Lecture 18: Deep Generative Models III: VAE & GAN

Xuming He SIST, ShanghaiTech Fall, 2018



Outline

- VAEs
 - □ Inverse graphics network
 - Attribute2Image
- Generative Adversarial Networks
 - Implicit generative models
 - □ Adversarial learning

Acknowledgement: Feifei Li et al's cs231n notes

The Variational Autencoder: overview

Learning:

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

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

□ 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



VAE objective

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)

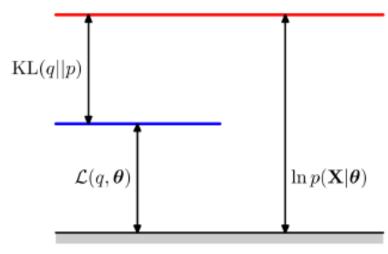


Review: VAEs

Main ideas:

- $\hfill\Box$ Introduce a parametric model $\,q_\phi(z\mid x)$ to approximate the true posterior $p_\theta(z\mid x)$
- Jointly learn approximate posterior with the deep latent variable model
- Variational EM: lower-bound of the Maximum Likelihood

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





Review: VAEs

Main ideas:

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- Jointly learn approximate posterior with the deep latent variable model
- Variational EM: lower-bound of the Maximum Likelihood

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

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

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

regularization term

reconstruction term



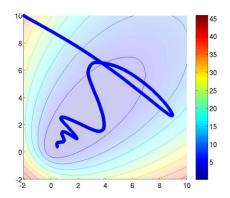
VAE learning

- 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 $\mathcal{L}(q^{(t)}, \theta)$

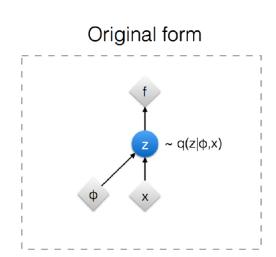
$$\mathcal{L}(x, \phi, \theta) = E_{q_{\phi}(z|x)}[\log p_{\theta}(x, z) - \log q_{\phi}(z|x)]$$

Two views of Learning VAE

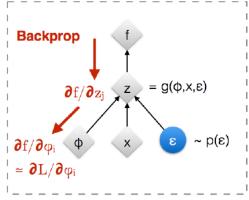
- Optimization interpretation
 - □ Stochastic gradient-based



- 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

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

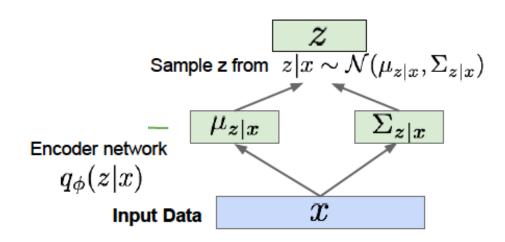


VAE Example

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

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

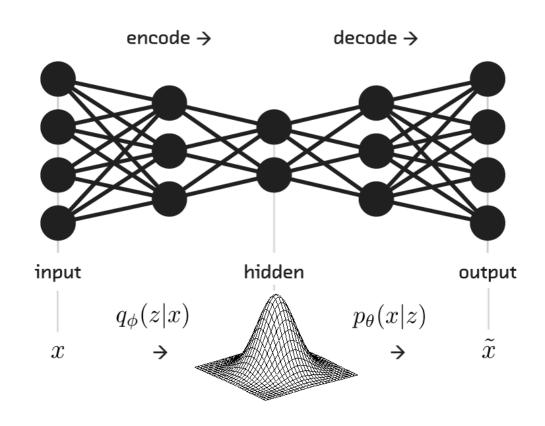
$$\mathbb{E}_{\mathcal{N}(z;\mu,\sigma^2)}\left[f(z)\right] = \mathbb{E}_{\mathcal{N}(\epsilon;0,1)}\left[f(\mu+\sigma\epsilon)\right] \simeq \frac{1}{L} \sum_{l=1}^{L} f(\mu+\sigma\epsilon^{(l)})$$



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

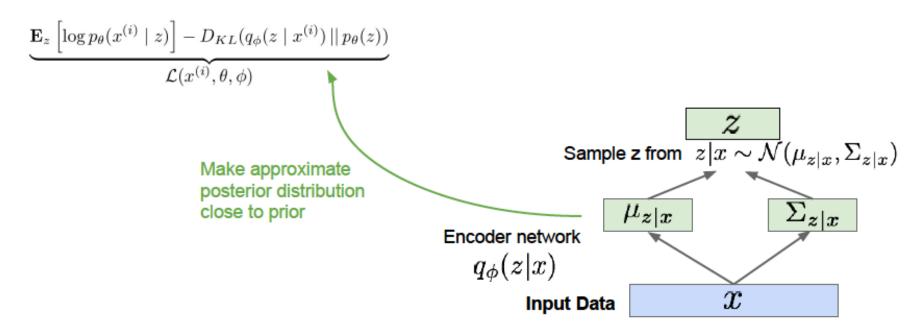




VAE Example

Learning objective

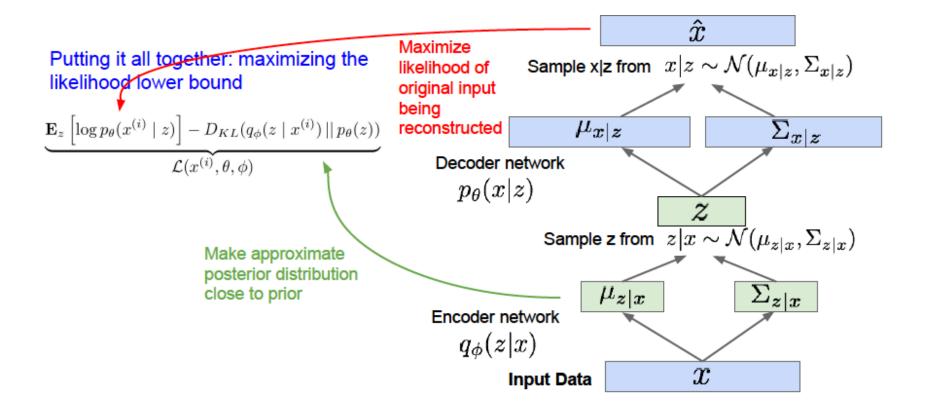
Putting it all together: maximizing the likelihood lower bound





VAE Example

Learning objective

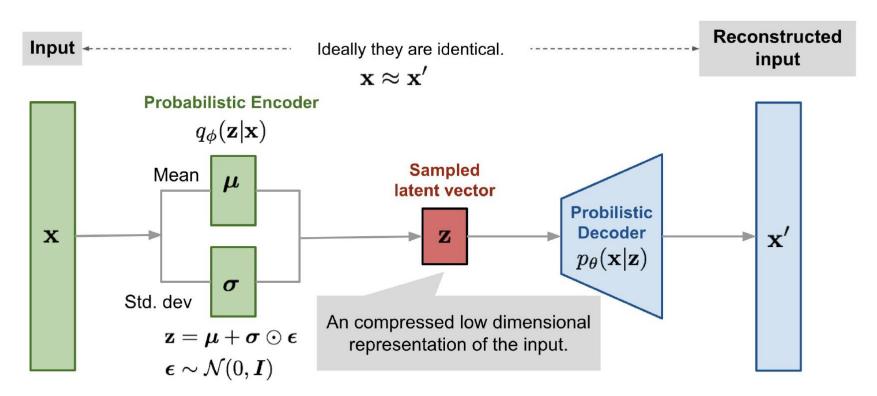


Autoencoder Interpretation

• 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.

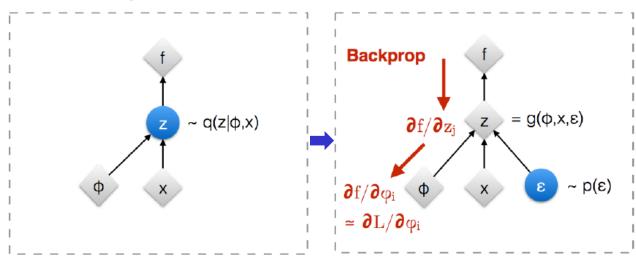
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Network interpretation

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

Original form

Reparameterised form



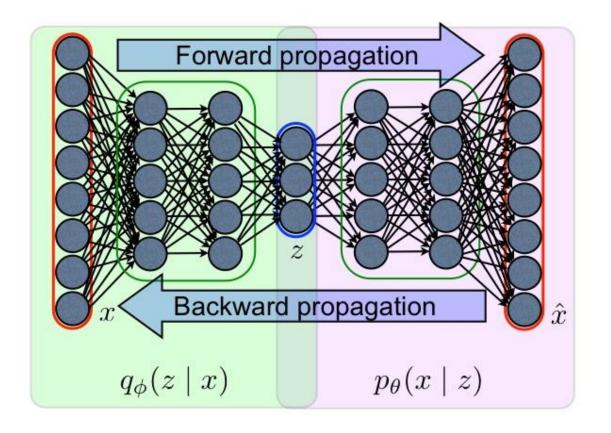
: Deterministic node

: 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.



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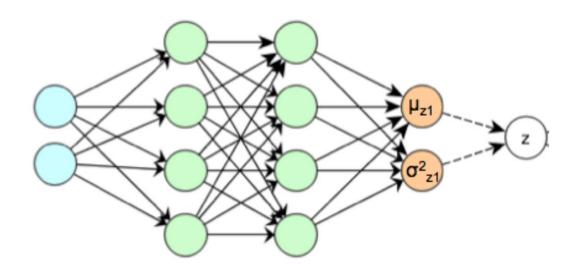


1D Gaussian Case

We can compute the KL regularization in close form

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

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

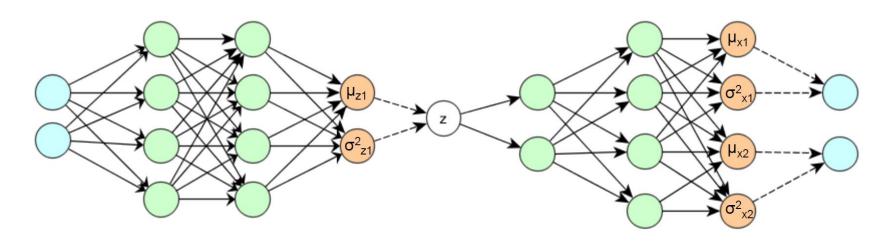




1D Gaussian Case

Overall loss function for BP

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



Cost: Regularisation

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

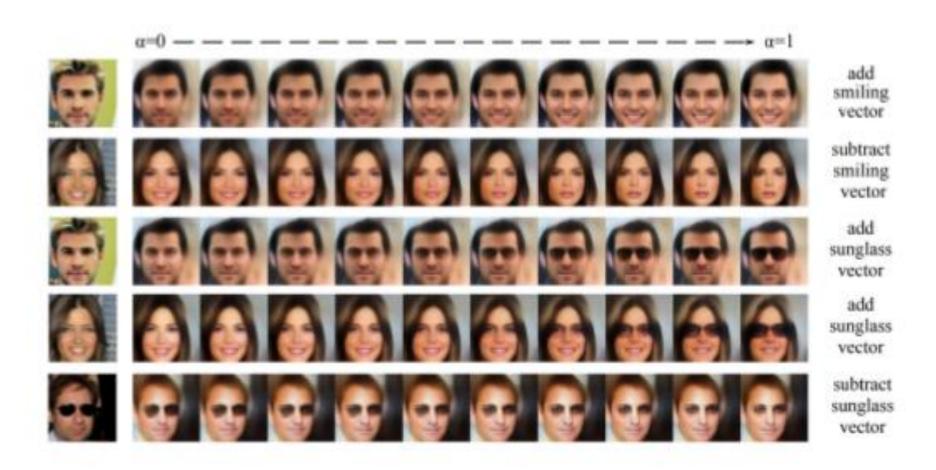
Cost: Reproduction

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

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

Least Square for constant variance

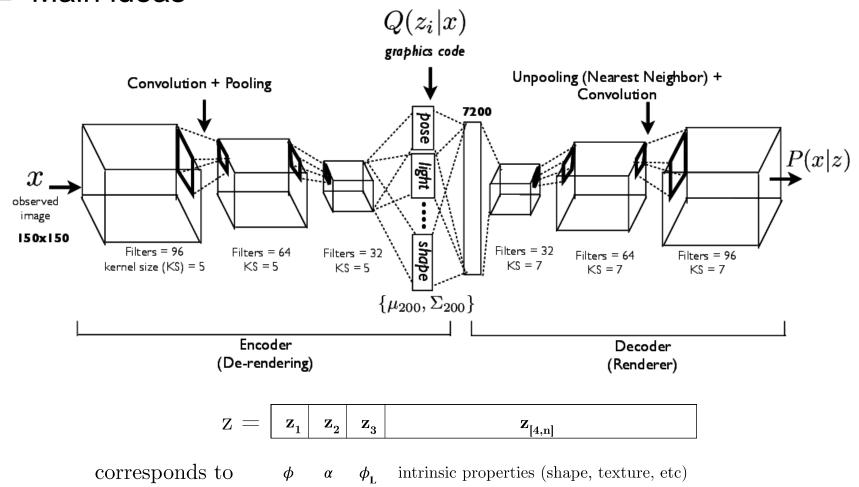
Interpreting the latent space



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

Vision task I – Inverse graphics network

Main ideas



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Vision task I – Inverse graphics network

Mini-batch training

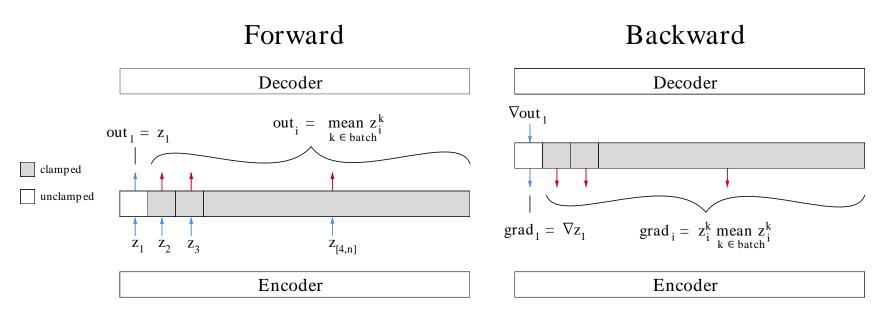
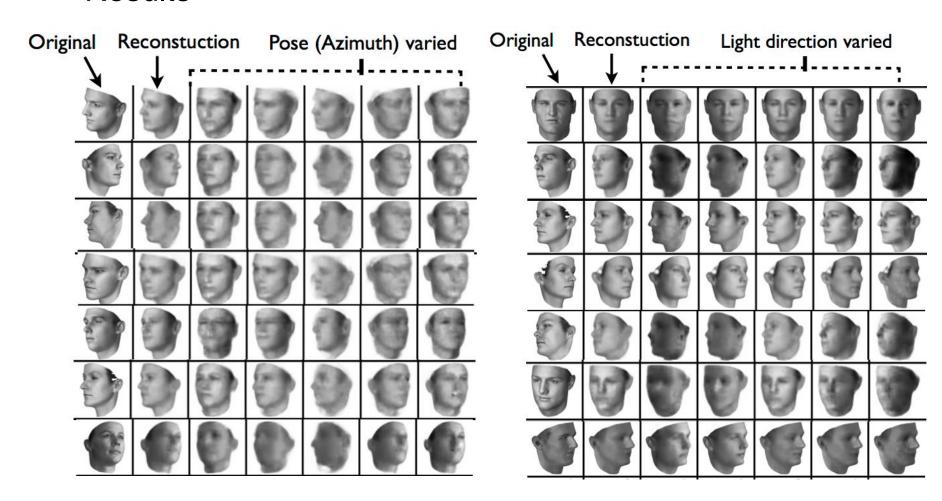


Figure 3: Training on a minibatch in which only ϕ , the azimuth angle of the face, changes. During the forward step, the output from each component $z_i \neq z_1$ of the encoder is altered to be the same for each sample in the batch. This reflects the fact that the generating variables of the image (e.g. the identity of the face) which correspond to the desired values of these latents are unchanged throughout the batch. By holding these outputs constant throughout the batch, the single neuron z_1 is forced to explain all the variance within the batch, i.e. the full range of changes to the image caused by changing ϕ . During the backward step z_1 is the only neuron which receives a gradient signal from the attempted reconstruction, and all $z_i \neq z_1$ receive a signal which nudges them to be closer to their respective averages over the batch. During the complete training process, after this batch, another batch is selected at random; it likewise contains variations of only one of ϕ , α , ϕ_L , intrinsic; all neurons which do not correspond to the selected latent are clamped; and the training proceeds.

Vision task I – Inverse graphics network

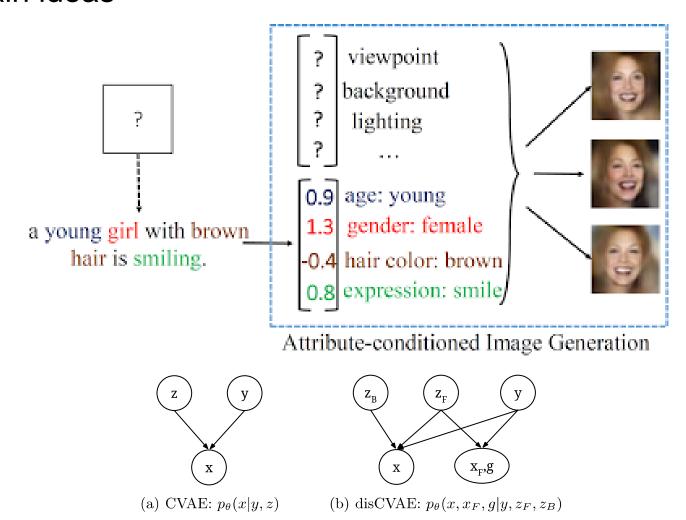
Results



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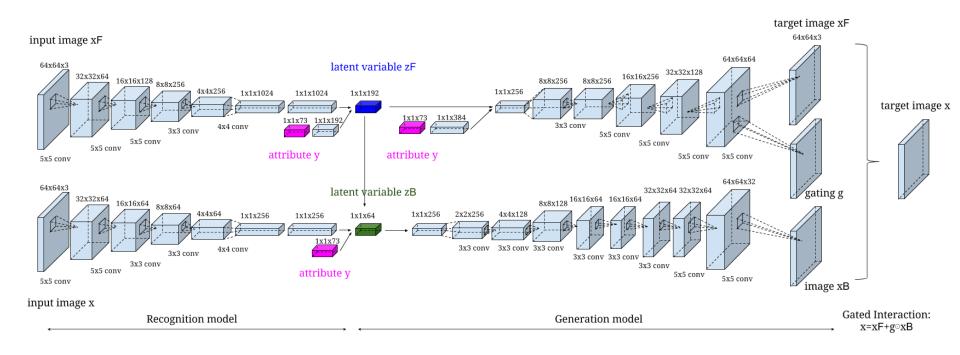
Vision task II – Attribute2Image

Main ideas



Vision task II – Attribute2Image

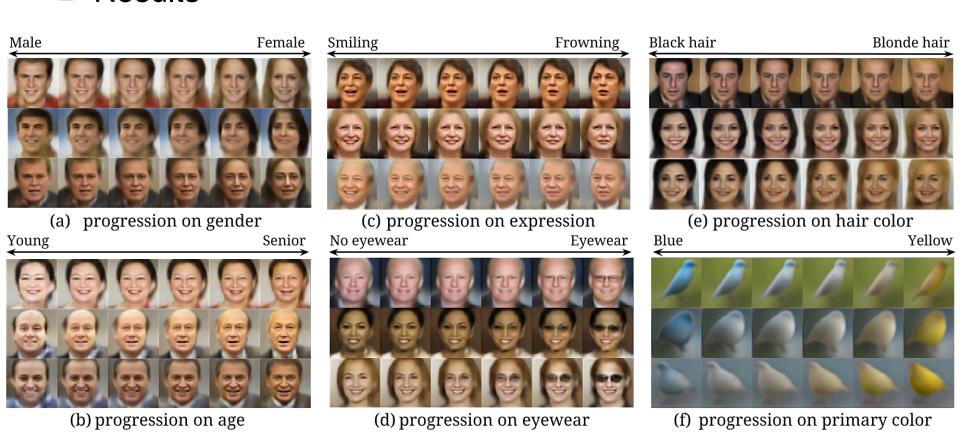
Network structure



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Vision task II – Attribute2Image

Results





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

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



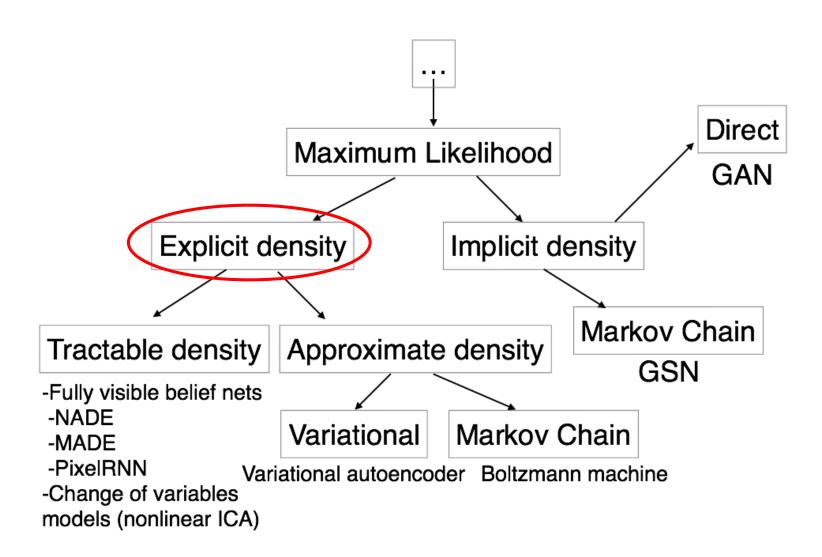
Outline

- Vision applications of VAEs
 - □ Inverse graphics network
 - ☐ Attribute2Image
- Generative Adversarial Networks
 - Implicit generative models
 - □ Adversarial learning

Acknowledgement: Feifei Li et al's cs231n notes

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Taxonomy of Generative Models





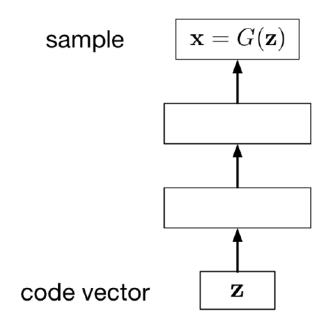
Implicit Generative Models

- Working with explicit model p(x) could be expensive
 - Variational Autoencoder (variational inference)
 - □ Boltzmann Machines (MCMC)
- Representation learning may not require p(x)
 - Sometimes we are more interested in taking samples from p(x) instead of p itself



Implicit Generative Models

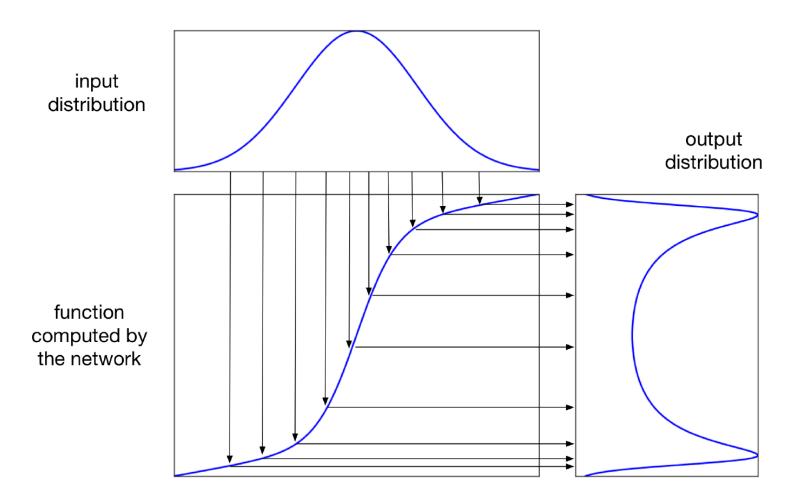
- Implicitly define a probability distribution
- Start by sampling the code vector z from a fixed, simple distribution
- A generator network computes a differentiable function G mapping z to an x in data space



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Implicit Generative Models

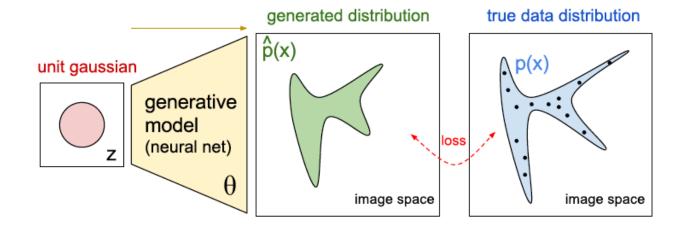
Intuition: 1D example





Implicit Generative Models

Intuition

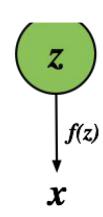


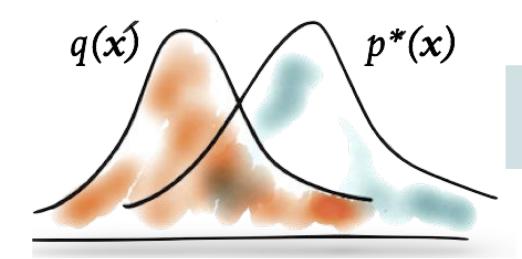
advocate/penalize samples within the blue/white region.

Learning by comparison

Basic idea

For some models, we only have access to an unnormalised probability, partial knowledge of the distribution, or a simulator of data.



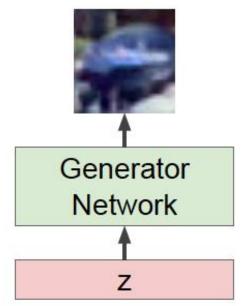


We compare the estimated distribution q(x) to the true distribution $p^*(x)$ using samples.

Generative Adversarial Networks

Using a neural network to generate data

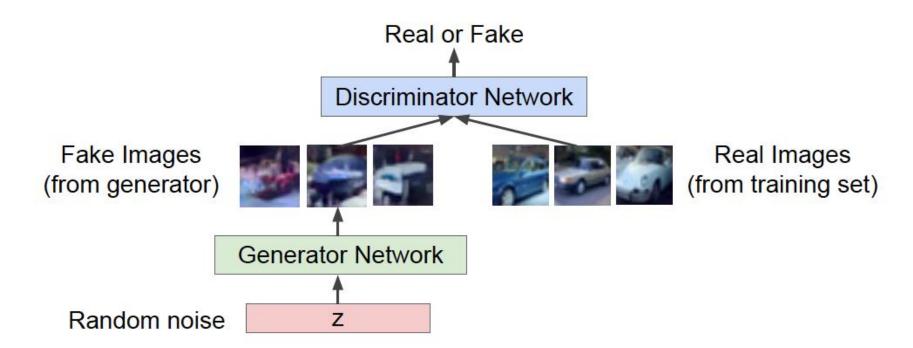
Output: Sample from training distribution



Input: Random noise

Generative Adversarial Networks

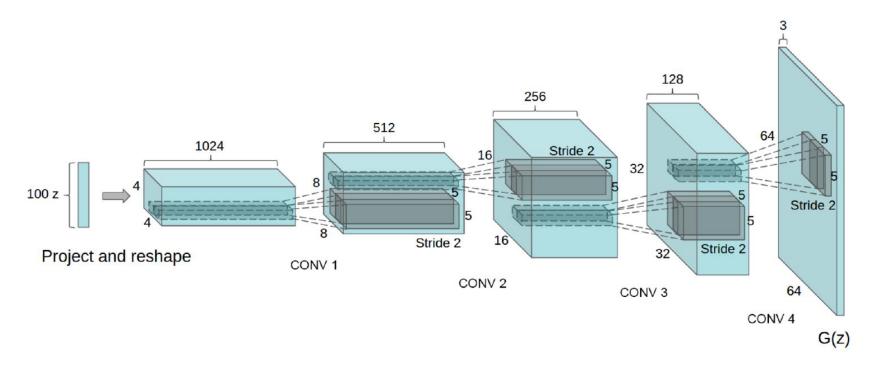
 Using another neural network to determine if the data is real or not





Typical generator architecture

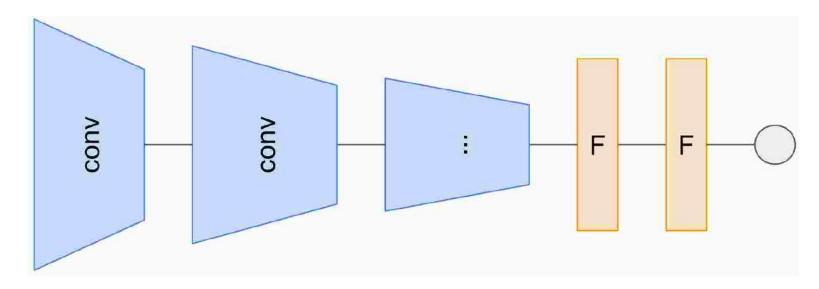
For images



- ▶ Unit Gaussian distribution on z, typically 10-100 dim.
- Up-convolutional deep network (reverse recognition CNN)

Typical discriminator architecture

For images



- Recognition CNN model
- ▶ Binary classification output: real / synthetic



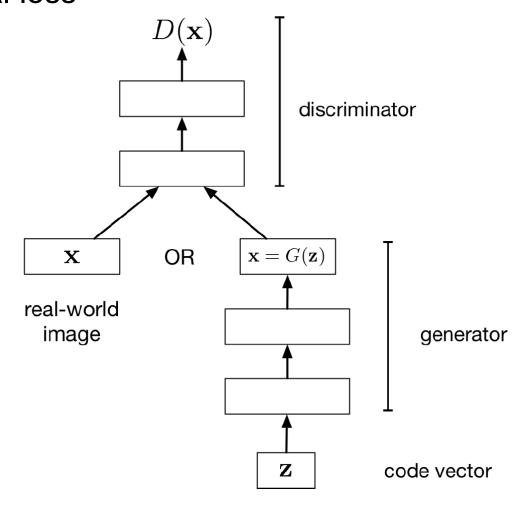
Adversarial learning

- GAN objective for the generator is some complicated objective function defined by a neural network.
 - □ This means a new way of thinking about "distance".
 - □ We are training networks to minimize the "distance" or "divergence" between generated images and real images.
 - ☐ Instead of some hand-crafted distance metric like L1 or L2, we can make something completely new.
 - □ A neural network, with the right architecture, is arguably the definition of perceptual similarity (assuming our visual system is some sort of neural network).



Adversarial Learning

Adversarial loss





Adversarial Learning

- Let D denote the discriminator's predicted probability of being real data
- Discriminator's cost function: cross-entropy loss for task of classifying real vs. fake images

$$\mathcal{J}_D = \mathbb{E}_{\mathbf{x} \sim \mathcal{D}}[-\log D(\mathbf{x})] + \mathbb{E}_{\mathbf{z}}[-\log(1 - D(G(\mathbf{z})))]$$

 One possible cost function for the generator: the opposite of the discriminator's

$$\mathcal{J}_G = -\mathcal{J}_D$$

= const + $\mathbb{E}_{\mathbf{z}}[\log(1 - D(G(\mathbf{z})))]$



Two-player game

Minimax formulation

 The generator and discriminator are playing a zero-sum game against each other

$$\max_{G} \min_{D} \mathcal{J}_{D}$$

Using parametric models

Discriminator outputs likelihood in (0,1) of real image

Minimax objective function:

$$\min_{\theta_g} \max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log (1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$
Discriminator output for for real data x generated fake data G(z)