Deep Generative Models
Lecture 7

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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 $\mathbf{x}$).

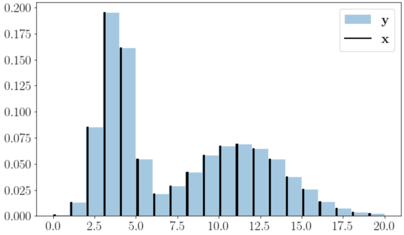
By fitting a continuous density model to discrete data, one can produce a degenerate solution with all probability mass on discrete values.

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:

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

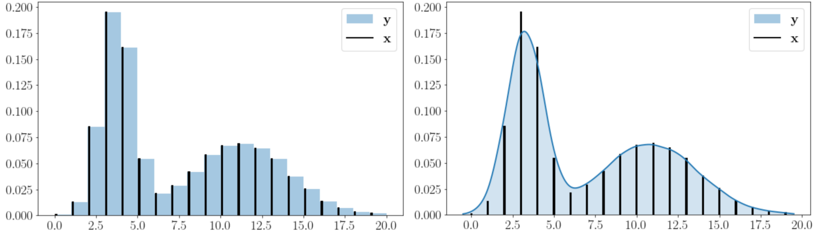
Thus, the maximisation of continuous model log-likelihood on $\mathbf{y}$ can't lead to the a collapse onto the discrete data (the objective is bounded above by the discrete model log-likelihood).

Proof

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

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

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

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

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

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

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

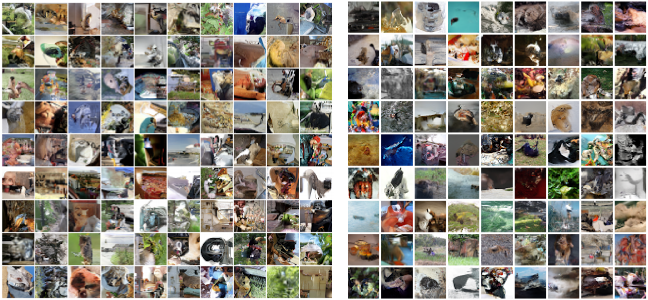
- If $p(\mathbf{x} + \mathbf{u}|\boldsymbol{\theta})$ is also a flow model, it is straightforward to calculate stochastic gradient of this ELBO.
- Uniform dequantization is a special case of variational dequantization ($q(\mathbf{u}|\mathbf{x}) = U[0, 1]$). The gap between $\log P(\mathbf{x}|\boldsymbol{\theta})$ 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

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

- Average reconstruction minus KL to prior

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

ELBO surgery, 2016

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

Theorem

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

where i is treated as random variable:

$$q(i, \mathbf{z}) = q(i)q(\mathbf{z}|i); \quad p(i, \mathbf{z}) = p(i)p(\mathbf{z}); \quad q(i) = p(i) = \frac{1}{n}; \quad q(\mathbf{z}|i) = q(\mathbf{z}|\mathbf{x}_i).$$

$$q(\mathbf{z}) = \sum_{i=1}^{n} q(i, \mathbf{z}) = \frac{1}{n} \sum_{i=1}^{n} q(\mathbf{z}|\mathbf{x}_i); \quad \mathbb{I}_{q(i,\mathbf{z})}[i, \mathbf{z}] = \mathbb{E}_{q(i,\mathbf{z})} \log \frac{q(i, \mathbf{z})}{q(i)q(\mathbf{z})}.$$

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

ELBO surgery, 2016

Theorem

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

Proof

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

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

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

$$= KL(q(\mathbf{z})||p(\mathbf{z})) - \mathbb{E}_{q(\mathbf{z})}\mathbb{H}\left[q(i|\mathbf{z})\right] + \log n.$$

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

ELBO surgery, 2016

Theorem

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

Proof (continued)

$$\frac{1}{n}\sum_{i=1}^{n} KL(q(\mathbf{z}_i|\mathbf{x}_i)||p(\mathbf{z}_i)) = KL(q(\mathbf{z})||p(\mathbf{z})) - \mathbb{E}_{q(\mathbf{z})}\mathbb{H}\left[q(i|\mathbf{z})\right] + \log n$$

$$\mathbb{I}_{q(i,\mathbf{z})}[i, \mathbf{z}] = \mathbb{E}_{q(i,\mathbf{z})} \log \frac{q(i, \mathbf{z})}{q(i)q(\mathbf{z})} = \mathbb{E}_{q(\mathbf{z})}\mathbb{E}_{q(i|\mathbf{z})} \log \frac{q(i|\mathbf{z})q(\mathbf{z})}{q(i)q(\mathbf{z})} =$$
$$= \mathbb{E}_{q(\mathbf{z})}\mathbb{E}_{q(i|\mathbf{z})} \log \frac{q(i|\mathbf{z})}{q(i)} = -\mathbb{E}_{q(\mathbf{z})}\mathbb{H}\left[q(i|\mathbf{z})\right] + \log n.$$

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

ELBO surgery, 2016

Theorem

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

ELBO revisiting

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

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

$$= \underbrace{\frac{1}{n}\sum_{i=1}^{n} \mathbb{E}_{q(\mathbf{z}_i|\mathbf{x}_i)} \log p(\mathbf{x}_i|\mathbf{z}_i, \boldsymbol{\theta})}_{\text{Reconstruction loss}} - \underbrace{\left(\log n - \mathbb{E}_{q(\mathbf{z})}\mathbb{H}\left[q(i|\mathbf{z})\right]\right)}_{0 \leq \text{Mutual info} \leq \log n} - \underbrace{KL(q(\mathbf{z})||p(\mathbf{z}))}_{\text{Marginal KL}}$$

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

ELBO surgery, 2016

ELBO revisiting

$$\sum_{i=1}^{n} \mathcal{L}(q, \boldsymbol{\theta}) = \underbrace{\frac{1}{n} \sum_{i=1}^{n} \mathbb{E}_{q(\mathbf{z}_i|\mathbf{x}_i)} \log p(\mathbf{x}_i|\mathbf{z}_i, \boldsymbol{\theta})}_{\text{Reconstruction loss}} -$$

$$- \underbrace{\left(\log n - \mathbb{E}_{q(\mathbf{z})} \mathbb{H}\left[q(i|\mathbf{z})\right]\right)}_{0 \leq \text{Mutual info} \leq \log n} - \underbrace{KL(q(\mathbf{z}) || p(\mathbf{z}))}_{\text{Marginal KL}}$$

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

	ELBO	Avg. KL	Mutual info. 2	Marg. KL 3
2D latents	-129.63	7.41	7.20	0.21
10D latents	-88.95	19.17	10.82	8.35
20D latents	-87.45	20.2	10.67	9.53

$$\log n \approx 11.0021$$

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

VAE prior

ELBO revisiting

$$\sum_{i=1}^{n} \mathcal{L}(q, \boldsymbol{\theta}) = \underbrace{\frac{1}{n} \sum_{i=1}^{n} \mathbb{E}_{q(\mathbf{z}_i|\mathbf{x}_i)} \log p(\mathbf{x}_i|\mathbf{z}_i, \boldsymbol{\theta})}_{\text{Reconstruction loss}} -$$

$$- \underbrace{\Big(\log n - \mathbb{E}_{q(\mathbf{z})} \mathbb{H}\left[q(i|\mathbf{z})\right]\Big)}_{0 \leq \text{Mutual info} \leq \log n} - \underbrace{KL(q(\mathbf{z})||p(\mathbf{z}))}_{\text{Marginal KL}}$$

How to choose the optimal $p(\mathbf{z})$?

- SG: $p(\mathbf{z}) = \mathcal{N}(0, I) \Rightarrow$ over-regularization;
- MoG: $p(\mathbf{z}|\boldsymbol{\lambda}) = \frac{1}{K} \sum_{k=1}^{K} \mathcal{N}(\boldsymbol{\mu}_k, \boldsymbol{\sigma}_k^2) \Rightarrow$ (*), (**);
- $p(\mathbf{z}) = q(\mathbf{z}) = \frac{1}{n} \sum_{i=1}^{n} q(\mathbf{z}|\mathbf{x}_i) \Rightarrow$ overfitting and highly expensive.

(*) Dilokthanakul N. et al. Deep Unsupervised Clustering with Gaussian Mixture Variational Autoencoders, 2016
(**) Nalisnick E., Hertel L., Smyth P. Approximate Inference for Deep Latent Gaussian Mixtures, 2016

VampPrior

Variational Mixture of posteriors

$$p(\mathbf{z}|\boldsymbol{\lambda}) = \frac{1}{K}\sum_{k=1}^{K} q(\mathbf{z}|\mathbf{u}_k),$$

where $\boldsymbol{\lambda} = \{\mathbf{u}_1, \ldots, \mathbf{u}_K\}$ are trainable preudo-inputs.

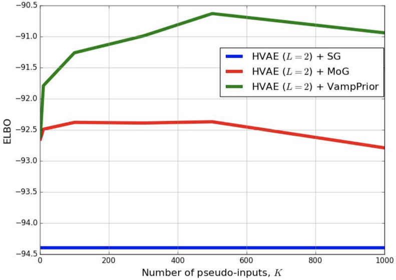
- Multimodal $\Rightarrow$ prevents over-regularization;.
- $K \ll n \Rightarrow$ prevents from potential overfitting $+$ less expensive to train.
- Pseudo-inputs are prior hyperparameters $\Rightarrow$ connection to the Empirical Bayes.

Tomczak J. M., Welling M. VAE with a VampPrior, 2017

VampPrior

- Do we equally need the multimodal prior?
- Is it beneficial to couple the prior with the variational posterior or MoG is enough?

Model	LL
VAE $(L=1)$ + NF [32]	-85.10
VAE $(L=2)$ [6]	-87.86
IWAE $(L=2)$ [6]	-85.32
HVAE $(L=2)$ + SG	-85.89
HVAE $(L=2)$ + MoG	-85.07
HVAE $(L=2)$ + VampPrior *data*	-85.71
HVAE $(L=2)$ + VampPrior	$\mathbf{-83.19}$
AVB + AC $(L=1)$ [28]	-80.20
VLAE [7]	$\mathbf{-79.03}$
VAE + IAF [18]	-79.88
convHVAE $(L=2)$ + VampPrior	-81.09
PixelHVAE $(L=2)$ + VampPrior	-79.78

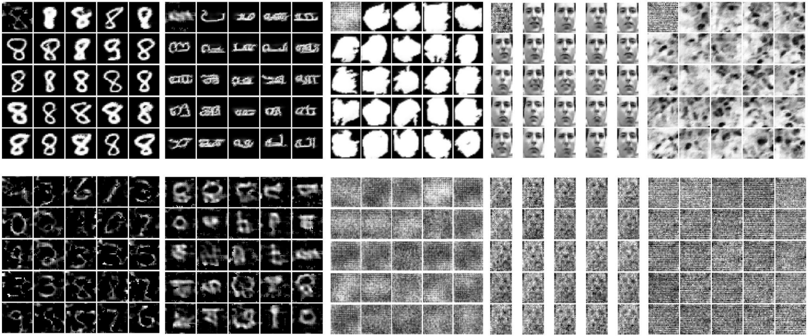


Tomczak J. M., Welling M. VAE with a VampPrior, 2017

VampPrior

Top row: gennerateddd images by PixelHVAE + VampPrior for chosen pseudo-input in the left top corner.

Bottom row: pseudo-inputs for different datasets.



MNIST Omniglot Caltech 101 Silhouettes Frey Faces Histopathology

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Tomczak J. M., Welling M. VAE with a VampPrior, 2017

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

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

Posterior collapse: toy example

Let define latent variable model in the following way:

$$p(\mathbf{x}|\boldsymbol{\theta}) = \int p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta}) d\mathbf{z} = \int p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) p(\mathbf{z}) d\mathbf{z}$$

- prior distribution $p(\mathbf{z}) = \mathcal{N}(\mathbf{z}|0, \mathbf{I})$;
- probabilistic model $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{z}), \boldsymbol{\sigma}_{\boldsymbol{\theta}}(\mathbf{z}))$ (diagonal covariance);
- variational posterior $q(\mathbf{z}|\mathbf{x}, \phi) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_{\boldsymbol{\phi}}(\mathbf{x}), \boldsymbol{\sigma}_{\phi}(\mathbf{x}))$ (diagonal covariance).

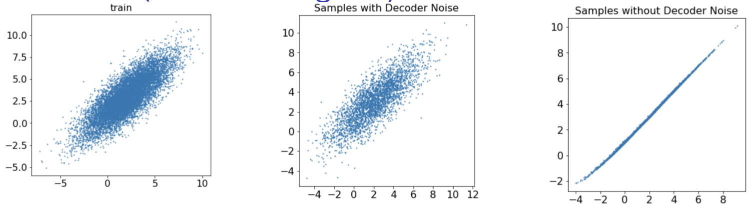
Let data distribution is $\pi(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma})$. Possible cases:

- covariance matrix $\boldsymbol{\Sigma}$ is diagonal (univariate case);
- covariance matrix $\boldsymbol{\Sigma}$ is **not** diagonal (multivariate case).

What is the difference?

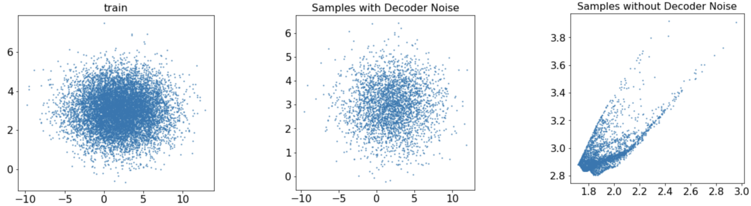
Posterior collapse: toy example

Multivariate ($\mathbf{\Sigma}$ is non-diagonal)



The encoder uses latent variables to model data.

Univariate ($\mathbf{\Sigma}$ is diagonal)



Latent variables are not used, since the decoder could model the data without the encoder.

Posterior collapse

Representation learning

"Identifies and disentangles the underlying causal factors of the data, so that it becomes easier to understand the data, to classify it, or to perform other tasks".

$$p(\mathbf{x}|\boldsymbol{\theta}) = \int p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta}) d\mathbf{z} = \int p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) p(\mathbf{z}) d\mathbf{z}$$

If the decoder model $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})$ is powerful enough to model $p(\mathbf{x}|\boldsymbol{\theta})$ the latent variables $\mathbf{z}$ becames irrelevant.

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

Early in the training the approximate posterior $q(\mathbf{z}|\mathbf{x})$ carries little information about $\mathbf{x}$ and the model sets the posterior to the prior to avoid paying any cost $KL(q(\mathbf{z}|\mathbf{x})||p(\mathbf{z}))$.

PixelVAE

$$p(\mathbf{x}|\boldsymbol{\theta}) = \int p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta}) d\mathbf{z} = \int p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) p(\mathbf{z}) d\mathbf{z}$$

- More powerful $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})$ leads to more powerful generative model $p(\mathbf{x}|\boldsymbol{\theta})$.
- Too powerful $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})$ could lead to posterior collapse, where variational posterior $q(\mathbf{z}|\mathbf{x})$ will not carry any information about data and close to prior $p(\mathbf{z})$.

How to make the generative model $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})$ more powerful?

Autoregressive decoder

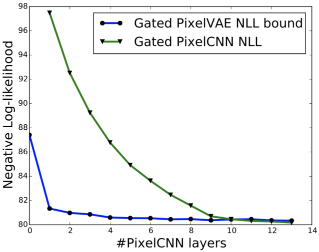
$$p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = \prod_{i=1}^{n} p(x_i|\mathbf{x}_{1:i-1}, \mathbf{z}, \boldsymbol{\theta})$$

Gulrajani I. et al. PixelVAE: A Latent Variable Model for Natural Images, 2016

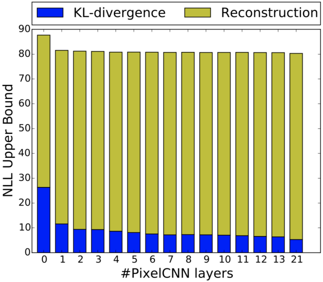
PixelVAE

VAE model with autoregressive PixelCNN decoder with few autoregressive layers.

- Global structure is captured by latent variables.
- Local statistics are captured by limited receptive field autoregressive model.



(a)



(b)

Gulrajani I. et al. PixelVAE: A Latent Variable Model for Natural Images, 2016

PixelVAE

MNIST

Model	NLL Test
DRAW (Gregor et al., 2016)	≤ 80.97
Discrete VAE (Rolfe, 2016)	$= 81.01$
IAF VAE (Kingma et al., 2016)	≈ 79.88
PixelCNN (van den Oord et al., 2016a)	$= 81.30$
PixelRNN (van den Oord et al., 2016a)	$= 79.20$
Convolutional VAE	≤ 87.41
PixelVAE	≤ 80.64
Gated PixelCNN (our implementation)	$= 80.10$
Gated PixelVAE	≈ 79.48 (≤ 80.02)
Gated PixelVAE without upsampling	$\approx$ **79.02** (≤ 79.66)

ImageNet 64x64

Model	NLL Validation (Train)
Convolutional DRAW (Gregor et al., 2016)	≤ 4.10 (4.04)
Real NVP (Dinh et al., 2016)	$= 4.01$ (3.93)
PixelRNN (van den Oord et al., 2016a)	$= 3.63$ (3.57)
Gated PixelCNN (van den Oord et al., 2016b)	$=$ **3.57** (3.48)
Hierarchical PixelVAE	≤ 3.66 (3.59)

Gulrajani I. et al. PixelVAE: A Latent Variable Model for Natural Images, 2016

Decoder weakening

$$p(\mathbf{x}|\boldsymbol{\theta}) = \int p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta}) d\mathbf{z} = \int p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) p(\mathbf{z}) d\mathbf{z}$$

Powerful decoder $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})$ makes the model expressive, but posterior collapse is possible.
PixelVAE model uses the autoregressive PixelCNN model with small number of layers to limit receptive field.
How to force the model encode information about $\mathbf{x}$ into $\mathbf{z}$?

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

What we get if $\beta = 1$ ($\beta = 0$)?

KL annealing

- Start training with $\beta = 0$.
- Increase it until $\beta = 1$ during training process.

Bowman S. R. et al. Generating Sentences from a Continuous Space, 2015

Decoder weakening

Free bits

- Divide the latent dimensions into the K subsets.
- Ensure the use of less than λ nats of information per subset j.

$$\hat{\mathcal{L}}(q, \boldsymbol{\theta}) = \mathbb{E}_{q(\mathbf{Z}|\mathbf{X})} \log p(\mathbf{X}|\mathbf{Z}, \boldsymbol{\theta}) - \sum_{j=1}^{K} \max(\lambda, KL(q(\mathbf{Z}_j|\mathbf{X})||p(\mathbf{Z}_j))).$$

Increasing the latent information is advantageous for the reconstruction term.

This results in $KL(q(\mathbf{Z}_j|\mathbf{x})||p(\mathbf{Z}_j)) \geq \lambda$ for all j, in practice.

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

Variational Lossy AutoEncoder, 2016

Lossy code via explicit information placement

$$p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = \prod_{i=1}^{m} p(x_i|\mathbf{z}, \mathbf{x}_{\text{WindowAround}(i)}, \boldsymbol{\theta}).$$

- WindowAround(i) restricts the receptive field (it forbids to represent arbitrarily complex distribution over $\mathbf{x}$ without dependence on $\mathbf{z}$).
- Local statistics of 2D images (texture) will be modeled by a small local window.
- Global structural information (shapes) is long-range dependency that can only be communicated through latent code $\mathbf{z}$.

Chen X. et al. Variational Lossy Autoencoder, 2016

Variational Lossy AutoEncoder, 2016

ELBO revisiting

$$\mathcal{L}(q, \boldsymbol{\theta}) = \underbrace{\frac{1}{n}\sum_{i=1}^{n} \mathbb{E}_{q(\mathbf{z}_i|\mathbf{x}_i)} \log p(\mathbf{x}_i|\mathbf{z}_i, \boldsymbol{\theta})}_{\text{Reconstruction loss}} - \underbrace{\left(\log n - \mathbb{E}_{q(\mathbf{z})}\mathbb{H}\left[q(i|\mathbf{z})\right]\right)}_{0 \leq \text{Mutual info} \leq \log N} - \underbrace{KL(q(\mathbf{z})||p(\mathbf{z}))}_{\text{Marginal KL}}$$

VampPrior

$$p(\mathbf{z}|\boldsymbol{\lambda}) = \frac{1}{K}\sum_{k=1}^{K} q(\mathbf{z}|\mathbf{u}_k),$$

where $\mathbf{u}_1, \dots \mathbf{u}_K$ is trainable preudo-inputs.

Autoregressive flow prior

$$\log p(\mathbf{z}|\boldsymbol{\lambda}) = \log p(\boldsymbol{\epsilon}) + \log \det \left|\frac{d\boldsymbol{\epsilon}}{d\mathbf{z}}\right|$$

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

Chen X. et al. Variational Lossy Autoencoder, 2016

Variational Lossy AutoEncoder, 2016

Theorem

VAE with the AF prior for latent code $\mathbf{z}$ is equivalent to using the IAF posterior for latent code $\boldsymbol{\epsilon}$.

Proof

$$\begin{aligned}
\mathcal{L}(q, \boldsymbol{\theta}) &= \mathbb{E}_{q(\mathbf{z}|\mathbf{x})} \left[\log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) + \log p(\mathbf{z}, \boldsymbol{\lambda}) - q(\mathbf{z}|\mathbf{x})\right] \\
&= \mathbb{E}_{\mathbf{z}\sim q(\mathbf{z}|\mathbf{x})} \Bigg[\log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) + \underbrace{\left(\log p(f(\mathbf{z}, \boldsymbol{\lambda})) + \log \left|\det \frac{\partial f(\mathbf{z}, \boldsymbol{\lambda})}{\partial \mathbf{z}}\right|\right)}_{\text{AF prior}} - q(\mathbf{z}|\mathbf{x})\Bigg] \\
&= \mathbb{E}_{\mathbf{z}\sim q(\mathbf{z}|\mathbf{x})} \Bigg[\log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) + \log p(f(\mathbf{z}, \boldsymbol{\lambda})) - \underbrace{\left(q(\mathbf{z}|\mathbf{x}) - \log \left|\det \frac{\partial f(\mathbf{z}, \boldsymbol{\lambda})}{\partial \mathbf{z}}\right|\right)}_{\text{IAF posterior}}\Bigg]
\end{aligned}$$

Chen X. et al. Variational Lossy Autoencoder, 2016

Variational Lossy AutoEncoder, 2016

Autoregressive flow prior

$$\mathcal{L}(q, \boldsymbol{\theta}) = \mathbb{E}_{\mathbf{z} \sim q(\mathbf{z}|\mathbf{x})} \left[\log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) + \underbrace{\left(\log p(f(\mathbf{z}, \boldsymbol{\lambda})) + \log \left| \det \frac{\partial f(\mathbf{z}, \boldsymbol{\lambda})}{\partial \mathbf{z}} \right| \right)}_{\text{AF prior}} - q(\mathbf{z}|\mathbf{x}) \right]$$

$$= \mathbb{E}_{\mathbf{z} \sim q(\mathbf{z}|\mathbf{x})} \left[\log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) + \log p(f(\mathbf{z}, \boldsymbol{\lambda})) - \underbrace{\left(q(\mathbf{z}|\mathbf{x}) - \log \left| \det \frac{\partial f(\mathbf{z}, \boldsymbol{\lambda})}{\partial \mathbf{z}} \right| \right)}_{\text{IAF posterior}} \right]$$

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

The AF prior and the IAF posterior have the same computation cost, so using the AF prior makes the model more expressive at no training time cost.

Chen X. et al. Variational Lossy Autoencoder, 2016

Variational Lossy AutoEncoder, 2016

- Can VLAE learn lossy codes that encode global statistics?
- Does using AF priors improves upon using IAF posteriors as predicted by theory?
- Does using autoregressive decoding distributions improve density estimation performance?

MNIST

Model	**NLL Test**
Normalizing flows (Rezende & Mohamed, 2015)	85.10
DRAW (Gregor et al., 2015)	< 80.97
Discrete VAE (Rolfe, 2016)	81.01
PixelRNN (van den Oord et al., 2016a)	79.20
IAF VAE (Kingma et al., 2016)	79.88
AF VAE	79.30
VLAE	**79.03**

CIFAR10

Method	bits/dim $\leq$
Results with tractable likelihood models:	
Uniform distribution [1]	8.00
Multivariate Gaussian [1]	4.70
NICE [2]	4.48
Deep GMMs [3]	4.00
Real NVP [4]	3.49
PixelCNN [1]	3.14
Gated PixelCNN [5]	3.03
PixelRNN [1]	3.00
PixelCNN++ [6]	**2.92**
Results with variationally trained latent-variable models:	
Deep Diffusion [7]	5.40
Convolutional DRAW [8]	3.58
ResNet VAE with IAF [9]	3.11
ResNet VLAE	3.04
DenseNet VLAE	**2.95**

Chen X. et al. Variational Lossy Autoencoder, 2016

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

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

Importance Sampling

Generative model

$$
\begin{aligned}
p(\mathbf{x}|\boldsymbol{\theta}) &= \int p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta}) d\mathbf{z} = \int \left[\frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z}|\mathbf{x})} \right] q(\mathbf{z}|\mathbf{x}) d\mathbf{z} \\
&= \int f(\mathbf{x}, \mathbf{z}) q(\mathbf{z}|\mathbf{x}) d\mathbf{z} = \mathbb{E}_{\mathbf{z} \sim q(\mathbf{z}|\mathbf{x})} f(\mathbf{x}, \mathbf{z})
\end{aligned}
$$

Here $f(\mathbf{x}, \mathbf{z}) = \frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z}|\mathbf{x})}$.

ELBO

$$
\begin{aligned}
\log p(\mathbf{x}|\boldsymbol{\theta}) = \log \mathbb{E}_{\mathbf{z} \sim q(\mathbf{z}|\mathbf{x})} f(\mathbf{x}, \mathbf{z}) \geq \mathbb{E}_{\mathbf{z} \sim q(\mathbf{z}|\mathbf{x})} \log f(\mathbf{x}, \mathbf{z}) = \\
= \mathbb{E}_{\mathbf{z} \sim q(\mathbf{z}|\mathbf{x})} \log \frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z}|\mathbf{x})} = \mathcal{L}(q, \boldsymbol{\theta}).
\end{aligned}
$$

Could we choose better $f(\mathbf{x}, \mathbf{z})$?

IWAE

Let define

$$f(\mathbf{x}, \mathbf{z}_1, \dots, \mathbf{z}_K) = \frac{1}{K} \sum_{k=1}^{K} \frac{p(\mathbf{x}, \mathbf{z}_k | \boldsymbol{\theta})}{q(\mathbf{z}_k | \mathbf{x})}$$

$$\mathbb{E}_{\mathbf{z}_1, \dots, \mathbf{z}_K \sim q(\mathbf{z}|\mathbf{x})} f(\mathbf{x}, \mathbf{z}_1, \dots, \mathbf{z}_K) = p(\mathbf{x}|\boldsymbol{\theta})$$

ELBO

$$\begin{aligned}
\log p(\mathbf{x}|\boldsymbol{\theta}) = \log \mathbb{E}_{\mathbf{z}_1, \dots, \mathbf{z}_K \sim q(\mathbf{z}|\mathbf{x})} f(\mathbf{x}, \mathbf{z}, \dots, \mathbf{z}_K) \geq \\
\geq \mathbb{E}_{\mathbf{z}_1, \dots, \mathbf{z}_K \sim q(\mathbf{z}|\mathbf{x})} \log f(\mathbf{x}, \mathbf{z}, \dots, \mathbf{z}_K) = \\
= \mathbb{E}_{\mathbf{z}_1, \dots, \mathbf{z}_K \sim q(\mathbf{z}|\mathbf{x})} \log \left[\frac{1}{K} \sum_{k=1}^{K} \frac{p(\mathbf{x}, \mathbf{z}_k | \boldsymbol{\theta})}{q(\mathbf{z}_k | \mathbf{x})} \right] = \mathcal{L}_K(q, \boldsymbol{\theta}).
\end{aligned}$$

Burda Y., Grosse R., Salakhutdinov R. Importance Weighted Autoencoders, 2015

IWAE

VAE objective

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

$$\mathcal{L}(q, \boldsymbol{\theta}) = \mathbb{E}_{\mathbf{z}_1, \dots, \mathbf{z}_K \sim q(\mathbf{z}|\mathbf{x})} \left(\frac{1}{K} \sum_{k=1}^{K} \log \frac{p(\mathbf{x}, \mathbf{z}_k|\boldsymbol{\theta})}{q(\mathbf{z}_k|\mathbf{x})} \right) \rightarrow \max_{q, \boldsymbol{\theta}}.$$

IWAE objective

$$\mathcal{L}_K(q, \boldsymbol{\theta}) = \mathbb{E}_{\mathbf{z}_1, \dots, \mathbf{z}_K \sim q(\mathbf{z}|\mathbf{x})} \log \left(\frac{1}{K} \sum_{k=1}^{K} \frac{p(\mathbf{x}, \mathbf{z}_k|\boldsymbol{\theta})}{q(\mathbf{z}_k|\mathbf{x})} \right) \rightarrow \max_{q, \boldsymbol{\theta}}.$$

If $K = 1$, these objectives coincide.

Burda Y., Grosse R., Salakhutdinov R. Importance Weighted Autoencoders, 2015

IWAE

Theorem

1. $\log p(\mathbf{x}|\boldsymbol{\theta}) \geq \mathcal{L}_K(q, \boldsymbol{\theta}) \geq \mathcal{L}_M(q, \boldsymbol{\theta}), \quad \text{for } K \geq M;$
2. $\log p(\mathbf{x}|\boldsymbol{\theta}) = \lim_{K \to \infty} \mathcal{L}_K(q, \boldsymbol{\theta})$ if $\frac{p(\mathbf{x},\mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z}|\mathbf{x})}$ is bounded.

Proof of 1.

$$
\begin{aligned}
\mathcal{L}_K(q, \boldsymbol{\theta}) &= \mathbb{E}_{\mathbf{z}_1, \dots, \mathbf{z}_K} \log \left(\frac{1}{K} \sum_{k=1}^{K} \frac{p(\mathbf{x}, \mathbf{z}_k|\boldsymbol{\theta})}{q(\mathbf{z}_k|\mathbf{x})} \right) = \\
&= \mathbb{E}_{\mathbf{z}_1, \dots, \mathbf{z}_K} \log \mathbb{E}_{k_1, \dots, k_M} \left(\frac{1}{M} \sum_{m=1}^{M} \frac{p(\mathbf{x}, \mathbf{z}_{k_m}|\boldsymbol{\theta})}{q(\mathbf{z}_{k_m}|\mathbf{x})} \right) \geq \\
&\geq \mathbb{E}_{\mathbf{z}_1, \dots, \mathbf{z}_K} \mathbb{E}_{k_1, \dots, k_m} \log \left(\frac{1}{M} \sum_{m=1}^{M} \frac{p(\mathbf{x}, \mathbf{z}_{k_m}|\boldsymbol{\theta})}{q(\mathbf{z}_{k_m}|\mathbf{x})} \right) = \\
&= \mathbb{E}_{\mathbf{z}_1, \dots, \mathbf{z}_M} \log \left(\frac{1}{M} \sum_{m=1}^{M} \frac{p(\mathbf{x}, \mathbf{z}_m|\boldsymbol{\theta})}{q(\mathbf{z}_m|\mathbf{x})} \right) = \mathcal{L}_M(q, \boldsymbol{\theta})
\end{aligned}
$$

Burda Y., Grosse R., Salakhutdinov R. Importance Weighted Autoencoders, 2015

IWAE

Theorem

1. $\log p(\mathbf{x}|\boldsymbol{\theta}) \geq \mathcal{L}_K(q, \boldsymbol{\theta}) \geq \mathcal{L}_M(q, \boldsymbol{\theta}), \quad \text{for} K \geq M;$
2. $\log p(\mathbf{x}|\boldsymbol{\theta}) = \lim_{K \to \infty} \mathcal{L}_K(q, \boldsymbol{\theta})$ if $\frac{p(\mathbf{x},\mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z}|\mathbf{x})}$ is bounded.

Proof of 2.

Consider r.v. $\xi_K = \frac{1}{K} \sum_{k=1}^{K} \frac{p(\mathbf{x},\mathbf{z}_k|\boldsymbol{\theta})}{q(\mathbf{z}_k|\mathbf{x})}$.

If summands are bounded, then (from the strong law of large numbers)

$$\xi_K \xrightarrow[K \to \infty]{a.s.} \mathbb{E}_{q(\mathbf{z}|\mathbf{x})} \frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z}|\mathbf{x})} = p(\mathbf{x}|\boldsymbol{\theta}).$$

Hence $\mathcal{L}_K(q, \boldsymbol{\theta}) = \mathbb{E} \log \xi_K$ converges to $\log p(\mathbf{x}|\boldsymbol{\theta})$ as $K \to \infty$.

Burda Y., Grosse R., Salakhutdinov R. Importance Weighted Autoencoders, 2015

IWAE

$$\log p(\mathbf{x}|\boldsymbol{\theta}) \geq \mathcal{L}_K(q, \boldsymbol{\theta}) \geq \mathcal{L}(q, \boldsymbol{\theta})$$

If $K > 1$ the bound could be tighter.

$$\mathcal{L}(q, \boldsymbol{\theta}) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x})} \log \frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z}|\mathbf{x})};$$

$$\mathcal{L}_K(q, \boldsymbol{\theta}) = \mathbb{E}_{\mathbf{z}_1, \dots, \mathbf{z}_K \sim q(\mathbf{z}|\mathbf{x})} \log \left(\frac{1}{K} \sum_{k=1}^{K} \frac{p(\mathbf{x}, \mathbf{z}_k|\boldsymbol{\theta})}{q(\mathbf{z}_k|\mathbf{x})} \right).$$

- $\mathcal{L}_1(q, \boldsymbol{\theta}) = \mathcal{L}(q, \boldsymbol{\theta})$;
- $\mathcal{L}_\infty(q, \boldsymbol{\theta}) = \log p(\mathbf{x}|\boldsymbol{\theta})$.

Which $q(\mathbf{z}|\mathbf{x})$ gives $\mathcal{L}(q, \boldsymbol{\theta}) = \log p(\mathbf{x}|\boldsymbol{\theta})$?

Which $q(\mathbf{z}|\mathbf{x})$ gives $\mathcal{L}(q, \boldsymbol{\theta}) = \mathcal{L}_K(q, \boldsymbol{\theta})$?

Burda Y., Grosse R., Salakhutdinov R. Importance Weighted Autoencoders, 2015

IWAE

Theorem

The VAE objective is equal to IWAE objective

$$\mathcal{L}(q_{EW}, \boldsymbol{\theta}) = \mathcal{L}_K(q, \boldsymbol{\theta})$$

for the following variational distribution

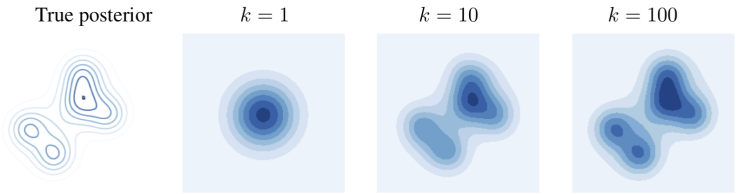
$$q_{EW}(\mathbf{z}|\mathbf{x}) = \mathbb{E}_{\mathbf{z}_2, \dots, \mathbf{z}_K \sim q(\mathbf{z}|\mathbf{x})} q_{IW}(\mathbf{z}|\mathbf{x}, \mathbf{z}_{2:K}),$$

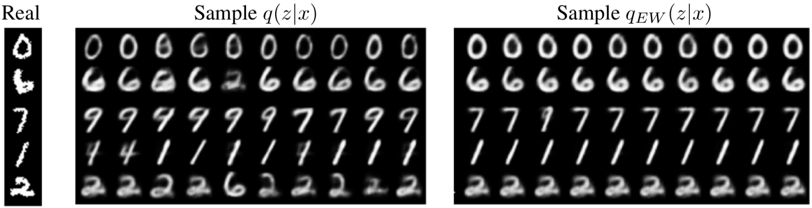
where

$$q_{IW}(\mathbf{z}|\mathbf{x}, \mathbf{z}_{2:K}) = \frac{\frac{p(\mathbf{x},\mathbf{z})}{q(\mathbf{z}|\mathbf{x})}}{\frac{1}{K}\sum_{k=1}^{K}\frac{p(\mathbf{x},\mathbf{z}_k)}{q(\mathbf{z}_k|\mathbf{x})}} q(\mathbf{z}|\mathbf{x}) = \frac{p(\mathbf{x}, \mathbf{z})}{\frac{1}{K}\left(\frac{p(\mathbf{x},\mathbf{z})}{q(\mathbf{z}|\mathbf{x})} + \sum_{k=2}^{K}\frac{p(\mathbf{x},\mathbf{z}_k)}{q(\mathbf{z}_k|\mathbf{x})}\right)}.$$

Cremer C., Morris Q., Duvenaud D. Reinterpreting Importance-Weighted Autoencoders, 2017, 2017

IWAE





Cremer C., Morris Q., Duvenaud D. Reinterpreting Importance-Weighted Autoencoders, 2017, 2017

Summary

- Uniform dequantization is the simplest form of dequantization. Variational dequantization is a more natural type that was proposed in Flow++ model.
- The ELBO surgery reveals insights about a prior distribution in VAE. The optimal prior is the aggregated posterior.
- VampPrior proposes to use a variational mixture of posteriors as the prior to approximate the aggregated posterior.
- More powerful decoder in VAE leads to more expressive generative model. However, too expressive decoder could lead to the posterior collapse.
- The decoder weakening is a set of techniques to avoid the posterior collapse.
- The autoregressive flows could be used as the prior. This is equivalent to the use of the IAF posterior.
- The importance sampling could get the tighter lower bound to the likelihood.

IWAE

$$\frac{a_1 + \cdots + a_K}{K} = \mathbb{E}_{i_1,\ldots,i_M} \frac{a_{i_1} + \cdots + a_{i_M}}{M}, \quad i_1, \ldots, i_M \sim U[1, K]$$