Deep Generative Models

Lecture 8

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Recap of previous lecture

Let our data $\mathbf{y}$ comes from discrete distribution $\Pi(\mathbf{y})$.

Discrete model

- Use **discrete** model (e.x. $P(\mathbf{y}|\boldsymbol{\theta}) = \text{Cat}(\boldsymbol{\pi}(\boldsymbol{\theta}))$).
- Minimize any suitable divergence measure $D(\Pi, P)$.

Continuous model

Use **continuous** model (e.x. $p(\mathbf{x}|\boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{x}), \boldsymbol{\sigma}^2_{\boldsymbol{\theta}}(\mathbf{x}))$), but

- **discretize** model (make the model outputs discrete): transform $p(\mathbf{x}|\boldsymbol{\theta})$ to $P(\mathbf{y}|\boldsymbol{\theta})$;
- **dequantize** data (make the data continuous): transform $\Pi(\mathbf{y})$ to $\pi(\mathbf{x})$.

Model discretization through CDF

$$F(\mathbf{x}|\boldsymbol{\theta}) = \int_{-\infty}^{\mathbf{x}} p(\mathbf{x}'|\boldsymbol{\theta}) d\mathbf{x}'; \quad P(\mathbf{y}|\boldsymbol{\theta}) = F(\mathbf{y} + 0.5|\boldsymbol{\theta}) - F(\mathbf{y} - 0.5|\boldsymbol{\theta})$$

Salimans T. et al. PixelCNN++: Improving the PixelCNN with Discretized Logistic Mixture Likelihood and Other Modifications, 2017

Recap of previous lecture

Uniform dequantization bound

Let dequantize discrete distribution $\Pi(\mathbf{y})$ to continuous distribution $\pi(\mathbf{x})$ in the following way: $\mathbf{x} = \mathbf{y} + \mathbf{u}$, where $\mathbf{u} \sim U[0, 1]$.

Theorem

Fitting continuous model $p(\mathbf{x}|\boldsymbol{\theta})$ on uniformly dequantized data is equivalent to maximization of a lower bound on log-likelihood for a discrete model:

$$P(\mathbf{y}|\boldsymbol{\theta}) = \int_{U[0,1]} p(\mathbf{y} + \mathbf{u}|\boldsymbol{\theta}) d\mathbf{u}$$

Variational dequantization bound

Introduce variational dequantization noise distribution $q(\mathbf{u}|\mathbf{y})$ and treat it as an approximate posterior.

$$\log P(\mathbf{y}|\boldsymbol{\theta}) \geq \int q(\mathbf{u}|\mathbf{y}) \log \frac{p(\mathbf{y} + \mathbf{u}|\boldsymbol{\theta})}{q(\mathbf{u}|\mathbf{y})} d\mathbf{u} = \mathcal{L}(q, \boldsymbol{\theta}).$$

Ho J. et al. Flow++: Improving Flow-Based Generative Models with Variational Dequantization and Architecture Design, 2019

Recap of previous lecture

Theorem

$$\frac{1}{n}\sum_{i=1}^{n} KL(q(\mathbf{z}|\mathbf{x}_i)||p(\mathbf{z})) = KL(q_{\text{agg}}(\mathbf{z})||p(\mathbf{z})) + \mathbb{I}_q[\mathbf{x}, \mathbf{z}].$$

ELBO surgery

$$\frac{1}{n}\sum_{i=1}^{n} \mathcal{L}_i(q, \boldsymbol{\theta}) = \underbrace{\frac{1}{n}\sum_{i=1}^{n} \mathbb{E}_{q(\mathbf{z}|\mathbf{x}_i)} \log p(\mathbf{x}_i|\mathbf{z}, \boldsymbol{\theta})}_{\text{Reconstruction loss}} - \underbrace{\mathbb{I}_q[\mathbf{x}, \mathbf{z}]}_{\text{MI}} - \underbrace{KL(q_{\text{agg}}(\mathbf{z})||p(\mathbf{z}))}_{\text{Marginal KL}}$$

Optimal prior

$$KL(q_{\text{agg}}(\mathbf{z})||p(\mathbf{z})) = 0 \quad \Leftrightarrow \quad p(\mathbf{z}) = q_{\text{agg}}(\mathbf{z}) = \frac{1}{n}\sum_{i=1}^{n} q(\mathbf{z}|\mathbf{x}_i).$$

The optimal prior distribution $p(\mathbf{z})$ is aggregated posterior $q(\mathbf{z})$.

Hoffman M. D., Johnson M. J. ELBO surgery: yet another way to carve up the variational evidence lower bound, 2016

Recap of previous lecture

- Standard Gaussian $p(\mathbf{z}) = \mathcal{N}(0, I) \Rightarrow$ over-regularization;
- $p(\mathbf{z}) = q_{\text{agg}}(\mathbf{z}) = \frac{1}{n}\sum_{i=1}^{n} q(\mathbf{z}|\mathbf{x}_i) \Rightarrow$ overfitting and highly expensive.

ELBO revisiting

$$\frac{1}{n}\sum_{i=1}^{n}\mathcal{L}_i(q, \boldsymbol{\theta}) = \text{RL} - \text{MI} - KL(q_{\text{agg}}(\mathbf{z})||p(\mathbf{z}|\boldsymbol{\lambda}))$$

It is Forward KL with respect to $p(\mathbf{z}|\boldsymbol{\lambda})$.

ELBO with flow-based VAE prior

$$\mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta}) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})}\left[\log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) + \log p(\mathbf{z}|\boldsymbol{\lambda}) - \log q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})\right]$$
$$= \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})}\Bigg[\log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) + \underbrace{\Big(\log p(f(\mathbf{z}, \boldsymbol{\lambda})) + \log |\det(\mathbf{J}_f)|\Big)}_{\text{flow-based prior}} - \log q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})\Bigg]$$

$$\mathbf{z} = f^{-1}(\mathbf{z}^*, \boldsymbol{\lambda}) = g(\mathbf{z}^*, \boldsymbol{\lambda}), \quad \mathbf{z}^* \sim p(\mathbf{z}^*) = \mathcal{N}(0, 1)$$

Chen X. et al. Variational Lossy Autoencoder, 2016

Outline

1. VAE limitations: posterior distribution
2. Likelihood-free learning
3. Generative adversarial networks (GAN)

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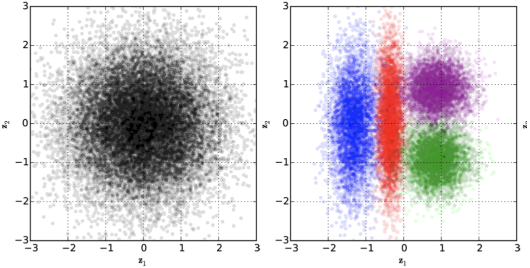
Variational posterior

ELBO decomposition

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \mathcal{L}(q, \boldsymbol{\theta}) + KL(q(\mathbf{z}|\mathbf{x}, \phi)||p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta})).$$

- E-step of EM-algorithm: $KL(q(\mathbf{z}|\mathbf{x}, \phi)||p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta})) = 0$.
  (In this case the lower bound is tight $\log p(\mathbf{x}|\boldsymbol{\theta}) = \mathcal{L}(q, \boldsymbol{\theta})$).
- $q(\mathbf{z}|\mathbf{x}, \phi) = \mathcal{N}(\mathbf{z}|\boldsymbol{\mu}_\phi(\mathbf{x}), \boldsymbol{\sigma}^2_\phi(\mathbf{x}))$ is a unimodal distribution (not expressive enough).



(a) Prior distribution (b) Posteriors in standard VAE

Rezende D. J., Mohamed S. Variational Inference with Normalizing Flows, 2015

Normalizing Flows in VAE posterior

$$\mathcal{L}(\phi, \boldsymbol{\theta}) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \phi)} \left[\log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) + \log p(\mathbf{z}|\boldsymbol{\lambda}) - \log q(\mathbf{z}|\mathbf{x}, \phi) \right]$$

Let apply NF to VAE posterior!
Assume $q(\mathbf{z}|\mathbf{x}, \phi)$ (VAE encoder) is a base distribution for a flow model.

Flow model in latent space

$$\log q(\mathbf{z}^*|\mathbf{x}, \phi, \boldsymbol{\lambda}) = \log q(\mathbf{z}|\mathbf{x}, \phi) + \log \left| \det \left(\frac{d\mathbf{z}}{d\mathbf{z}^*} \right) \right|$$

$$\mathbf{z}^* = f(\mathbf{z}, \boldsymbol{\lambda}) = g^{-1}(\mathbf{z}, \boldsymbol{\lambda})$$

- Encoder outputs base distribution $q(\mathbf{z}|\mathbf{x}, \phi)$.
- Flow model $\mathbf{z}^* = f(\mathbf{z}, \boldsymbol{\lambda})$ transforms the base distribution $q(\mathbf{z}|\mathbf{x}, \phi)$ to the distribution $q(\mathbf{z}^*|\mathbf{x}, \phi, \boldsymbol{\lambda})$.
- Distribution $q(\mathbf{z}^*|\mathbf{x}, \phi, \boldsymbol{\lambda})$ is used as a variational distribution for ELBO maximization.
- Here ϕ – encoder parameters, $\boldsymbol{\lambda}$ – flow parameters.

Rezende D. J., Mohamed S. Variational Inference with Normalizing Flows, 2015

Normalizing Flows in VAE posterior

ELBO with flow-based VAE posterior

$$
\begin{aligned}
\mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta}, \boldsymbol{\lambda}) &= \mathbb{E}_{q(\mathbf{z}^*|\mathbf{x}, \phi, \boldsymbol{\lambda})} \log p(\mathbf{x}|\mathbf{z}^*, \boldsymbol{\theta}) - KL(q(\mathbf{z}^*|\mathbf{x}, \phi, \boldsymbol{\lambda}) || p(\mathbf{z}^*)) = \\
&= \mathbb{E}_{q(\mathbf{z}^*|\mathbf{x}, \phi, \boldsymbol{\lambda})} \left[\log p(\mathbf{x}|\mathbf{z}^*, \boldsymbol{\theta}) + \log p(\mathbf{z}^*) - \log q(\mathbf{z}^*|\mathbf{x}, \phi, \boldsymbol{\lambda}) \right] = \\
&= \mathbb{E}_{q(\mathbf{z}^*|\mathbf{x}, \phi, \boldsymbol{\lambda})} \Bigg[\log p(\mathbf{x}|\mathbf{z}^*, \boldsymbol{\theta}) + \log p(\mathbf{z}^*) - \\
&\quad - \Big(\log q(g(\mathbf{z}^*, \boldsymbol{\lambda})|\mathbf{x}, \phi) + \log |\det(\mathbf{J}_g)| \Big) \Bigg].
\end{aligned}
$$

KL term in ELBO is **reverse** KL divergence with respect to $\boldsymbol{\lambda}$.

- RealNVP with coupling layers.
- Inverse autoregressive flow (slow $f(\mathbf{z}, \boldsymbol{\lambda})$, fast $g(\mathbf{z}^*, \boldsymbol{\lambda})$).
- Is it OK to use AF for VAE posterior?

Rezende D. J., Mohamed S. Variational Inference with Normalizing Flows, 2015

Flows in VAE posterior

Theorem (flow KL duality, Lecture 5)

$$KL(\pi(\mathbf{x})||p(\mathbf{x}|\boldsymbol{\theta})) = KL(p(\mathbf{z}|\boldsymbol{\theta})||p(\mathbf{z})).$$

ELBO with flow-based VAE posterior

$$\begin{aligned}\mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta}, \boldsymbol{\lambda}) &= \mathbb{E}_{q(\mathbf{z}^*|\mathbf{x},\phi,\boldsymbol{\lambda})} \log p(\mathbf{x}|\mathbf{z}^*, \boldsymbol{\theta}) - KL(q(\mathbf{z}^*|\mathbf{x}, \phi, \boldsymbol{\lambda})||p(\mathbf{z}^*)) \\ &= \mathbb{E}_{q(\mathbf{z}|\mathbf{x},\phi)} \log p(\mathbf{x}|f(\mathbf{z}, \boldsymbol{\lambda}), \boldsymbol{\theta}) - KL(q(\mathbf{z}|\mathbf{x}, \phi)||p(\mathbf{z}|\boldsymbol{\lambda})).\end{aligned}$$

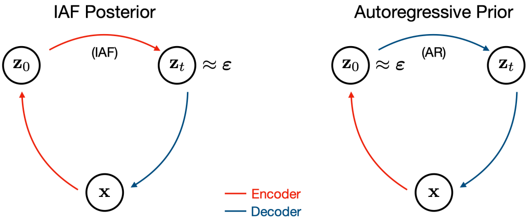
(Here we use Flow KL duality theorem and LOTUS trick.)

ELBO with flow-based VAE prior

$$\mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta}, \boldsymbol{\lambda}) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x},\phi)} \log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) - KL(q(\mathbf{z}|\mathbf{x}, \phi)||p(\mathbf{z}|\boldsymbol{\lambda}))$$

Chen X. et al. Variational Lossy Autoencoder, 2016

Flows-based VAE prior vs posterior



- Flow-based posterior decoder path: $\mathbf{z} \sim p(\mathbf{z})$, $\mathbf{x} \sim p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})$.
- Flow-based prior decoder path: $\mathbf{z}^* \sim p(\mathbf{z}^*)$, $\mathbf{z} = f(\mathbf{z}^*, \boldsymbol{\lambda})$, $\mathbf{x} \sim p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})$.

image credit: https://courses.cs.washington.edu/courses/cse599i/20au

VAE limitations

- Poor generative distribution (decoder)

$$p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{z}), \boldsymbol{\sigma}^2_{\boldsymbol{\theta}}(\mathbf{z})) \quad \text{or} \quad = \text{Softmax}(\boldsymbol{\pi}_{\boldsymbol{\theta}}(\mathbf{z})).$$

- Loose lower bound

$$\log p(\mathbf{x}|\boldsymbol{\theta}) - \mathcal{L}(q, \boldsymbol{\theta}) = (?).$$

- Poor prior distribution

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

- Poor variational posterior distribution (encoder)

$$q(\mathbf{z}|\mathbf{x}, \phi) = \mathcal{N}(\mathbf{z}|\boldsymbol{\mu}_{\phi}(\mathbf{x}), \boldsymbol{\sigma}^2_{\phi}(\mathbf{x})).$$

Outline

1. VAE limitations: posterior distribution
2. Likelihood-free learning
3. Generative adversarial networks (GAN)

Likelihood based models

Poor likelihood
Great samples

$$p_1(\mathbf{x}) = \frac{1}{n}\sum_{i=1}^{n}\mathcal{N}(\mathbf{x}|\mathbf{x}_i, \epsilon\mathbf{I})$$

For small ϵ this model will generate samples with great quality, but likelihood will be very poor.

Great likelihood
Poor samples

$$p_2(\mathbf{x}) = 0.01p(\mathbf{x}) + 0.99p_{\text{noise}}(\mathbf{x})$$

$$\log\left[0.01p(\mathbf{x}) + 0.99p_{\text{noise}}(\mathbf{x})\right] \geq$$
$$\geq \log\left[0.01p(\mathbf{x})\right] = \log p(\mathbf{x}) - \log 100$$

Noisy irrelevant samples, but for high dimensions $\log p(\mathbf{x})$ becomes proportional to m.

- Likelihood is not a perfect quality measure for generative model.
- Likelihood could be intractable.

Theis L., Oord A., Bethge M. A note on the evaluation of generative models, 2015

Likelihood-free learning

Where did we start

We would like to approximate true data distribution $\pi(\mathbf{x})$. Instead of searching true $\pi(\mathbf{x})$ over all probability distributions, learn function approximation $p(\mathbf{x}|\boldsymbol{\theta}) \approx \pi(\mathbf{x})$.

Imagine we have two sets of samples

- $\mathcal{S}_1 = \{\mathbf{x}_i\}_{i=1}^{n_1} \sim \pi(\mathbf{x})$ – real samples;
- $\mathcal{S}_2 = \{\mathbf{x}_i\}_{i=1}^{n_2} \sim p(\mathbf{x}|\boldsymbol{\theta})$ – generated (or fake) samples.

Let define discriminative model (classifier):

$$p(y = 1|\mathbf{x}) = P\bigl(\{\mathbf{x} \sim \pi(\mathbf{x})\}\bigr); \quad p(y = 0|\mathbf{x}) = P\bigl(\{\mathbf{x} \sim p(\mathbf{x}|\boldsymbol{\theta})\}\bigr)$$

Assumption

Generative distribution $p(\mathbf{x}|\boldsymbol{\theta})$ equals to the true distribution $\pi(\mathbf{x})$ if we can not distinguish them using discriminative model $p(y|\mathbf{x})$. It means that $p(y = 1|\mathbf{x}) = 0.5$ for each sample $\mathbf{x}$.

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Likelihood-free learning

The more powerful discriminative model we will have, the more likely we got the "best" generative distribution $p(\mathbf{x}|\boldsymbol{\theta})$.
The most common way to learn a classifier is to minimize cross entropy loss.

- **Generator:** generative model $\mathbf{x} = G(\mathbf{z})$, which makes generated sample more realistic. Here $\mathbf{z}$ comes from the base (known) distribution $p(\mathbf{z})$ and $\mathbf{x} \sim p(\mathbf{x}|\boldsymbol{\theta})$. Generator tries to **minimize** cross entropy.
- **Discriminator:** a classifier $p(y = 1|\mathbf{x}) = D(\mathbf{x}) \in [0, 1]$, which distinguishes real samples from generated samples. Discriminator tries to **maximize** cross entropy (tries to enhance discriminative model).

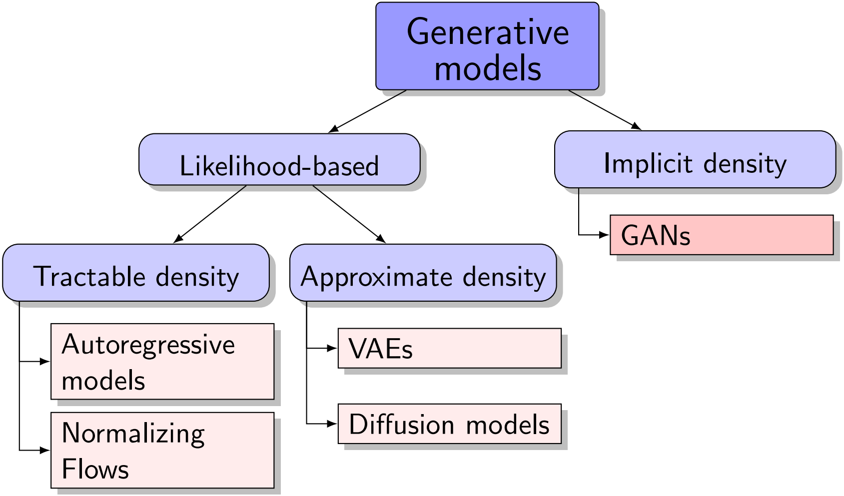
Generative adversarial network (GAN) objective

$$\min_G \max_D \left[\mathbb{E}_{\pi(\mathbf{x})} \log D(\mathbf{x}) + \mathbb{E}_{p(\mathbf{x}|\boldsymbol{\theta})} \log(1 - D(\mathbf{x}))\right]$$

$$\min_G \max_D \left[\mathbb{E}_{\pi(\mathbf{x})} \log D(\mathbf{x}) + \mathbb{E}_{p(\mathbf{z})} \log(1 - D(G(\mathbf{z})))\right]$$

Goodfellow I. J. et al. Generative Adversarial Networks, 2014

Generative models zoo



GAN optimality

Theorem

The minimax game

$$\min_G \max_D \Big[\underbrace{\mathbb{E}_{\pi(\mathbf{x})} \log D(\mathbf{x}) + \mathbb{E}_{p(\mathbf{z})} \log(1 - D(G(\mathbf{z})))}_{V(G,D)} \Big]$$

has the global optimum $\pi(\mathbf{x}) = p(\mathbf{x}|\boldsymbol{\theta})$, in this case $D^*(\mathbf{x}) = 0.5$.

Proof (fixed G)

$$\begin{aligned} V(G, D) &= \mathbb{E}_{\pi(\mathbf{x})} \log D(\mathbf{x}) + \mathbb{E}_{p(\mathbf{x}|\boldsymbol{\theta})} \log(1 - D(\mathbf{x})) \\ &= \int \underbrace{[\pi(\mathbf{x}) \log D(\mathbf{x}) + p(\mathbf{x}|\boldsymbol{\theta}) \log(1 - D(\mathbf{x})]}_{y(D)} d\mathbf{x} \end{aligned}$$

$$\frac{dy(D)}{dD} = \frac{\pi(\mathbf{x})}{D(\mathbf{x})} - \frac{p(\mathbf{x}|\boldsymbol{\theta})}{1 - D(\mathbf{x})} = 0 \quad \Rightarrow \quad D^*(\mathbf{x}) = \frac{\pi(\mathbf{x})}{\pi(\mathbf{x}) + p(\mathbf{x}|\boldsymbol{\theta})}$$

Goodfellow I. J. et al. Generative Adversarial Networks, 2014

GAN optimality

Proof continued (fixed $D = D^*$)

$$V(G, D^*) = \mathbb{E}_{\pi(\mathbf{x})} \log \frac{\pi(\mathbf{x})}{\pi(\mathbf{x}) + p(\mathbf{x}|\boldsymbol{\theta})} + \mathbb{E}_{p(\mathbf{x}|\boldsymbol{\theta})} \log \frac{p(\mathbf{x}|\boldsymbol{\theta})}{\pi(\mathbf{x}) + p(\mathbf{x}|\boldsymbol{\theta})}$$

$$= KL\left(\pi(\mathbf{x})||\frac{\pi(\mathbf{x}) + p(\mathbf{x}|\boldsymbol{\theta})}{2}\right) + KL\left(p(\mathbf{x}|\boldsymbol{\theta})||\frac{\pi(\mathbf{x}) + p(\mathbf{x}|\boldsymbol{\theta})}{2}\right) - 2\log 2$$

$$= 2JSD(\pi(\mathbf{x})||p(\mathbf{x}|\boldsymbol{\theta})) - 2\log 2.$$

Jensen-Shannon divergence (symmetric KL divergence)

$$JSD(\pi(\mathbf{x})||p(\mathbf{x}|\boldsymbol{\theta})) = \frac{1}{2}\left[KL\left(\pi(\mathbf{x})||\frac{\pi(\mathbf{x}) + p(\mathbf{x}|\boldsymbol{\theta})}{2}\right) + KL\left(p(\mathbf{x}|\boldsymbol{\theta})||\frac{\pi(\mathbf{x}) + p(\mathbf{x}|\boldsymbol{\theta})}{2}\right)\right]$$

Could be used as a distance measure!

$$V(G^*, D^*) = -2\log 2, \quad \pi(\mathbf{x}) = p(\mathbf{x}|\boldsymbol{\theta}), \quad D^*(\mathbf{x}) = 0.5.$$

Goodfellow I. J. et al. Generative Adversarial Networks, 2014

GAN optimality

Theorem

The minimax game

$$\min_G \max_D \Big[\underbrace{\mathbb{E}_{\pi(\mathbf{x})} \log D(\mathbf{x}) + \mathbb{E}_{p(\mathbf{z})} \log(1 - D(G(\mathbf{z})))}_{V(G,D)}\Big]$$

has the global optimum $\pi(\mathbf{x}) = p(\mathbf{x}|\boldsymbol{\theta})$, in this case $D^*(\mathbf{x}) = 0.5$.

Expectations

If the generator could be **any** function and the discriminator is **optimal** at every step, then the generator is **guaranteed to converge** to the data distribution.

Reality

- Generator updates are made in parameter space, discriminator is not optimal at every step.
- Generator and discriminator loss keeps oscillating during GAN training.

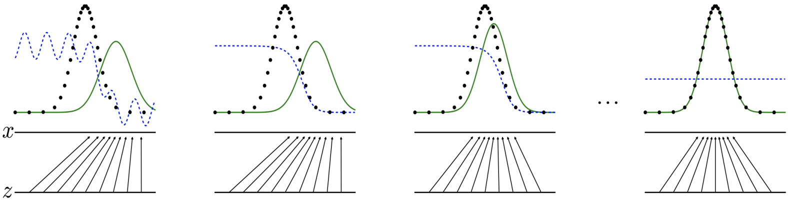
Goodfellow I. J. et al. Generative Adversarial Networks, 2014

GAN training

Let futher assume that generator and discriminator are parametric models: $D(\mathbf{x}, \phi)$ and $G(\mathbf{z}, \boldsymbol{\theta})$.

Objective

$$\min_{\boldsymbol{\theta}} \max_{\boldsymbol{\phi}} \left[\mathbb{E}_{\pi(\mathbf{x})} \log D(\mathbf{x}, \phi) + \mathbb{E}_{p(\mathbf{z})} \log(1 - D(G(\mathbf{z}, \boldsymbol{\theta}), \phi))\right]$$



(a) (b) (c) (d)

- $\mathbf{z} \sim p(\mathbf{z})$ is a latent variable.
- $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = \delta(\mathbf{x} - G(\mathbf{z}, \boldsymbol{\theta}))$ is deterministic decoder (like NF).
- We do not have encoder at all.

Goodfellow I. J. et al. Generative Adversarial Networks, 2014

Summary

- We could use flows to make variational posterior more expressive.
- It is possible to use flows in VAE prior and posterior. It is (almost) equivalent.
- Likelihood is not a perfect criteria to measure quality of generative model.
- Adversarial learning suggests to solve minimax problem to match the distributions.
- GAN tries to optimize Jensen-Shannon divergence (in theory).