Deep Generative Models

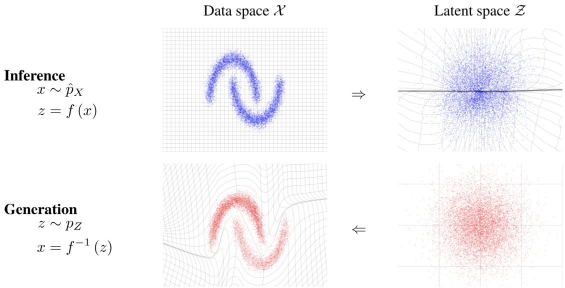
Lecture 6

Roman Isachenko

Moscow Institute of Physics and Technology

Autumn, 2021

Recap of previous lecture



Flow likelihood

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \log p(f(\mathbf{x}, \boldsymbol{\theta})) + \log \left| \det \left(\frac{\partial f(\mathbf{x}, \boldsymbol{\theta})}{\partial \mathbf{x}} \right) \right|$$

What we want

- Efficient computation of Jacobian $\frac{\partial f(\mathbf{x},\boldsymbol{\theta})}{\partial \mathbf{x}}$;
- Efficient sampling from the base distribution $p(\mathbf{z})$;
- Efficient inversion of $f(\mathbf{x}, \boldsymbol{\theta})$.

Dinh L., Sohl-Dickstein J., Bengio S. Density estimation using Real NVP, 2016

Recap of previous lecture

Planar flow

$$g(\mathbf{z}, \boldsymbol{\theta}) = \mathbf{z} + \mathbf{u}\, h(\mathbf{w}^T\mathbf{z} + b).$$

Sylvester flow

$$g(\mathbf{z}, \boldsymbol{\theta}) = \mathbf{z} + \mathbf{A}\, h(\mathbf{B}\mathbf{z} + \mathbf{b}).$$

NICE/RealNVP: Affine coupling law

$$\begin{cases} \mathbf{z}_{1:d} = \mathbf{x}_{1:d}; \\ \mathbf{z}_{d:m} = \mathbf{x}_{d:m} \odot \exp\left(c_1(\mathbf{x}_{1:d}, \boldsymbol{\theta})\right) + c_2(\mathbf{x}_{1:d}, \boldsymbol{\theta}). \end{cases}$$

Glow: invertible 1x1 conv

$$\mathbf{W} = \mathbf{P}\mathbf{L}(\mathbf{U} + \mathrm{diag}(\mathbf{s})).$$

Rezende D. J., Mohamed S. Variational Inference with Normalizing Flows, 2015
Berg R. et al. Sylvester normalizing flows for variational inference, 2018
Dinh L., Krueger D., Bengio Y. NICE: Non-linear Independent Components Estimation, 2014
Dinh L., Sohl-Dickstein J., Bengio S. Density estimation using Real NVP, 2016
Kingma D. P., Dhariwal P. Glow: Generative Flow with Invertible 1x1 Convolutions, 2018

Likelihood-based models

Exact likelihood evaluation

- Autoregressive models (PixelCNN, WaveNet);
- Flow models (NICE, RealNVP, Glow).

Approximate likelihood evaluation

- Latent variable models (VAE).

What are the pros and cons of each of them?

VAE recap

ELBO

$$\log p(\mathbf{x}|\boldsymbol{\theta}) \geq \mathcal{L}(\phi, \boldsymbol{\theta}) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x},\phi)} \log \frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z}|\mathbf{x}, \phi)} \to \max_{\phi,\boldsymbol{\theta}} .$$

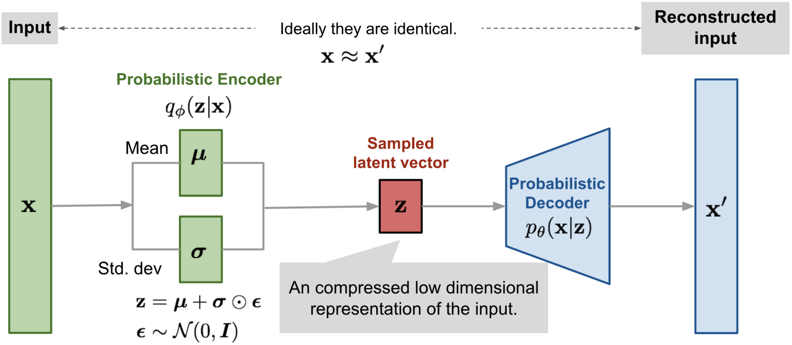


image credit:
https://lilianweng.github.io/lil-log/2018/08/12/from-autoencoder-to-beta-vae.html

VAE limitations

- Poor variational posterior distribution (encoder)

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

- Poor prior distribution

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

- Poor probabilistic model (decoder)

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

- Loose lower bound

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

Variational posterior

ELBO

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

- In E-step of EM-algorithm we wish $KL(q(\mathbf{z}|\mathbf{x}, \phi)||p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta})) = 0$.
  (In this case the lower bound is tight $\log p(\mathbf{x}|\boldsymbol{\theta}) = \mathcal{L}(q, \boldsymbol{\theta})$).
- Normal variational distribution $q(\mathbf{z}|\mathbf{x}, \phi) = \mathcal{N}(\mathbf{z}|\boldsymbol{\mu}_\phi(\mathbf{x}), \boldsymbol{\sigma}^2_\phi(\mathbf{x}))$ is poor (e.g. has only one mode).
- Flows models convert a simple base distribution to a compex one using invertible transformation with simple Jacobian. How to use flows in VAE?

Flows in VAE

Apply a sequence of transformations to the random variable

$$\mathbf{z}_0 \sim q(\mathbf{z}|\mathbf{x}, \phi) = \mathcal{N}(\mathbf{z}|\boldsymbol{\mu}_\phi(\mathbf{x}), \boldsymbol{\sigma}^2_\phi(\mathbf{x})).$$

Here, $q(\mathbf{z}|\mathbf{x}, \phi)$ (which is a VAE encoder) plays a role of a base distribution.

$$\mathbf{z}_0 \xrightarrow{g_1} \mathbf{z}_1 \xrightarrow{g_2} \dots \xrightarrow{g_K} \mathbf{z}_K, \quad \mathbf{z}_K = g(\mathbf{z}_0), \quad g = g_K \circ \dots \circ g_1.$$

Each g_k is a flow transformation (e.g. planar, coupling layer) parameterized by ϕ_k.

$$\log q_K(\mathbf{z}_K|\mathbf{x}, \phi, \{\phi_k\}_{k=1}^K) = \log q(\mathbf{z}_0|\mathbf{x}, \phi) - \sum_{k=1}^K \log \left| \det \left(\frac{\partial g_k(\mathbf{z}_{k-1}, \phi_k)}{\partial \mathbf{z}_{k-1}} \right) \right|.$$

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

Flows in VAE

ELBO

$$p(\mathbf{x}|\boldsymbol{\theta}) \geq \mathcal{L}(\phi, \boldsymbol{\theta}) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x},\phi)} \log \frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z}|\mathbf{x}, \phi)} \rightarrow \max_{\phi, \boldsymbol{\theta}}.$$

Flow model in latent space

$$\log q_K(\mathbf{z}_K|\mathbf{x}, \phi_*) = \log q(\mathbf{z}_0|\mathbf{x}, \phi) - \sum_{k=1}^{K} \log \left| \det \left(\frac{\partial g_k(\mathbf{z}_{k-1}, \phi_k)}{\partial \mathbf{z}_{k-1}} \right) \right|.$$

Let use $q_K(\mathbf{z}_K|\mathbf{x}, \phi_*)$, $\phi_* = \{\phi, \phi_1, \dots, \phi_K\}$ as a variational distribution. Here ϕ – encoder parameters, $\{\phi_k\}_{k=1}^K$ – flow parameters.

- Encoder outputs base distribution $q(\mathbf{z}_0|\mathbf{x}, \phi)$.
- Flow model $\mathbf{z}_K = g(\mathbf{z}_0, \{\phi_k\}_{k=1}^K)$ transforms the base distribution $q(\mathbf{z}_0|\mathbf{x}, \phi)$ to the distribution $q_K(\mathbf{z}_K|\mathbf{x}, \phi_*)$.
- Distribution $q_K(\mathbf{z}_K|\mathbf{x}, \phi_*)$ is used as a variational distribution for ELBO maximization.

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

Flows in VAE

Flow model in latent space

$$\log q_K(\mathbf{z}_K|\mathbf{x}, \phi_*) = \log q(\mathbf{z}_0|\mathbf{x}, \phi) - \sum_{k=1}^{K} \log \left| \det \left(\frac{\partial g_k(\mathbf{z}_{k-1}, \phi_k)}{\partial \mathbf{z}_{k-1}} \right) \right|.$$

ELBO objective

$$\begin{aligned}
\mathcal{L}(\phi, \boldsymbol{\theta}) &= \mathbb{E}_{q_K(\mathbf{z}_K|\mathbf{x},\phi_*)} \log \frac{p(\mathbf{x}, \mathbf{z}_K|\boldsymbol{\theta})}{q_K(\mathbf{z}_K|\mathbf{x}, \phi_*)} \\
&= \mathbb{E}_{q_K(\mathbf{z}_K|\mathbf{x},\phi_*)} \left[\log p(\mathbf{x}, \mathbf{z}_K|\boldsymbol{\theta}) - \log q_K(\mathbf{z}_K|\mathbf{x}, \phi_*) \right] \\
&= \mathbb{E}_{q_K(\mathbf{z}_K|\mathbf{x},\phi_*)} \log p(\mathbf{x}|\mathbf{z}_K, \boldsymbol{\theta}) - KL(q_K(\mathbf{z}_K|\mathbf{x}, \phi_*)||p(\mathbf{z}_K)).
\end{aligned}$$

The second term in ELBO is reverse KL divergence. Planar flows was originally proposed for variational inference in VAE.

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

Flows in VAE

Variational distribution

$$\log q_K(\mathbf{z}_K|\mathbf{x}, \phi_*) = \log q(\mathbf{z}_0|\mathbf{x}, \phi) - \sum_{k=1}^{K} \log \left| \det \left(\frac{\partial g_k(\mathbf{z}_{k-1}, \phi_k)}{\partial \mathbf{z}_{k-1}} \right) \right| .$$

ELBO objective

$$\begin{aligned}
\mathcal{L}(\phi, \boldsymbol{\theta}) &= \mathbb{E}_{q_K(\mathbf{z}_K|\mathbf{x}, \phi_*)} \big[\log p(\mathbf{x}, \mathbf{z}_K|\boldsymbol{\theta}) - \log q_K(\mathbf{z}_K|\mathbf{x}, \phi_*) \big] \\
&= \mathbb{E}_{q(\mathbf{z}_0|\mathbf{x}, \phi)} \left[\log p(\mathbf{x}, \mathbf{z}_K|\boldsymbol{\theta}) - \log q_K(\mathbf{z}_K|\mathbf{x}, \phi_*) \right] \Big|_{\mathbf{z}_K = g(\mathbf{z}_0, \{\phi_k\}_{k=1}^K)} \\
&= \mathbb{E}_{q(\mathbf{z}_0|\mathbf{x}, \phi)} \Bigg[\log p(\mathbf{x}, \mathbf{z}_K|\boldsymbol{\theta}) - \log q(\mathbf{z}_0|\mathbf{x}, \phi) + \\
&\qquad + \sum_{k=1}^{K} \log \left| \det \left(\frac{\partial g_k(\mathbf{z}_{k-1}, \phi_k)}{\partial \mathbf{z}_{k-1}} \right) \right| \Bigg] .
\end{aligned}$$

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

Flows in VAE

Variational distribution

$$\log q_K(\mathbf{z}_K|\mathbf{x}, \phi_*) = \log q(\mathbf{z}_0|\mathbf{x}, \phi) - \sum_{k=1}^{K} \log \left| \det \left(\frac{\partial g_k(\mathbf{z}_{k-1}, \phi_k)}{\partial \mathbf{z}_{k-1}} \right) \right|.$$

ELBO objective

$$\mathcal{L}(\phi, \boldsymbol{\theta}) = \mathbb{E}_{q(\mathbf{z}_0|\mathbf{x},\phi)} \Bigg[\log p(\mathbf{x}, \mathbf{z}_K|\boldsymbol{\theta}) - \log q(\mathbf{z}_0|\mathbf{x}, \phi) + \\ + \sum_{k=1}^{K} \log \left| \det \left(\frac{\partial g_k(\mathbf{z}_{k-1}, \phi_k)}{\partial \mathbf{z}_{k-1}} \right) \right| \Bigg].$$

- Obtain samples $\mathbf{z}_0$ from the encoder.
- Apply flow model $\mathbf{z}_K = g(\mathbf{z}_0, \{\phi_k\}_{k=1}^K)$.
- Compute likelihood for $\mathbf{z}_K$ using the decoder, base distribution for $\mathbf{z}_0$ and the Jacobian.
- We do not need inverse flow function, if we use flows in variational inference.

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

Recap of previous lecture

ELBO

$$p(\mathbf{x}|\boldsymbol{\theta}) \geq \mathcal{L}(\phi, \boldsymbol{\theta}) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x},\phi)} \log \frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z}|\mathbf{x}, \phi)} \rightarrow \max_{\phi,\boldsymbol{\theta}}.$$

- Normal variational distribution $q(\mathbf{z}|\mathbf{x}, \phi) = \mathcal{N}(\mathbf{z}|\boldsymbol{\mu}_\phi(\mathbf{x}), \boldsymbol{\sigma}^2_\phi(\mathbf{x}))$ is poor (e.g. has only one mode).
- Flows models convert a simple base distribution to a compex one using an invertible transformation with simple Jacobian.

Flow model in latent space

$$\log q_K(\mathbf{z}_K|\mathbf{x}, \phi_*) = \log q(\mathbf{z}_0|\mathbf{x}, \phi) - \sum_{k=1}^{K} \log \left| \det \left(\frac{\partial g_k(\mathbf{z}_{k-1}, \phi_k)}{\partial \mathbf{z}_{k-1}} \right) \right|.$$

Let's use $q_K(\mathbf{z}_K|\mathbf{x}, \phi_*)$, $\phi_* = \{\phi, \phi_1, \dots, \phi_K\}$ as a variational distribution. Here, ϕ – encoder parameters, $\{\phi_k\}_{k=1}^K$ – flow parameters.

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

Recap of previous lecture

Variational distribution

$$\log q_K(\mathbf{z}_K|\mathbf{x}, \phi_*) = \log q(\mathbf{z}_0|\mathbf{x}, \phi) - \sum_{k=1}^{K} \log \left| \det \left(\frac{\partial g_k(\mathbf{z}_{k-1}, \phi_k)}{\partial \mathbf{z}_{k-1}} \right) \right|.$$

ELBO objective

$$\mathcal{L}(\phi, \boldsymbol{\theta}) = \mathbb{E}_{q(\mathbf{z}_0|\mathbf{x},\phi)} \Bigg[\log p(\mathbf{x}, \mathbf{z}_K|\boldsymbol{\theta}) - \log q(\mathbf{z}_0|\mathbf{x}, \phi) + \\ + \sum_{k=1}^{K} \log \left| \det \left(\frac{\partial g_k(\mathbf{z}_{k-1}, \phi_k)}{\partial \mathbf{z}_{k-1}} \right) \right| \Bigg].$$

- Obtain samples $\mathbf{z}_0$ from the encoder.
- Apply flow model $\mathbf{z}_K = g(\mathbf{z}_0, \{\phi_k\}_{k=1}^K)$.
- Compute likelihood for $\mathbf{z}_K$ using the decoder, base distribution for $\mathbf{z}_0$ and the Jacobian.
- We do not need an inverse flow function if we use flows in variational inference.

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

Inverse autoregressive flow (IAF)

$$\mathbf{x} = g(\mathbf{z}, \boldsymbol{\theta}) \quad \Rightarrow \quad x_i = \tilde{\sigma}_i(\mathbf{z}_{1:i-1}) \cdot z_i + \tilde{\mu}_i(\mathbf{z}_{1:i-1}).$$

$$\mathbf{z} = f(\mathbf{x}, \boldsymbol{\theta}) \quad \Rightarrow \quad z_i = (x_i - \tilde{\mu}_i(\mathbf{z}_{1:i-1})) \cdot \frac{1}{\tilde{\sigma}_i(\mathbf{z}_{1:i-1})}.$$

Reverse KL for flow model

$$KL(p||\pi) = \mathbb{E}_{p(\mathbf{z})} \left[\log p(\mathbf{z}) - \log \left| \det \left(\frac{\partial g(\mathbf{z}, \boldsymbol{\theta})}{\partial \mathbf{z}} \right) \right| - \log \pi(g(\mathbf{z}, \boldsymbol{\theta})) \right]$$

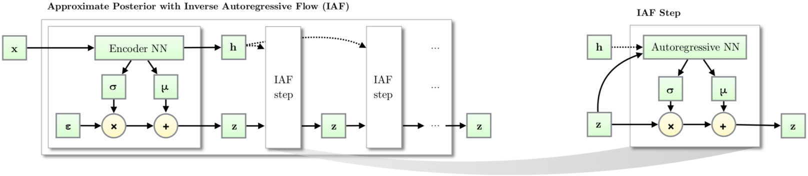
- We don't need to think about computing the function $f(\mathbf{x}, \boldsymbol{\theta})$.
- Inverse autoregressive flow is a natural choice for using flows in VAE:

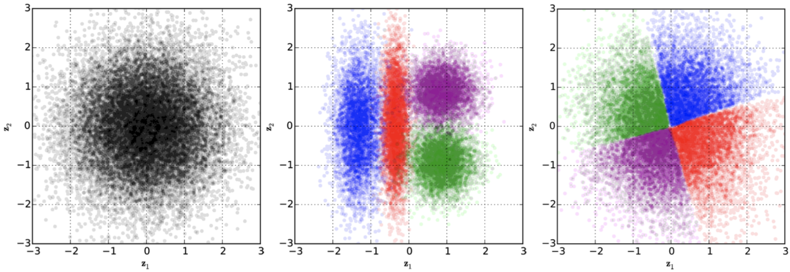
$$\mathbf{z}_0 = \boldsymbol{\sigma}(\mathbf{x}) \odot \boldsymbol{\epsilon} + \boldsymbol{\mu}(\mathbf{x}), \quad \boldsymbol{\epsilon} \sim \mathcal{N}(0, 1); \quad \sim q(\mathbf{z}_0 | \mathbf{x}, \phi).$$

$$\mathbf{z}_k = \tilde{\boldsymbol{\sigma}}_k(\mathbf{z}_{k-1}) \odot \mathbf{z}_{k-1} + \tilde{\boldsymbol{\mu}}_k(\mathbf{z}_{k-1}), \quad k \geq 1; \quad \sim q_k(\mathbf{z}_k | \mathbf{x}, \phi, \{\phi_j\}_{j=1}^k).$$

Kingma D. P. et al. Improving Variational Inference with Inverse Autoregressive Flow, 2016

Inverse autoregressive flow (IAF)





Kingma D. P. et al. Improving Variational Inference with Inverse Autoregressive Flow, 2016

MAF/IAF pros and cons

MAF

- Sampling is slow.
- Likelihood evaluation is fast.

IAF

- Sampling is fast.
- Likelihood evaluation is slow.

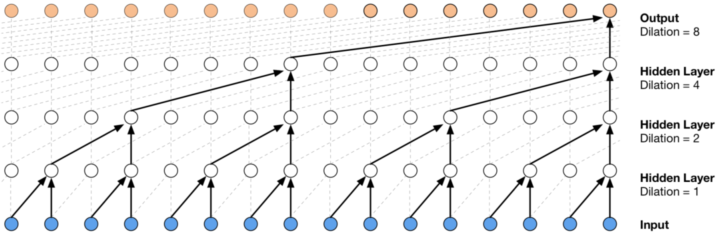
How to take the best of both worlds?

WaveNet (2016)

Autoregressive model for raw audio waveforms generation

$$p(\mathbf{x}|\boldsymbol{\theta}) = \prod_{t=1}^{T} p(x_t|\mathbf{x}_{1:t-1}, \boldsymbol{\theta}).$$

The model uses causal dilated convolutions.



Oord A. et al. Wavenet: A generative model for raw audio, 2016

Parallel WaveNet, 2017

Previous WaveNet model

- raw audio is high-dimensional (e.g. 16000 samples per second for 16kHz audio);
- WaveNet encodes 8-bit signal with 256-way categorical distribution.

Goal

- improved fidelity (24kHz instead of 16kHz) $\rightarrow$ increase dilated convolution filter size from 2 to 3;
- 16-bit signals $\rightarrow$ mixture of logistics instead of categorical distribution.

Oord A. et al. Parallel WaveNet: Fast High-Fidelity Speech Synthesis, 2017

Parallel WaveNet, 2017

Probability density distillation

1. Train usual WaveNet (MAF) via MLE (teacher network).
2. Train IAF WaveNet (student network), which attempts to match the probability of its own samples under the distribution learned by the teacher.

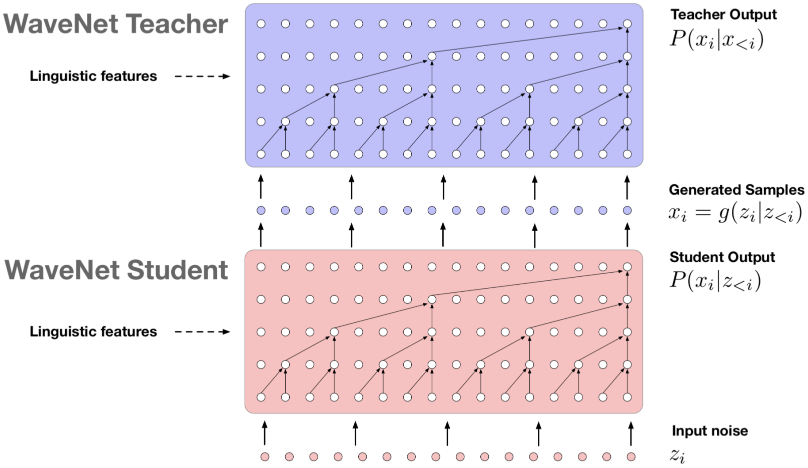
Student objective

$$KL(p_s || p_t) = H(p_s, p_t) - H(p_s).$$

More than 1000x speed-up relative to original WaveNet!

Oord A. et al. Parallel WaveNet: Fast High-Fidelity Speech Synthesis, 2017

Parallel WaveNet, 2017



Oord A. et al. Parallel WaveNet: Fast High-Fidelity Speech Synthesis, 2017

Flow KL duality

Theorem

Fitting flow model $p(\mathbf{x}|\boldsymbol{\theta})$ to the target distribution $\pi(\mathbf{x})$ using forward KL (MLE) is equivalent to fitting the induced distribution $p(\mathbf{z}|\boldsymbol{\theta})$ to the base $p(\mathbf{z})$ using reverse KL:

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

- $p(\mathbf{z})$ is a base distribution; $\pi(\mathbf{x})$ is a data distribution;
- $\mathbf{z} \sim p(\mathbf{z})$, $\mathbf{x} = g(\mathbf{z}, \boldsymbol{\theta})$, $\mathbf{x} \sim p(\mathbf{x}|\boldsymbol{\theta})$;
- $\mathbf{x} \sim \pi(\mathbf{x})$, $\mathbf{z} = f(\mathbf{x}, \boldsymbol{\theta})$, $\mathbf{z} \sim p(\mathbf{z}|\boldsymbol{\theta})$;

$$\log p(\mathbf{z}|\boldsymbol{\theta}) = \log \pi(g(\mathbf{z}, \boldsymbol{\theta})) + \log \left| \det \left(\frac{\partial g(\mathbf{z}, \boldsymbol{\theta})}{\partial \mathbf{z}} \right) \right|;$$

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \log p(f(\mathbf{x}, \boldsymbol{\theta})) + \log \left| \det \left(\frac{\partial f(\mathbf{x}, \boldsymbol{\theta})}{\partial \mathbf{x}} \right) \right|.$$

Papamakarios G. et al. Normalizing flows for probabilistic modeling and inference, 2019

MAF vs IAF

Theorem

Fitting flow model $p(\mathbf{x}|\boldsymbol{\theta})$ to the target distribution $\pi(\mathbf{x})$ using forward KL (MLE) is equivalent to fitting the induced distribution $p(\mathbf{z}|\boldsymbol{\theta})$ to the base $p(\mathbf{z})$ using reverse KL:

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

Proof

$$KL\left(p(\mathbf{z}|\boldsymbol{\theta})||\pi(\mathbf{z})\right) = \mathbb{E}_{p(\mathbf{z}|\boldsymbol{\theta})}\left[\log p(\mathbf{z}|\boldsymbol{\theta}) - \log p(\mathbf{z})\right] =$$

$$= \mathbb{E}_{p(\mathbf{z}|\boldsymbol{\theta})}\left[\log \pi(g(\mathbf{z},\boldsymbol{\theta})) + \log\left|\det\left(\frac{\partial g(\mathbf{z},\boldsymbol{\theta})}{\partial \mathbf{z}}\right)\right| - \log p(\mathbf{z})\right] =$$

$$= \mathbb{E}_{\pi(\mathbf{x})}\left[\log \pi(\mathbf{x}) - \log\left|\det\left(\frac{\partial f(\mathbf{x},\boldsymbol{\theta})}{\partial \mathbf{x}}\right)\right| - \log p(f(\mathbf{x},\boldsymbol{\theta}))\right].$$

Papamakarios G., Pavlakou T., Murray I. Masked Autoregressive Flow for Density Estimation, 2017

MAF vs IAF

Theorem

Fitting flow model $p(\mathbf{x}|\boldsymbol{\theta})$ to the target distribution $\pi(\mathbf{x})$ using forward KL (MLE) is equivalent to fitting the induced distribution $p(\mathbf{z}|\boldsymbol{\theta})$ to the base $p(\mathbf{z})$ using reverse KL:

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

Proof (continued)

$$KL\left(p(\mathbf{z}|\boldsymbol{\theta})||p(\mathbf{z})\right) =$$
$$= \mathbb{E}_{\pi(\mathbf{x})}\left[\log \pi(\mathbf{x}) - \log\left|\det\left(\frac{\partial f(\mathbf{x}, \boldsymbol{\theta})}{\partial \mathbf{x}}\right)\right| - \log p(f(\mathbf{x}, \boldsymbol{\theta}))\right] =$$
$$= \mathbb{E}_{\pi(\mathbf{x})}\left[\log \pi(\mathbf{x}) - \log p(\mathbf{x}|\boldsymbol{\theta})\right] = KL(\pi(\mathbf{x})||p(\mathbf{x}|\boldsymbol{\theta})).$$

Papamakarios G., Pavlakou T., Murray I. Masked Autoregressive Flow for Density Estimation, 2017

Dequantization

- Images are discrete data, pixels lie in the [0, 255] integer domain (the model is $P(\mathbf{x}|\boldsymbol{\theta}) = \text{Categorical}(\boldsymbol{\pi}(\boldsymbol{\theta}))$).
- Flow is a continuous model (it works with continuous data $\mathbf{x}$).

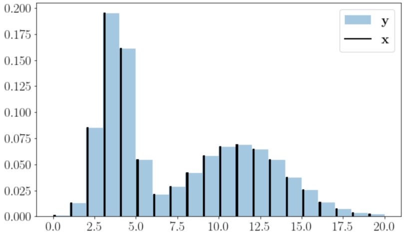
By fitting a continuous density model to discrete data, one can produce a degenerate solution with all probability mass on discrete values.

How to convert a discrete data distribution to a continuous one?

Uniform dequantization

$$\mathbf{x} \sim \text{Categorical}(\boldsymbol{\pi})$$
$$\mathbf{u} \sim U[0, 1]$$

$$\mathbf{y} = \mathbf{x} + \mathbf{u} \sim \text{Continuous}$$



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

Uniform dequantization

Statement

Fitting continuous model $p(\mathbf{y}|\boldsymbol{\theta})$ on uniformly dequantized data $\mathbf{y} = \mathbf{x} + \mathbf{u}$, $\mathbf{u} \sim U[0, 1]$ is equivalent to maximization of a lower bound on log-likelihood for a discrete model:

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

Thus, the maximisation of continuous model log-likelihood on $\mathbf{y}$ can't lead to the a collapse onto the discrete data (the objective is bounded above by the discrete model log-likelihood).

Proof

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

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

Summary

- Gaussian autoregressive model is a special type of flow.
- MAF is an example of such a model which is suitable for density estimation tasks. IAF uses an inverse autoregressive transformation for variational inference task.
- RealNVP is a special case of IAF and MAF.
- There is a duality between forward and reverse KL for flow models.
- To apply a continuous model to a discrete distribution it is standard practice to dequantize data at first.