Deep Generative Models

Lecture 7

Roman Isachenko

Moscow Institute of Physics and Technology

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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 complex one using invertible transformation with simple Jacobian. How to use flows in VAE?

Flows in VAE posterior

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.

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

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

Flows in VAE posterior

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 posterior

Flow model in latent space

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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 posterior

Variational distribution

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\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)} \big[\log p(\mathbf{x}, \mathbf{z}_K|\boldsymbol{\theta}) - \log q_K(\mathbf{z}_K|\mathbf{x}, \phi_*) \big] \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}$$

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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).
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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.

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

ELBO objective

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

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Inverse autoregressive flow (IAF)

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

Reverse KL for flow model

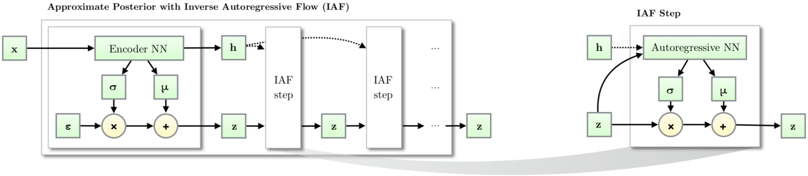
$$
KL(p||\pi) = \mathbb{E}_{p(\mathbf{z})} \left[\log p(\mathbf{z}) - \log \left| \det \left(\frac{\partial g(\mathbf{z}, \boldsymbol{\theta})}{\partial \mathbf{z}} \right) \right| - \log \pi(g(\mathbf{z}, \boldsymbol{\theta})) \right]
$$

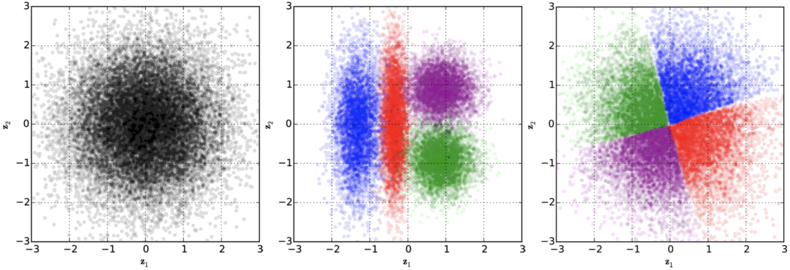
- We don't need to think about computing the function $f(\mathbf{x}, \boldsymbol{\theta})$.
- Inverse autoregressive flow is a natural choice for using flows in VAE:

$$
\begin{aligned}
&\mathbf{z}_0 = \boldsymbol{\sigma}(\mathbf{x}) \odot \boldsymbol{\epsilon} + \boldsymbol{\mu}(\mathbf{x}), \quad \boldsymbol{\epsilon} \sim \mathcal{N}(0, 1); \quad \sim q(\mathbf{z}_0|\mathbf{x}, \phi). \\
&\mathbf{z}_k = \tilde{\boldsymbol{\sigma}}_k(\mathbf{z}_{k-1}) \odot \mathbf{z}_{k-1} + \tilde{\boldsymbol{\mu}}_k(\mathbf{z}_{k-1}), \quad k \geq 1; \quad \sim q_k(\mathbf{z}_k|\mathbf{x}, \phi, \{\phi_j\}_{j=1}^k).
\end{aligned}
$$

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

Inverse autoregressive flow (IAF)





(a) Prior distribution (b) Posteriors in standard VAE (c) Posteriors in VAE with IAF

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

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 $\mathbf{x}$).

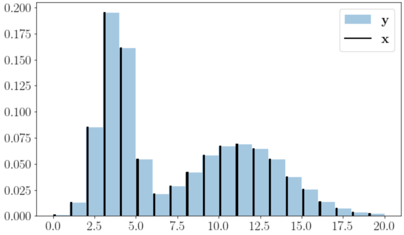
By fitting a continuous density model to discrete data, one can produce a degenerate solution with all probability mass on discrete values.

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

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

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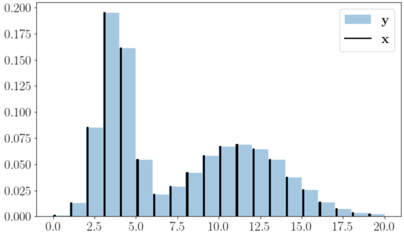

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$$P(\mathbf{x}|\boldsymbol{\theta}) = \int_{U[0,1]} p(\mathbf{x} + \mathbf{u}|\boldsymbol{\theta}) d\mathbf{u}$$

Proof

$$\mathbb{E}_\pi \log p(\mathbf{y}|\boldsymbol{\theta}) = \int \pi(\mathbf{y}) \log p(\mathbf{y}|\boldsymbol{\theta}) d\mathbf{y} =$$

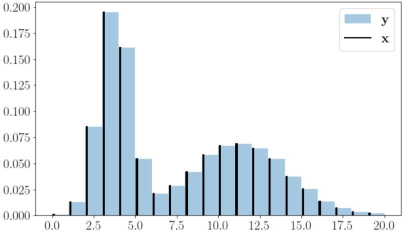
$$= \sum \pi(\mathbf{x}) \int_{U[0,1]} \log p(\mathbf{x} + \mathbf{u}|\boldsymbol{\theta}) d\mathbf{u} \leq$$

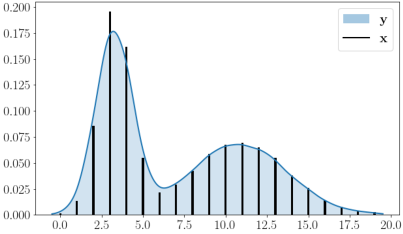
$$\leq \sum \pi(\mathbf{x}) \log \int_{U[0,1]} p(\mathbf{x} + \mathbf{u}|\boldsymbol{\theta}) d\mathbf{u} =$$

$$= \sum \pi(\mathbf{x}) \log P(\mathbf{x}|\boldsymbol{\theta}) = \mathbb{E}_\pi \log P(\mathbf{x}|\boldsymbol{\theta}).$$

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

Variational dequantization





- $p(\mathbf{y}|\boldsymbol{\theta})$ assign unifrom density to unit hypercubes $\mathbf{x} + U[0, 1]$ (left fig).
- Neural network density models are smooth function approximators (right fig).
- Smooth dequantization is more natural.

How to perform the smooth dequantization?

Flow++

Variational dequantization

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

Variational lower bound

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

Uniform dequantization bound

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

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

Flow++

Variational lower bound

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

Let $\mathbf{u} = h(\boldsymbol{\epsilon}, \boldsymbol{\phi})$ is a flow model with base distribution $\boldsymbol{\epsilon} \sim p(\boldsymbol{\epsilon}) = \mathcal{N}(0, \mathbf{I})$:

$$q(\mathbf{u}|\mathbf{x}) = p(h^{-1}(\mathbf{u}, \boldsymbol{\phi})) \cdot \left| \det \frac{\partial h^{-1}(\mathbf{u}, \boldsymbol{\phi})}{\partial \mathbf{u}} \right|.$$

Then

$$\log P(\mathbf{x}|\boldsymbol{\theta}) \geq \mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta}) = \int p(\boldsymbol{\epsilon}) \log \left(\frac{p(\mathbf{x} + h(\boldsymbol{\epsilon}, \boldsymbol{\phi})|\boldsymbol{\theta})}{p(\boldsymbol{\epsilon}) \cdot \left| \det \frac{\partial h(\boldsymbol{\epsilon}, \boldsymbol{\phi})}{\partial \boldsymbol{\epsilon}} \right|^{-1}} \right) d\boldsymbol{\epsilon}.$$

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

Flow++

Variational lower

$$\log P(\mathbf{x}|\boldsymbol{\theta}) \geq \int p(\boldsymbol{\epsilon}) \log \left(\frac{p(\mathbf{x} + h(\boldsymbol{\epsilon}, \phi))}{p(\boldsymbol{\epsilon}) \cdot \left| \det \frac{\partial h(\boldsymbol{\epsilon}, \phi)}{\partial \boldsymbol{\epsilon}} \right|^{-1}} \right) d\boldsymbol{\epsilon}.$$

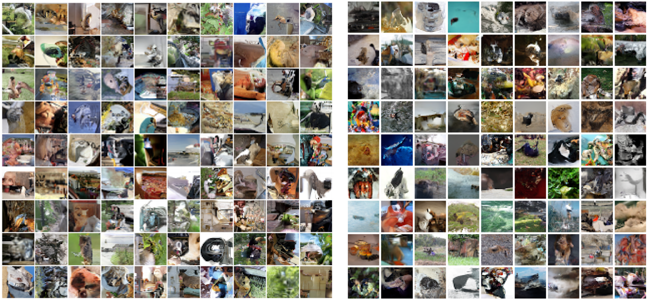
- If $p(\mathbf{x} + \mathbf{u}|\boldsymbol{\theta})$ is also a flow model, it is straightforward to calculate stochastic gradient of this ELBO.
- Uniform dequantization is a special case of variational dequantization ($q(\mathbf{u}|\mathbf{x}) = U[0, 1]$). The gap between $\log P(\mathbf{x}|\boldsymbol{\theta})$ and the derived ELBO is $KL(q(\mathbf{u}|\mathbf{x})||p(\mathbf{u}|\mathbf{x}))$.
- In the case of uniform dequantization the model unnaturally places uniform density over each hypercube $\mathbf{x} + U[0, 1]$ due to inexpressive distribution q.

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

Flow++

Table 1. Unconditional image modeling results in bits/dim

Model family	Model	CIFAR10	ImageNet 32x32	ImageNet 64x64
Non-autoregressive	RealNVP (Dinh et al., 2016)	3.49	4.28	–
	Glow (Kingma & Dhariwal, 2018)	3.35	4.09	3.81
	IAF-VAE (Kingma et al., 2016)	3.11	–	–
	Flow++ (ours)	**3.08**	**3.86**	**3.69**
Autoregressive	Multiscale PixelCNN (Reed et al., 2017)	–	3.95	3.70
	PixelCNN (van den Oord et al., 2016b)	3.14	–	–
	PixelRNN (van den Oord et al., 2016b)	3.00	3.86	3.63
	Gated PixelCNN (van den Oord et al., 2016c)	3.03	3.83	3.57
	PixelCNN++ (Salimans et al., 2017)	2.92	–	–
	Image Transformer (Parmar et al., 2018)	2.90	3.77	–
	PixelSNAIL (Chen et al., 2017)	2.85	3.80	3.52



(a) PixelCNN (b) Flow++

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

VAE limitations

- Poor variational posterior distribution (encoder)

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

- Poor prior distribution

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

- Poor probabilistic model (decoder)

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

- Loose lower bound

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

ELBO interpretations

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

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

- Evidence minus posterior KL

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

- Average negative energy plus entropy

$$\begin{aligned} \mathcal{L}(q, \boldsymbol{\theta}) &= \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \phi)} [\log p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta}) - \log q(\mathbf{z}|\mathbf{x}, \phi)] \\ &= \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \phi)} \log p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta}) + \mathbb{H} [q(\mathbf{z}|\mathbf{x}, \phi)] . \end{aligned}$$

- Average reconstruction minus KL to prior

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

ELBO surgery

$$
\frac{1}{n} \sum_{i=1}^{n} \mathcal{L}_i(q, \boldsymbol{\theta}) = \frac{1}{n} \sum_{i=1}^{n} \left[\mathbb{E}_{q(\mathbf{z}|\mathbf{x}_i)} \log p(\mathbf{x}_i | \mathbf{z}, \boldsymbol{\theta}) - KL(q(\mathbf{z}|\mathbf{x}_i) || p(\mathbf{z})) \right].
$$

Theorem

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

- $q(\mathbf{z}) = \frac{1}{n} \sum_{i=1}^{n} q(\mathbf{z}|\mathbf{x}_i)$ – **aggregated** posterior distribution.
- $\mathbb{I}_q[\mathbf{x}, \mathbf{z}]$ – mutual information between $\mathbf{x}$ and $\mathbf{z}$ under empirical data distribution and distribution $q(\mathbf{z}|\mathbf{x})$.
- First term pushes $q(\mathbf{z})$ towards the prior $p(\mathbf{z})$.
- Second term reduces the amount of information about $\mathbf{x}$ stored in $\mathbf{z}$.

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

ELBO surgery

Theorem

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

Proof

$$\frac{1}{n}\sum_{i=1}^{n} KL(q(\mathbf{z}|\mathbf{x}_i)||p(\mathbf{z})) = \frac{1}{n}\sum_{i=1}^{n}\int q(\mathbf{z}|\mathbf{x}_i)\log\frac{q(\mathbf{z}|\mathbf{x}_i)}{p(\mathbf{z})}d\mathbf{z} =$$

$$= \frac{1}{n}\sum_{i=1}^{n}\int q(\mathbf{z}|\mathbf{x}_i)\log\frac{q(\mathbf{z})q(\mathbf{z}|\mathbf{x}_i)}{p(\mathbf{z})q(\mathbf{z})}d\mathbf{z} = \int \frac{1}{n}\sum_{i=1}^{n} q(\mathbf{z}|\mathbf{x}_i)\log\frac{q(\mathbf{z})}{p(\mathbf{z})}d\mathbf{z} +$$

$$+ \frac{1}{n}\sum_{i=1}^{n}\int q(\mathbf{z}|\mathbf{x}_i)\log\frac{q(\mathbf{z}|\mathbf{x}_i)}{q(\mathbf{z})}d\mathbf{z} = KL(q(\mathbf{z})||p(\mathbf{z})) + \frac{1}{n}\sum_{i=1}^{n} KL(q(\mathbf{z}|\mathbf{x}_i)||q(\mathbf{z}))$$

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

ELBO surgery

Theorem

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

Proof (continued)

$$\frac{1}{n}\sum_{i=1}^{n} KL(q(\mathbf{z}|\mathbf{x}_i)||p(\mathbf{z}_i)) = KL(q(\mathbf{z})||p(\mathbf{z})) + \frac{1}{n}\sum_{i=1}^{n} KL(q(\mathbf{z}|\mathbf{x}_i)||q(\mathbf{z}))$$

It could be shown (exercise):

$$\mathbb{I}_q[\mathbf{x}, \mathbf{z}] = \frac{1}{n}\sum_{i=1}^{n} KL(q(\mathbf{z}|\mathbf{x}_i)||q(\mathbf{z})) \in [0, \log n].$$

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Summary

- Uniform dequantization is the simplest form of dequantization.
- Variational dequantization is a more natural type that was proposed in Flow++ model.
- The IWAE could get the tighter lower bound to the likelihood, but the training of such model becomes more difficult.
- The ELBO surgery reveals insights about a prior distribution in VAE. The optimal prior is the aggregated posterior.