Deep Generative Models

Lecture 8

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

Discrete model

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

Continuous model

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

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

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

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

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

Variational dequantization bound

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

$$\log P(\mathbf{x}|\boldsymbol{ heta}) \geq \int q(\mathbf{u}|\mathbf{x}) \log rac{p(\mathbf{x} + \mathbf{u}|oldsymbol{ heta})}{q(\mathbf{u}|\mathbf{x})} d\mathbf{u} = \mathcal{L}(q,oldsymbol{ heta}).$$

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

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

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

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(z) is aggregated posterior q(z).

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

ELBO revisiting

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

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

ELBO with flow-based VAE prior

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

- RealNVP with coupling layers.
- ▶ Autoregressive flow (fast $f(\mathbf{z}, \lambda)$, slow $g(\mathbf{z}^*, \lambda)$).

ELBO decomposition

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

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

Apply a sequence of transformations to the random variable

$$\mathbf{z} \sim q(\mathbf{z}|\mathbf{x}, oldsymbol{\phi}) = \mathcal{N}(\mathbf{z}|oldsymbol{\mu_{\phi}}(\mathbf{x}), oldsymbol{\sigma_{\phi}^2}(\mathbf{x})).$$

Let $q(\mathbf{z}|\mathbf{x}, \phi)$ (VAE encoder) be a base distribution for a flow model.

Outline

1. Flow-based VAE posterior vs flow-based VAE prior

2. Likelihood-free learning

3. Generative adversarial networks (GAN)

4. Vanishing gradients and mode collapse

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Flows in VAE posterior

- ▶ 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 $q(\mathbf{z}^*|\mathbf{x}, \phi, \lambda)$ is used as a variational distribution for ELBO maximization.
- ▶ Here ϕ encoder parameters, λ flow parameters.

Flow model in latent space

$$\log q(\mathbf{z}^*|\mathbf{x}, \boldsymbol{\phi}, \boldsymbol{\lambda}) = \log q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi}) + \log \left| \det \left(\frac{d\mathbf{z}}{d\mathbf{z}^*} \right) \right|$$
$$\mathbf{z}^* = f(\mathbf{z}, \boldsymbol{\lambda}) = g^{-1}(\mathbf{z}^*, \boldsymbol{\lambda})$$

ELBO with flow-based VAE posterior

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

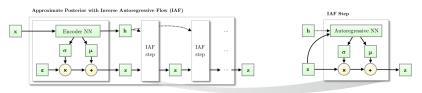
The second term in ELBO is **reverse** KL divergence with respect to $q(\mathbf{z}^*|\mathbf{x}, \phi, \lambda)$.

Flow-based VAE posterior

ELBO objective

$$\begin{split} \mathcal{L}(\phi, \theta, \boldsymbol{\lambda}) &= \mathbb{E}_{q(\mathbf{z}^* | \mathbf{x}, \phi, \boldsymbol{\lambda})} \big[\log p(\mathbf{x} | \mathbf{z}^*, \boldsymbol{\theta}) + \log p(\mathbf{z}^*) - \log q(\mathbf{z}^* | \mathbf{x}, \phi, \boldsymbol{\lambda}) \big] = \\ &= \mathbb{E}_{q(\mathbf{z}^* | \mathbf{x}, \phi, \boldsymbol{\lambda})} \bigg[\log p(\mathbf{x} | \mathbf{z}^*, \boldsymbol{\theta}) + \log p(\mathbf{z}^*) - \\ &- \bigg(\log q(g(\mathbf{z}^*, \boldsymbol{\lambda}) | \mathbf{x}, \phi) + \log |\det(\mathbf{J}_g)| \bigg) \bigg]. \end{split}$$

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



Flows-based VAE prior vs posterior

Theorem

VAE with the flow-based prior $p(\mathbf{z}|\lambda)$ for latent code \mathbf{z}^* is equivalent to VAE with flow-based posterior $q(\mathbf{z}|\mathbf{x}, \phi, \lambda)$ for latent code \mathbf{z} .

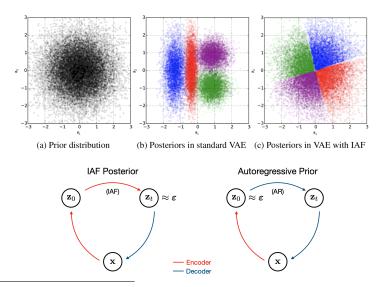
Proof

$$\begin{split} \mathcal{L}(\phi, \theta, \lambda) &= \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \phi)} \log p(\mathbf{x}|\mathbf{z}, \theta) - \underbrace{\mathcal{K}L(q(\mathbf{z}|\mathbf{x}, \phi)||p(\mathbf{z}|\lambda))}_{\text{flow-based prior}} \\ &= \mathbb{E}_{q(\mathbf{z}^*|\mathbf{x}, \phi, \lambda)} \log p(\mathbf{x}|f(\mathbf{z}^*, \lambda), \theta) - \underbrace{\mathcal{K}L(q(\mathbf{z}^*|\mathbf{x}, \phi, \lambda)||p(\mathbf{z}^*))}_{\text{flow-based posterior}} \end{split}$$

(Here we use Flow KL duality theorem from Lecture 5 and LOTUS)

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

Flows-based VAE prior vs posterior



Kingma D. P. et al. Improving Variational Inference with Inverse Autoregressive Flow, 2016 image credit: https://courses.cs.washington.edu/courses/cse599i/20au

VAE limitations

Poor generative distribution (decoder)

$$p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = \mathcal{N}(\mathbf{x}|\mu_{\boldsymbol{\theta}}(\mathbf{z}), \sigma_{\boldsymbol{\theta}}^2(\mathbf{z})) \quad \text{or } = \mathsf{Softmax}(\pi_{\boldsymbol{\theta}}(\mathbf{z})).$$

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)

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

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Likelihood based models

Is likelihood a good measure of model quality?

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

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

$$egin{aligned} \log\left[0.01p(\mathbf{x})+0.99p_{\mathsf{noise}}(\mathbf{x})
ight] \geq \\ \geq \log\left[0.01p(\mathbf{x})
ight] = \log p(\mathbf{x}) - \log 100 \end{aligned}$$

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

Likelihood-free learning

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

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 $p(\mathbf{x}|\theta) \approx \pi(\mathbf{x})$.

Imagine we have two sets of samples

- \triangleright $S_1 = \{\mathbf{x}_i\}_{i=1}^{n_1} \sim \pi(\mathbf{x})$ real samples;
- \triangleright $S_2 = \{\mathbf{x}_i\}_{i=1}^{n_2} \sim p(\mathbf{x}|\boldsymbol{\theta})$ generated (or fake) samples.

Two sample test

$$H_0: \pi(\mathbf{x}) = \rho(\mathbf{x}|\boldsymbol{\theta}), \quad H_1: \pi(\mathbf{x}) \neq \rho(\mathbf{x}|\boldsymbol{\theta})$$

Define test statistic $T(S_1, S_2)$. The test statistic is likelihood free. If $T(S_1, S_2) < \alpha$, then accept H_0 , else reject it.

Likelihood-free learning

Two sample test

$$H_0: \pi(\mathbf{x}) = p(\mathbf{x}|\boldsymbol{\theta}), \quad H_1: \pi(\mathbf{x}) \neq p(\mathbf{x}|\boldsymbol{\theta})$$

Desired behaviour

- \triangleright $p(\mathbf{x}|\theta)$ minimizes the value of test statistic $T(S_1, S_2)$.
- It is hard to find an appropriate test statistic in high dimensions. $T(S_1, S_2)$ could be learnable.

Generative adversarial network (GAN) objective

- ▶ **Generator:** generative model $\mathbf{x} = G(\mathbf{z})$, which makes generated sample more realistic. Here $\mathbf{z} \sim p(\mathbf{z})$, $\mathbf{x} \sim p(\mathbf{x}|\boldsymbol{\theta})$.
- ▶ **Discriminator:** a classifier $D(\mathbf{x}) \in [0,1]$, which distinguishes real samples from generated samples.

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

Outline

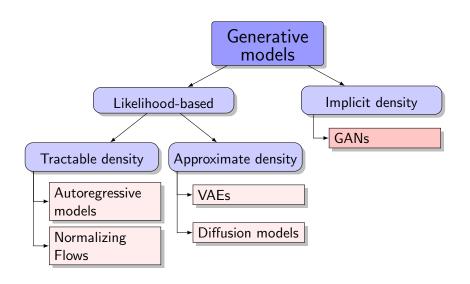
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Generative models zoo



GAN optimality

Theorem

The minimax game

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

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

Proof (fixed G)

$$V(G, D) = \mathbb{E}_{\pi(\mathbf{x})} \log D(\mathbf{x}) + \mathbb{E}_{p(\mathbf{x}|\boldsymbol{\theta})} \log(1 - D(\mathbf{x}))$$

$$= \int \underbrace{\left[\pi(\mathbf{x}) \log D(\mathbf{x}) + p(\mathbf{x}|\boldsymbol{\theta}) \log(1 - D(\mathbf{x})\right]}_{y(D)} d\mathbf{x}$$

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

GAN optimality

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

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

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

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

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!

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

GAN optimality

Theorem

The minimax game

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

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

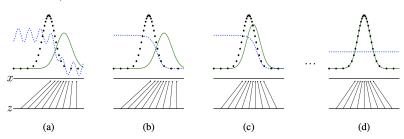
- Generator updates are made in parameter space, discriminator is not optimal at every step.
- Generator and discriminator loss keeps oscillating during GAN training.

GAN

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

Objective

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



- ightharpoonup $z \sim p(z)$ 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.

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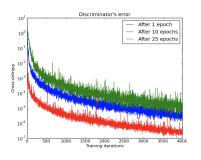
4. Vanishing gradients and mode collapse

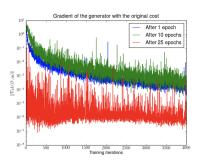
Vanishing gradients

Objective

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

Early in learning, G is poor, D can reject samples with high confidence. In this case, $\log(1 - D(G(\mathbf{z}, \theta), \phi))$ saturates.





Arjovsky M., Bottou L. Towards Principled Methods for Training Generative Adversarial Networks, 2017

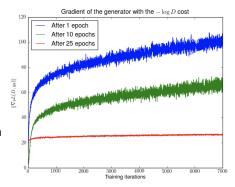
Vanishing gradients

Objective

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

Non-saturating GAN

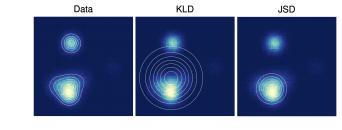
- Maximize $\log D(G(z))$ instead of minimizing $\log(1 D(G(z)))$.
- Gradients are getting much stronger, but the training is unstable (with increasing mean and variance).



Arjovsky M., Bottou L. Towards Principled Methods for Training Generative Adversarial Networks, 2017

Mode collapse

The phenomena where the generator of a GAN collapses to one or few distribution modes.





Alternate architectures, adding regularization terms, injecting small noise perturbations and other millions bags and tricks are used to avoid the mode collapse.

Goodfellow I. J. et al. Generative Adversarial Networks, 2014 Metz L. et al. Unrolled Generative Adversarial Networks, 2016

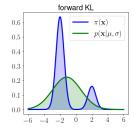
Jensen-Shannon vs Kullback-Leibler

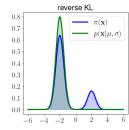
- $\blacktriangleright \pi(\mathbf{x})$ is a fixed mixture of 2 gaussians.
- \triangleright $p(\mathbf{x}|\mu,\sigma) \mathcal{N}(\mu,\sigma^2)$.

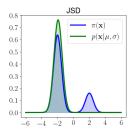
Mode covering vs mode seeking

$$\mathit{KL}(\pi||p) = \int \pi(\mathbf{x}) \log rac{\pi(\mathbf{x})}{p(\mathbf{x})} d\mathbf{x}, \quad \mathit{KL}(p||\pi) = \int p(\mathbf{x}) \log rac{p(\mathbf{x})}{\pi(\mathbf{x})} d\mathbf{x}$$

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







Summary

- ▶ It is possible to use flows in VAE prior and posterior. This is almost the same.
- 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).
- Mode collapse and vanishing gradients are the two main problems of vanilla GAN. Lots of tips and tricks has to be used to make the GAN training is stable and scalable.