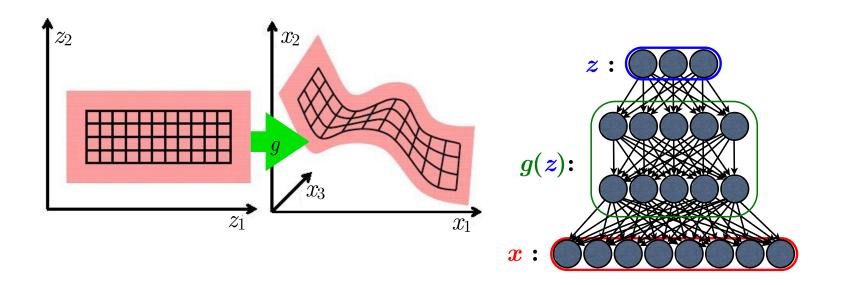


http://www.dpkingma.com/sgvb_mnist_demo/demo.html

Deep Latent Variable Models

Leverage neural networks in a latent variable model

$$p(\boldsymbol{x}, \boldsymbol{z}) = p(\boldsymbol{x} \mid \boldsymbol{z})p(\boldsymbol{z})$$
 $p(\boldsymbol{x} \mid \boldsymbol{z}) = g(\boldsymbol{z})$



Can represent complicated data distribution and conditional dependencies



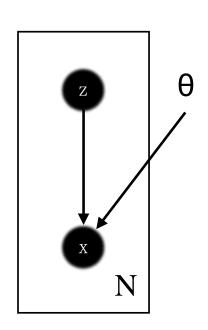
An example

$$p(z) = N(0, I)$$

- $P_{ heta}(x|z) = N(\mu, \sigma^2)$ $\mu = f_{ heta}(z) = ext{multilayer neural net}$
- With flexible neural net,

$$p_{ heta}(x) = \int_z p_{ heta}(x|z) p(z) dz$$

- Can be arbitrarily complicated
- The multilayer network can capture complex dependencies in the data generation process





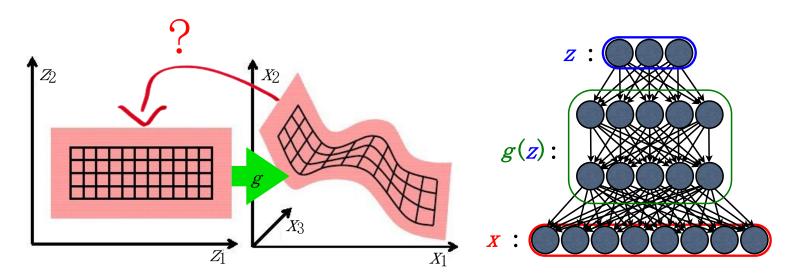
Challenges in Deep LVM

Inference:

- \square Given an observation $oldsymbol{x}$, what is the probable $oldsymbol{z}$?
- \square Computing the posterior $p(\mathbf{z}|\mathbf{x})$ (intractable)

Learning:

- oxdot Given a large dataset of observations $\mathbf{X} = \{\mathbf{x}^{(1)}, \cdots, \mathbf{x}^{(N)}\}$
- ☐ Estimating the parameters in Deep LVM (inefficient/intractable)



The Variational Autencoder: overview

- Auto-Encoding Variational Bayes
- ICLR2014, and ICLR 2024 Test of Time Award



Durk Kingma



Max Welling





The Variational Autencoder: overview

Inference:

- $\hfill\Box$ Introduce a parametric model $\,q_\phi(z\mid x)$ to approximate the true posterior $p_\theta(z\mid x)$
- □ Variational inference or Amortized inference

$$\forall x_i \quad \arg\min_{q_i} D_{KL}(q_i(z)||p_{\theta}(z|x_i))$$

$$\Rightarrow \forall x_i \quad \arg\min_{\phi} D_{KL}(q_{\phi}(z|x_i)||p_{\theta}(z|x_i))$$

 Replacing datum-wise posterior distribution by a parametric family of conditional densities.



The Variational Autencoder: overview

Inference:

- Introduce a parametric model $q_{\phi}(z \mid x)$ to approximate the true posterior $p_{\theta}(z \mid x)$
- Variational inference or Amortized inference

Learning:

Based on Maximum Likelihood

$$\max \sum_{i=1}^{N} \log p(x^{(i)})$$

- Direct optimization is challenging: use EM learning strategy
- Jointly learning inference model with the deep latent variable model



Recall lower bound of the data log likelihood

$$\begin{split} \log p_{\theta}(x) &= \log \int_{z} p_{\theta}(x,z) dz \\ &= \log \int_{z} q_{\phi}(z|x) \frac{p_{\theta}(x,z)}{q_{\phi}(z|x)} dz \\ &\geq \int_{z} q_{\phi}(z|x) \log \frac{p_{\theta}(x,z)}{q_{\phi}(z|x)} dz \quad \text{(Jensen's Inequality)} \\ &= \mathbf{E}_{q_{\phi}(z|x)} \left[\log p_{\theta}(x,z) - \log q_{\phi}(z|x) \right] = \mathcal{L}(x;\theta,\phi) \\ &\log p_{\theta}(x) = \boxed{\mathcal{L}(x;\theta,\phi)} + D_{KL}(q_{\phi}(z|x)||p_{\theta}(z|x)) \end{split}$$

- Learning: maximize the lower bound of data likelihood
- ☐ The evidence lower bound (ELBO)



From the EM perspective

$$\log p_{\theta}(x) = \log \frac{p_{\theta}(x \mid z)p(z)}{p_{\theta}(z \mid x)} = \log \frac{p_{\theta}(x \mid z)p(z)q_{\phi}(z \mid x)}{p_{\theta}(z \mid x)q_{\phi}(z \mid x)}$$

$$= E_z[\log p_{\theta}(x|z)] - E_z \left[\log \frac{q_{\phi}(z|x)}{p(z)}\right] + E_z \left[\log \frac{q_{\phi}(z|x)}{p_{\theta}(z|x)}\right]$$

$$= E_{z \sim q_{\phi}(z|x)}[\log p_{\theta}(x|z)] - D_{KL}(q_{\phi}(z|x), p(z)) + D_{KL}(q_{\phi}(z|x), p_{\theta}(z|x))$$

Data reconstruction

KL divergence between prior, and samples from the encoder network

KL divergence between encoder and posterior of decoder



From the EM perspective

$$\log p_{\theta}(x) = \log \frac{p_{\theta}(x \mid z)p(z)}{p_{\theta}(z \mid x)} = \log \frac{p_{\theta}(x \mid z)p(z)q_{\phi}(z \mid x)}{p_{\theta}(z \mid x)q_{\phi}(z \mid x)}$$

$$= E_{z}[\log p_{\theta}(x|z)] - E_{z} \left[\log \frac{q_{\phi}(z|x)}{p(z)}\right] + E_{z} \left[\log \frac{q_{\phi}(z|x)}{p_{\theta}(z|x)}\right]$$

$$=E_{z\sim q_\phi(z|x)}[\log p_\theta(x|z)]-D_{KL}\left(q_\phi(z|x),p(z)\right)+D_{KL}(q_\phi(z|x),p_\theta(z|x))$$

Data reconstruction

- How well does my decoder reconstruct a data point given the latent vector z
- We need to sample from z

KL divergence between prior, and samples from the encoder network

 Measures how good my latent distribution is with respect to my Gaussian prior KL divergence between encoder and posterior of decoder

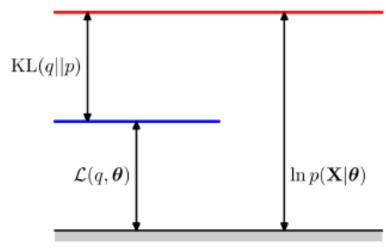
Free energy, >= 0

28



Visualizing ELBO

$$\log p_{ heta}(x) = \mathcal{L}(x; heta, \phi) + D_{KL}(q_{\phi}(z|x)||p_{ heta}(z|x))$$



Bishop - Pattern Recognition and Machine Learning

- Note: all we have done so far is decompose the log probability of the data, we still have exact equality
- This holds for any distribution q

29



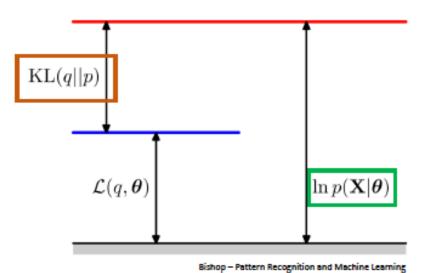
VAE learning

- EM perspective
 - Expectation Maximization alternately optimizes the ELBO, $\mathcal{L}(q,\theta)$, with respect to q (the E step) and θ (the M step)
 - Initialize $\theta^{(0)}$
 - At each iteration t=1,...
 - E step: Hold $\theta^{(t-1)}$ fixed, find $q^{(t)}$ which maximizes $\mathcal{L}(q, \theta^{(t-1)})$
 - M step: Hold $q^{(t)}$ fixed, find $\theta^{(t)}$ which maximizes $\mathcal{L}(q^{(t)}, \theta)$

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EM perspective

The E step



- The first term does not involve q, and we know the KL divergence must be non-negative
- The best we can do is to make the KL divergence 0
- Thus the solution is to set $q^{(t)}(z) \leftarrow p(z|x, \theta^{(t-1)})$

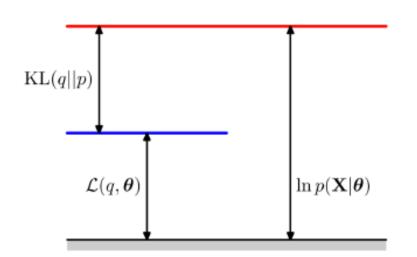
• Suppose we are at iteration t of our algorithm. How do we maximize $\mathcal{L}(q, \theta^{(t-1)})$ with respect to q? We know that:

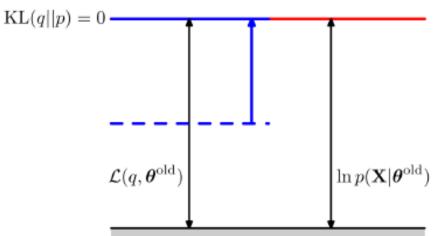
$$\operatorname{argmax}_{q} \mathcal{L}(q, \theta^{(t-1)}) = \operatorname{argmax}_{q} \log p(x|\theta^{(t-1)}) - \operatorname{KL}(q(z)||p(z|x, \theta^{(t-1)}))$$



EM perspective

The E step



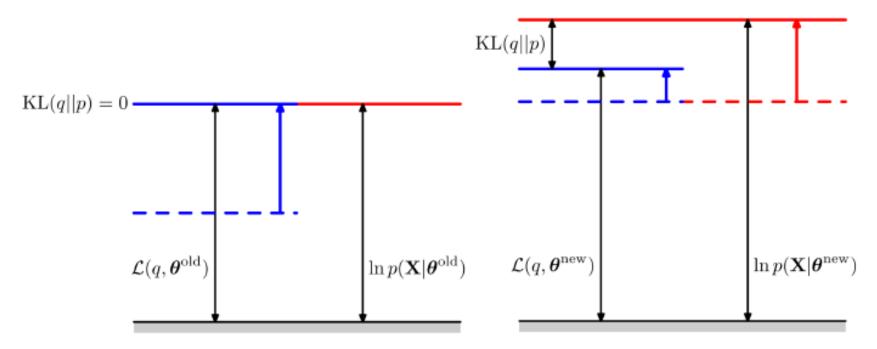


Bishop – Pattern Recognition and Machine Learning

• Suppose we are at iteration t of our algorithm. How do we maximize $\mathcal{L}(q, \theta^{(t-1)})$ with respect to q? $q^{(t)}(z) \leftarrow p(z|x, \theta^{(t-1)})$

EM perspective

The M step



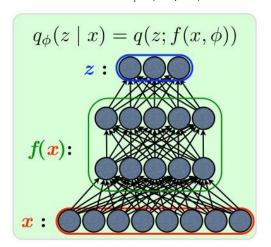
Bishop - Pattern Recognition and Machine Learning

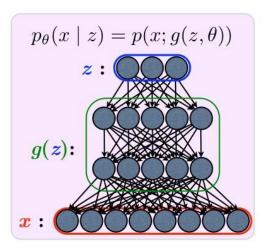
• After applying the E step, we increase the likelihood of the data by finding better parameters according to: $\theta^{(t)} \leftarrow \operatorname{argmax}_{\theta} \mathbb{E}_{q^{(t)}(z)}[\log p(x,z \mid \theta)]$



VAE learning

- What is $q_{\phi}(z|x)$?
 - \square Parametrize $q_{\phi}(z|x)$ with another neural network





Interpreting VAE objective

$$\mathcal{L}(\theta, \phi, x) = \mathbb{E}_{q_{\phi}(z|x)} \left[\log p_{\theta}(x, z) - \log q_{\phi}(z \mid x) \right]$$

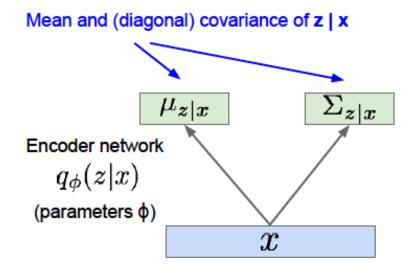
$$= \mathbb{E}_{q_{\phi}(z|x)} \left[\log p_{\theta}(x \mid z) + \log p_{\theta}(z) - \log q_{\phi}(z \mid x) \right]$$

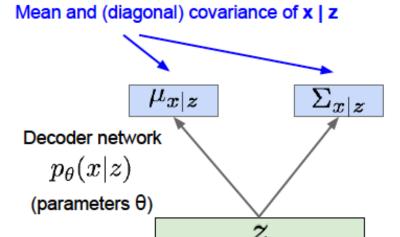
$$= \left(-D_{\text{KL}} \left(q_{\phi}(z \mid x) \| p_{\theta}(z) \right) + \mathbb{E}_{q_{\phi}(z|x)} \left[\log p_{\theta}(x \mid z) \right] \right)$$



VAE Example

Conditionals Gaussians





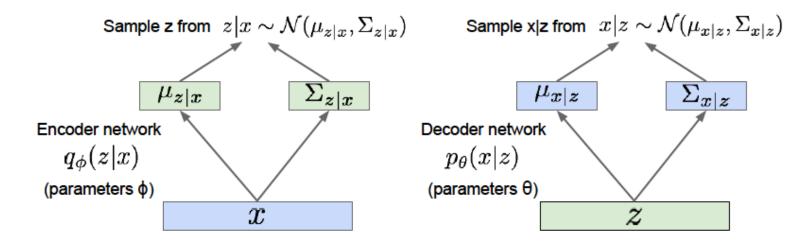


VAE Example

- Conditionals Gaussians
- Jointly train encoder q and decoder p to maximize the Evidence Lower Bound (ELBO)

$$\log p_{\theta}(x) \ge E_{z \sim q_{\phi}(z|x)}[\log p_{\theta}(x|z)] - D_{KL}\left(q_{\phi}(z|x), p(z)\right)$$

Since we're modeling probabilistic generation of data, encoder and decoder networks are probabilistic



Encoder and decoder networks also called "recognition"/"inference" and "generation" networks

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

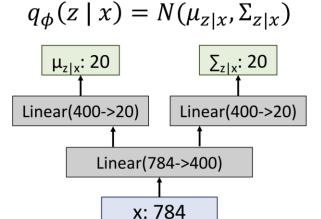


Toy example: Fully-Connected VAE

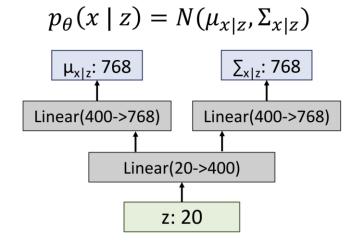
x: 28x28 image, flattened to 784-dim vector

z: 20-dim vector

Encoder Network



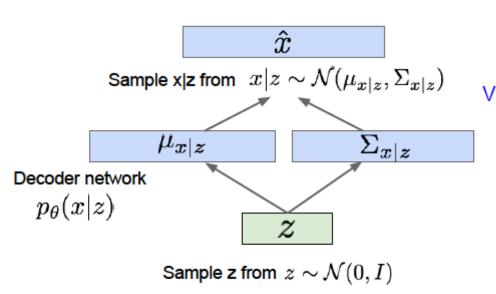
Decoder Network





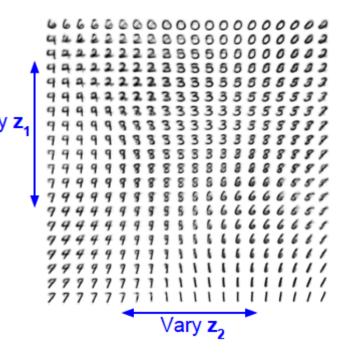
Generating data

Use decoder network. Now sample z from prior!



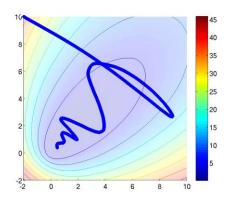
Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Data manifold for 2-d z

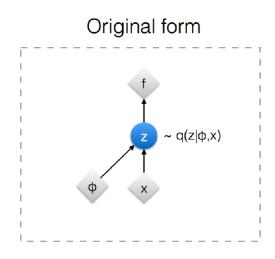


Two views of Learning VAE

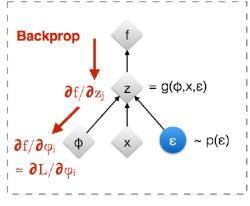
- Optimization interpretation
 - Stochastic gradient-based



- Network interpretation
 - □ Backpropagation



Reparameterised form



Optimization interpretation

Recall VAE objective

$$\mathcal{L}(x, \phi, \theta) = E_{q_{\phi}(z|x)}[\log p_{\theta}(x, z) - \log q_{\phi}(z|x)]$$

- \square Or rewrite as $\mathcal{L}(x,\phi,\theta)=E_{q_{\phi}(z|x)}[f_{\phi,\theta}(x,z)]$
- Often no analytic solution to exact gradient

$$\nabla_{\phi,\theta} \mathcal{L}(x,\phi,\theta)$$

- □ Solution: stochastic gradient ascent
- Requires unbiased estimates of gradient
- Can use small minibatches or single point of data

$$\nabla_{\phi} \mathcal{L}(x, \phi, \theta) \approx \nabla_{\phi} f_{\phi, \theta}(x, z^{(i)}), \quad z^{(i)} \sim q_{\phi}(z|x)$$

High variance for gradient estimation



Reparameterization trick

■ Reparameterize $\mathbf{z}^{(i)} \sim q_{\phi}(\mathbf{z}|\mathbf{x})$ using a differentiable transformation of an auxiliary noise variable ϵ

$$\mathbf{z} = g_{\phi}(\epsilon, \mathbf{x})$$
 with $\epsilon \sim q(\epsilon)$

□ Then we can write the ELBO as

$$\mathcal{L}(x,\phi,\theta) = E_{q_{\phi}(z|x)}[f_{\phi,\theta}(x,z)] = E_{q(\epsilon)}[f_{\phi,\theta}(x,g_{\phi}(\epsilon,\mathbf{x}))]$$

□ And its gradient estimation with L samples

$$\nabla_{\phi} \mathcal{L}(x, \phi, \theta) = E_{q(\epsilon)}[\nabla_{\phi} f_{\phi, \theta}(x, z)] \approx \frac{1}{L} \sum_{i=1}^{L} \nabla_{\phi} f_{\phi, \theta}(x, g_{\phi}(\epsilon^{(i)}, x)), \quad \boxed{\epsilon^{(i)} \sim q(\epsilon)}$$

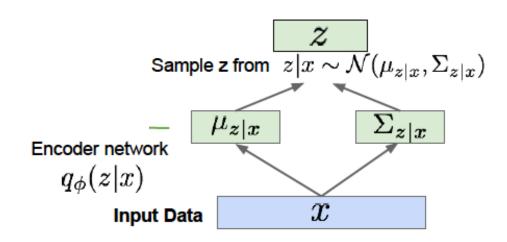


Univariate Gaussian $z \sim p(z|x) = \mathcal{N}(\mu, \sigma^2)$

$$z \sim p(z|x) = \mathcal{N}(\mu, \sigma^2)$$

$$z = \mu + \sigma \epsilon$$
 $\epsilon \sim \mathcal{N}(0, 1)$

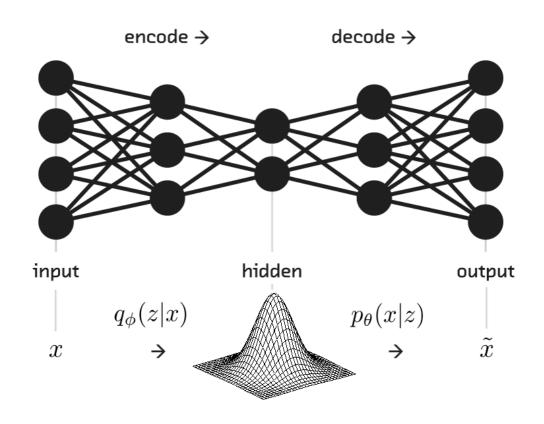
$$\mathbb{E}_{\mathcal{N}(z;\mu,\sigma^2)}\left[f(z)\right] = \mathbb{E}_{\mathcal{N}(\epsilon;0,1)}\left[f(\mu+\sigma\epsilon)\right] \simeq \frac{1}{L} \sum_{l=1}^{L} f(\mu+\sigma\epsilon^{(l)})$$





Objective $\mathcal{L}(x,\phi,\theta) = -D_{KL}(q_{\phi}(z|x)||p_{\theta}(z)) + E_{q_{\phi}(z|x)}[\log p_{\theta}(x|z)]$

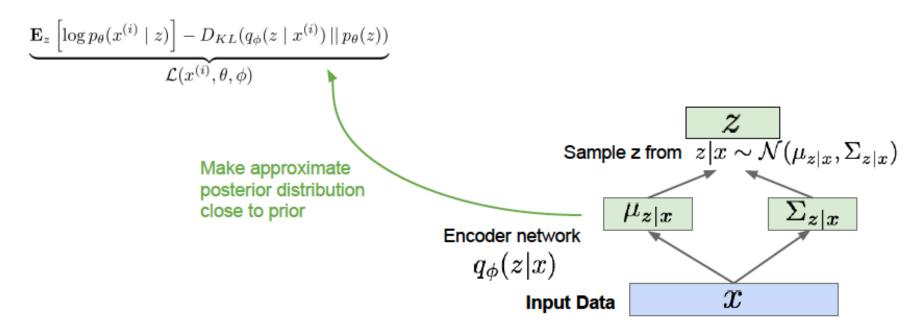
Regularization term Reconstruction term





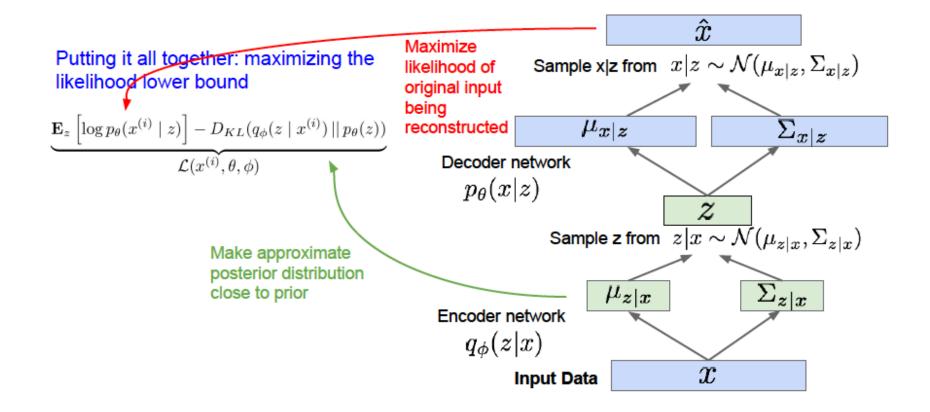
Learning objective

Putting it all together: maximizing the likelihood lower bound





Learning objective





Variational Autoencoders

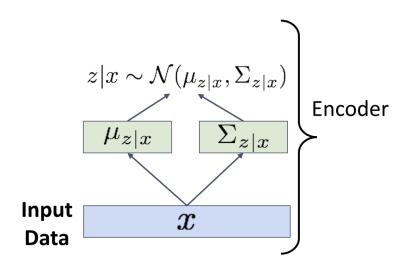
Train by maximizing the variational lower bound

$$E_{z \sim q_{\phi}(z|x)}[\log p_{\theta}(x|z)] - D_{KL}(q_{\phi}(z|x), p(z))$$

- Run input data through encoder to get a distribution over latent codes
- 2. Encoder output should match the prior p(z)!

$$\begin{split} -D_{KL}\left(q_{\phi}(z|x), p(z)\right) &= \int_{Z} q_{\phi}(z|x) \log \frac{p(z)}{q_{\phi}(z|x)} dz \\ &= \int_{Z} N\left(z; \mu_{z|x}, \Sigma_{z|x}\right) \log \frac{N(z; 0, I)}{N\left(z; \mu_{z|x}, \Sigma_{z|x}\right)} dz \\ &= \frac{1}{2} \sum_{i=1}^{J} \left(1 + \log \left(\left(\Sigma_{z|x}\right)_{j}^{2}\right) - \left(\mu_{z|x}\right)_{j}^{2} - \left(\Sigma_{z|x}\right)_{j}^{2}\right) \end{split}$$

Closed form solution when q_{ϕ} is diagonal Gaussian and p is unit Gaussian! (Assume z has dimension J)

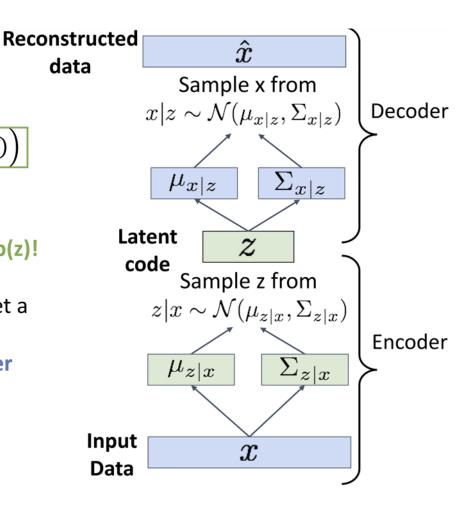


Variational Autoencoders

Train by maximizing the variational lower bound

$$E_{z \sim q_{\phi}(z|x)}[\log p_{\theta}(x|z)] - D_{KL}(q_{\phi}(z|x), p(z))$$

- Run input data through encoder to get a distribution over latent codes
- Encoder output should match the prior p(z)!
- 3. Sample code z from encoder output
- 4. Run sampled code through **decoder** to get a distribution over data samples
- 5. Original input data should be likely under the distribution output from (4)!
- 6. Can sample a reconstruction from (4)

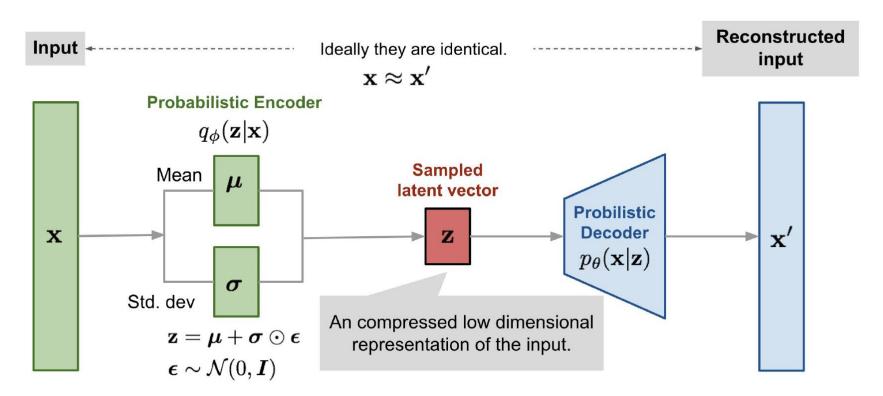


Autoencoder Interpretation

• Objective $\mathcal{L}(x,\phi,\theta) = -D_{KL}(q_{\phi}(z|x)||p_{\theta}(z)) + E_{q_{\phi}(z|x)}[\log p_{\theta}(x|z)]$

Regularization term

Reconstruction term



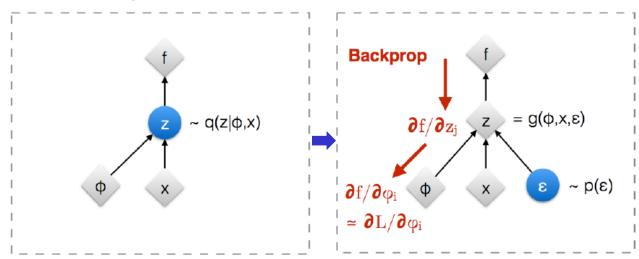
The objective function can be represented as an Autoencoderlike computation graph.

Network interpretation

$$\begin{split} \mathcal{L}(x,\phi,\theta) &= E_{q_{\phi}(z|x)}[f_{\phi,\theta}(x,z)] \\ & \qquad \qquad \downarrow \\ \mathcal{L}(x,\phi,\theta) &= E_{q(\epsilon)}[f_{\phi,\theta}(x,z)] \approx \frac{1}{L} \sum_{i=1}^{L} f_{\phi,\theta}(x,g_{\phi}(\epsilon^{(i)},x)), \quad \epsilon^{(i)} \sim q(\epsilon) \end{split}$$

Original form

Reparameterised form



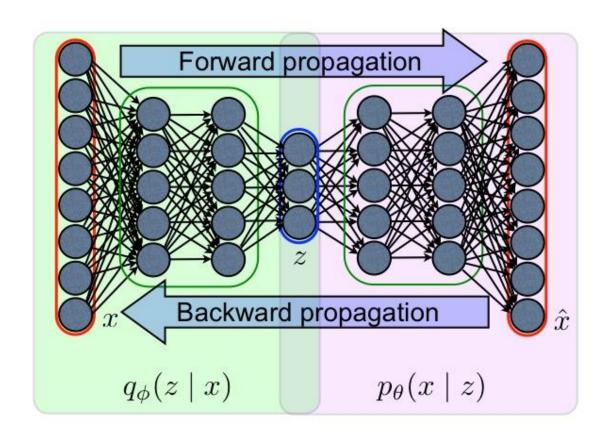
: Deterministic node

: Random node

[Kingma, 2013] [Bengio, 2013] [Kingma and Welling 2014] [Rezende et al 2014]

Training with Backpropagation

Due to reparametrization trick, we can simultaneously train both the generative model and the inference model by optimizing the variational bound using the gradient backpropagation.



50

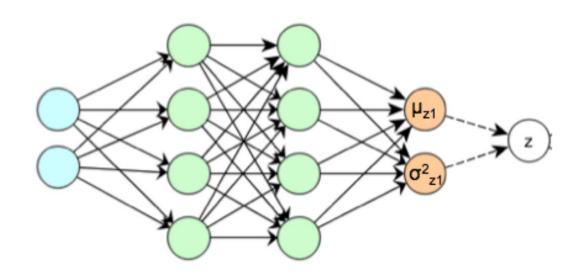


1D Gaussian Case

We can compute the KL regularization in close form

Use N(0,1) as prior for p(z) $q(z|x^{(i)}) \text{ is Gaussian with parameters } (\mu^{(i)},\sigma^{(i)}) \text{ determined by NN}$

$$-D_{\text{KL}}\left(q(z|x^{(i)})||p(z)\right) = \frac{1}{2}\sum_{j=1}^{J}\left(1 + \log(\sigma_{z_j}^{(i)^2}) - \mu_{z_j}^{(i)^2} - \sigma_{z_j}^{(i)^2}\right)$$



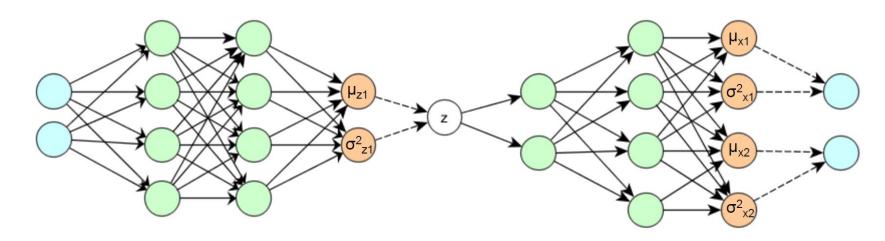
51



1D Gaussian Case

Overall loss function for BP

Prior $p(z) \sim N(0,1)$ and p, q Gaussian, extension to dim(z) > 1 trivial



Cost: Regularisation

$$-D_{\text{KL}}\left(q(z|x^{(i)})||p(z)\right) = \frac{1}{2}\sum_{j=1}^{J}\left(1 + \log(\sigma_{z_j}^{(i)^2}) - \mu_{z_j}^{(i)^2} - \sigma_{z_j}^{(i)^2}\right)$$

Cost: Reproduction

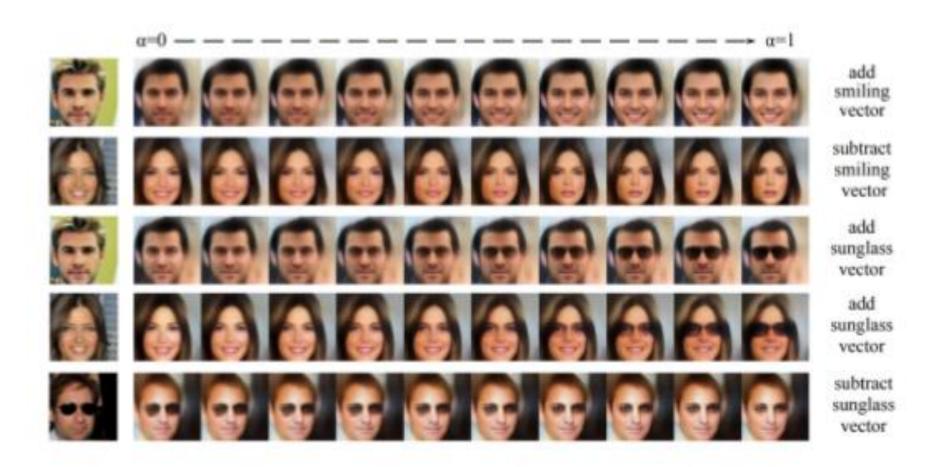
$$-\log(p(x^{(i)}|z^{(i)})) = \sum_{j=1}^{D} \frac{1}{2}\log(\sigma_{x_j}^2) + \frac{(x_j^{(i)} - \mu_{x_j})^2}{2\sigma_{x_j}^2}$$

We use mini batch gradient decent to optimize the cost function over all $x^{(i)}$ in the mini batch

Least Square for constant variance

52

Interpreting the latent space



https://arxiv.org/pdf/1610.00291.pdf



Problems of VAE

- Model capacity
 - Note that the VAE requires 2 tractable distributions to be used:
 - The prior distribution p(z) must be easy to sample from
 - The conditional likelihood $p(x|z,\theta)$ must be computable
 - In practice this means that the 2 distributions of interest are often simple, for example uniform, Gaussian, or even isotropic Gaussian

M

Problems of VAE

Blurry images





https://blog.openai.com/generative-models/

- The samples from the VAE look blurry
- Three plausible explanations for this
 - Maximizing the likelihood
 - Restrictions on the family of distributions
 - The lower bound approximation



Problems of VAE

Blurry images

- Recent investigations suggest that both the simple probability distributions and the variational approximation lead to blurry images
- Kingma & colleages: Improving Variational Inference with Inverse Autoregressive Flow
- Zhao & colleagues: Towards a Deeper Understanding of Variational Autoencoding Models
- Nowozin & colleagues: f-gan: Training generative neural samplers using variational divergence minimization



Summary

- Autoencoders (AEs)
 - □ Representation learning
- Variational Autoencoders (VAEs)
 - VAE objective
 - □ Reparametrization trick
- Next time:
 - □ VAE: Vision applications
 - GAN
- Reading material
 - http://www.cs.columbia.edu/~blei/talks/Blei_VI_tutorial.pdf
 - http://www.cs.toronto.edu/~rgrosse/courses/csc421_2019/slides/lec17.pdf
 - https://dvl.in.tum.de/slides/adl4cv-ws18/6.Bayesian&VAE.pdf
 - https://arxiv.org/pdf/1312.6114.pdf

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