Deep Generative Models
Lecture 5

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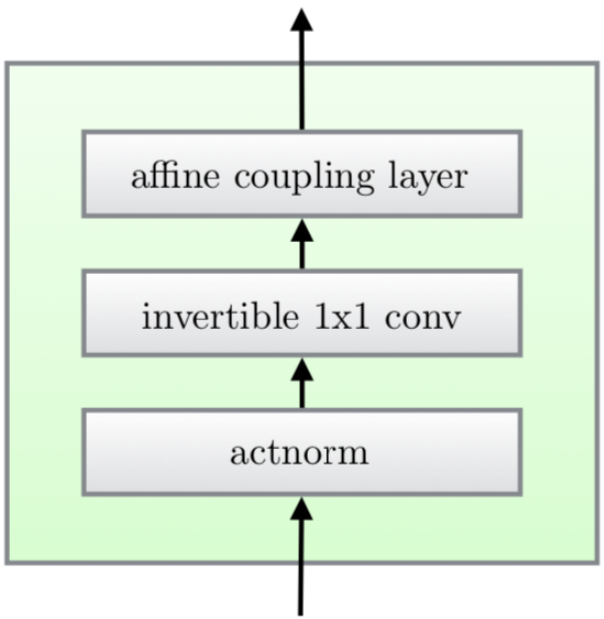
2020

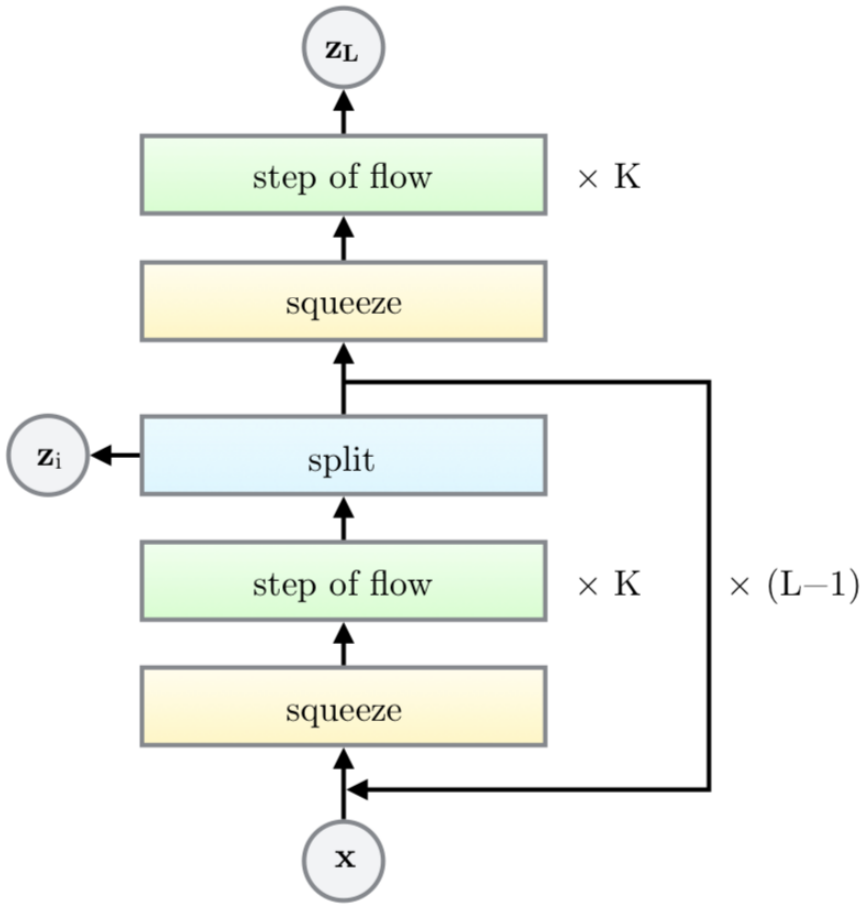
Glow, 2018

https://arxiv.org/pdf/1807.03039.pdf

Glow, 2018

Model architecture





https://arxiv.org/pdf/1807.03039.pdf

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NICE

$$\begin{cases} \mathbf{z}_1 = \mathbf{x}_1; \\ \mathbf{z}_2 = \mathbf{x}_2 + \mathcal{F}(\mathbf{x}_1, \theta); \end{cases} \Leftrightarrow \begin{cases} \mathbf{x}_1 = \mathbf{z}_1; \\ \mathbf{x}_2 = \mathbf{z}_2 - \mathcal{F}(\mathbf{z}_1, \theta). \end{cases}$$

First step is a **split** operator which decouples variable into 2 subparts (usualy channel-wise). The order of decoupling should be manually changed between layers.
Could we use more general operator?
Let use rotation matrix via 1x1 invertible convolution.
$\mathbf{W} \in \mathbb{R}^{c \times c}$ - kernel of 1x1 convolution with c input and output channels.
The cost of computing or differentiating $\det(\mathbf{W})$ is $O(c^3)$.

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https://arxiv.org/pdf/1807.03039.pdf

Glow, 2018

Description	Function	Reverse Function	Log-determinant
Actnorm. See Section 3.1.	$\forall i,j : \mathbf{y}_{i,j} = \mathbf{s} \odot \mathbf{x}_{i,j} + \mathbf{b}$	$\forall i,j : \mathbf{x}_{i,j} = (\mathbf{y}_{i,j} - \mathbf{b})/\mathbf{s}$	$h \cdot w \cdot \texttt{sum}(\log \lvert\mathbf{s}\rvert)$
Invertible 1×1 convolution. $\mathbf{W} : [c \times c]$. See Section 3.2.	$\forall i,j : \mathbf{y}_{i,j} = \mathbf{W}\mathbf{x}_{i,j}$	$\forall i,j : \mathbf{x}_{i,j} = \mathbf{W}^{-1}\mathbf{y}_{i,j}$	$h \cdot w \cdot \log \lvert\det(\mathbf{W})\rvert$ or $h \cdot w \cdot \texttt{sum}(\log \lvert\mathbf{s}\rvert)$ (see eq. (10))
Affine coupling layer. See Section 3.3 and (Dinh et al., 2014)	$\mathbf{x}_a, \mathbf{x}_b = \texttt{split}(\mathbf{x})$ $(\log \mathbf{s}, \mathbf{t}) = \texttt{NN}(\mathbf{x}_b)$ $\mathbf{s} = \exp(\log \mathbf{s})$ $\mathbf{y}_a = \mathbf{s} \odot \mathbf{x}_a + \mathbf{t}$ $\mathbf{y}_b = \mathbf{x}_b$ $\mathbf{y} = \texttt{concat}(\mathbf{y}_a, \mathbf{y}_b)$	$\mathbf{y}_a, \mathbf{y}_b = \texttt{split}(\mathbf{y})$ $(\log \mathbf{s}, \mathbf{t}) = \texttt{NN}(\mathbf{y}_b)$ $\mathbf{s} = \exp(\log \mathbf{s})$ $\mathbf{x}_a = (\mathbf{y}_a - \mathbf{t})/\mathbf{s}$ $\mathbf{x}_b = \mathbf{y}_b$ $\mathbf{x} = \texttt{concat}(\mathbf{x}_a, \mathbf{x}_b)$	$\texttt{sum}(\log(\lvert\mathbf{s}\rvert))$

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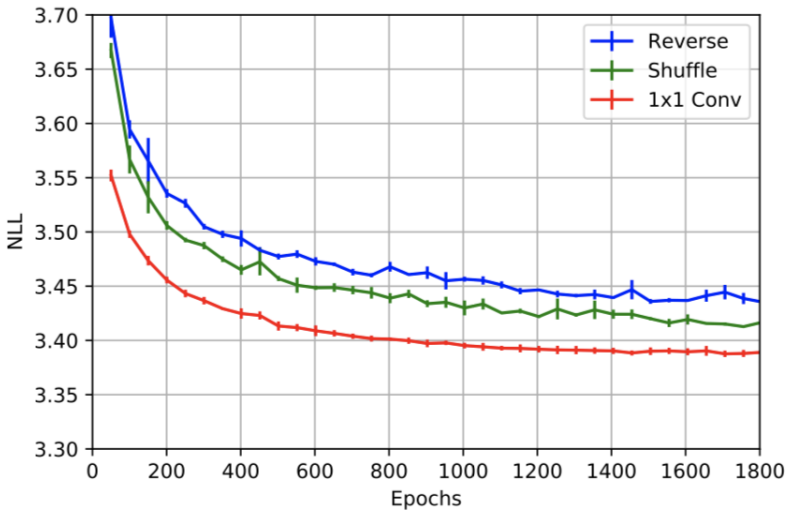
Invertible 1x1 conv

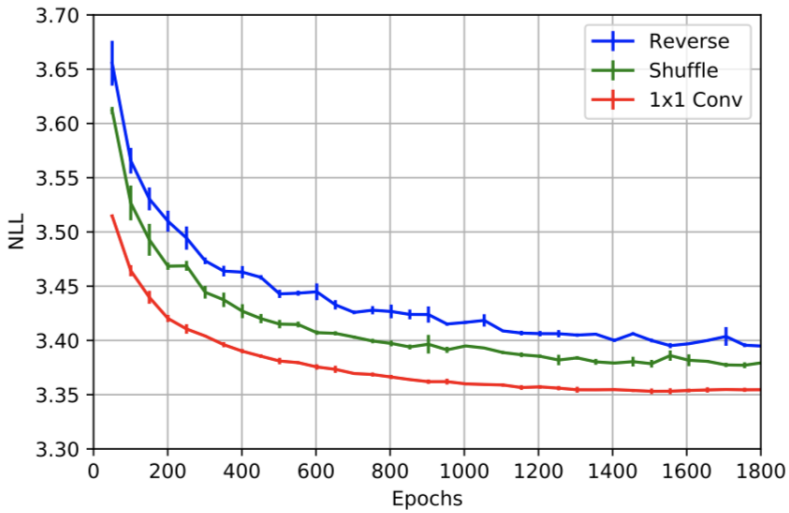
Cost to compute $\det(\mathbf{W})$ is $O(c^3)$. LU-decomposition reduces the cost to $O(c)$:

$$\mathbf{W} = \mathbf{PL}(\mathbf{U} + \text{diag}(\mathbf{s})),$$

where $\mathbf{P}$ is a permutation matrix, $\mathbf{L}$ is a lower triangular matrix with ones on the diagonal, $\mathbf{U}$ is an upper triangular matrix with zeros on the diagonal, and $\mathbf{s}$ is a vector.



(a) Additive coupling.



(b) Affine coupling.

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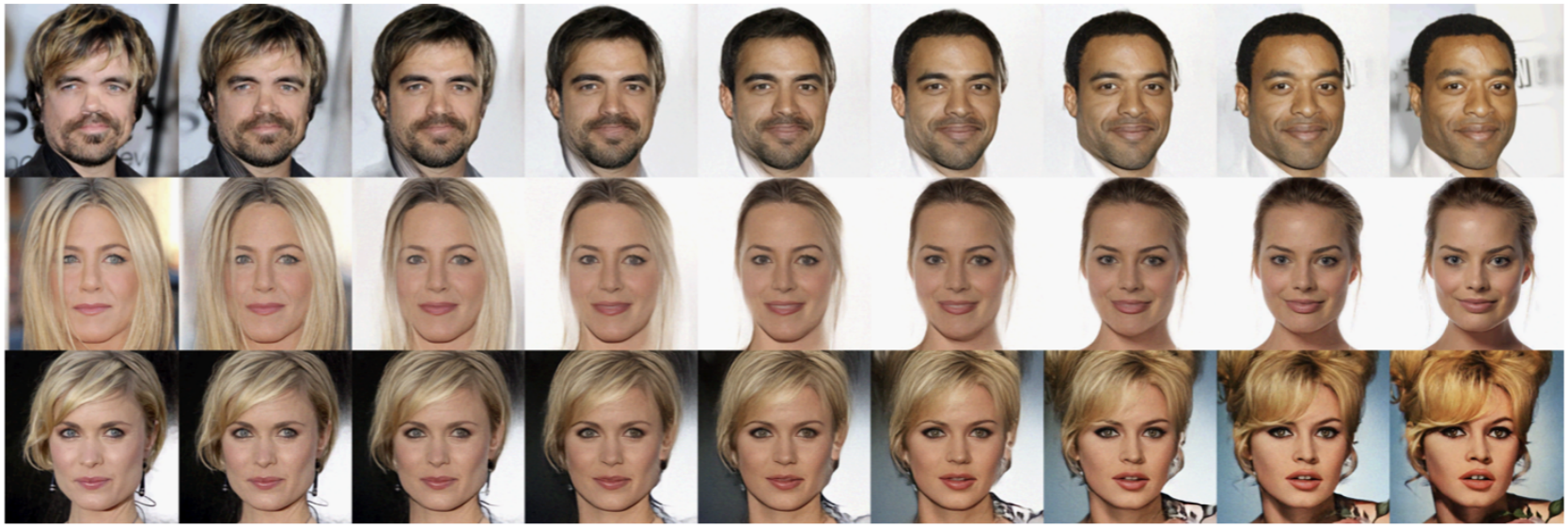
Face interpolation



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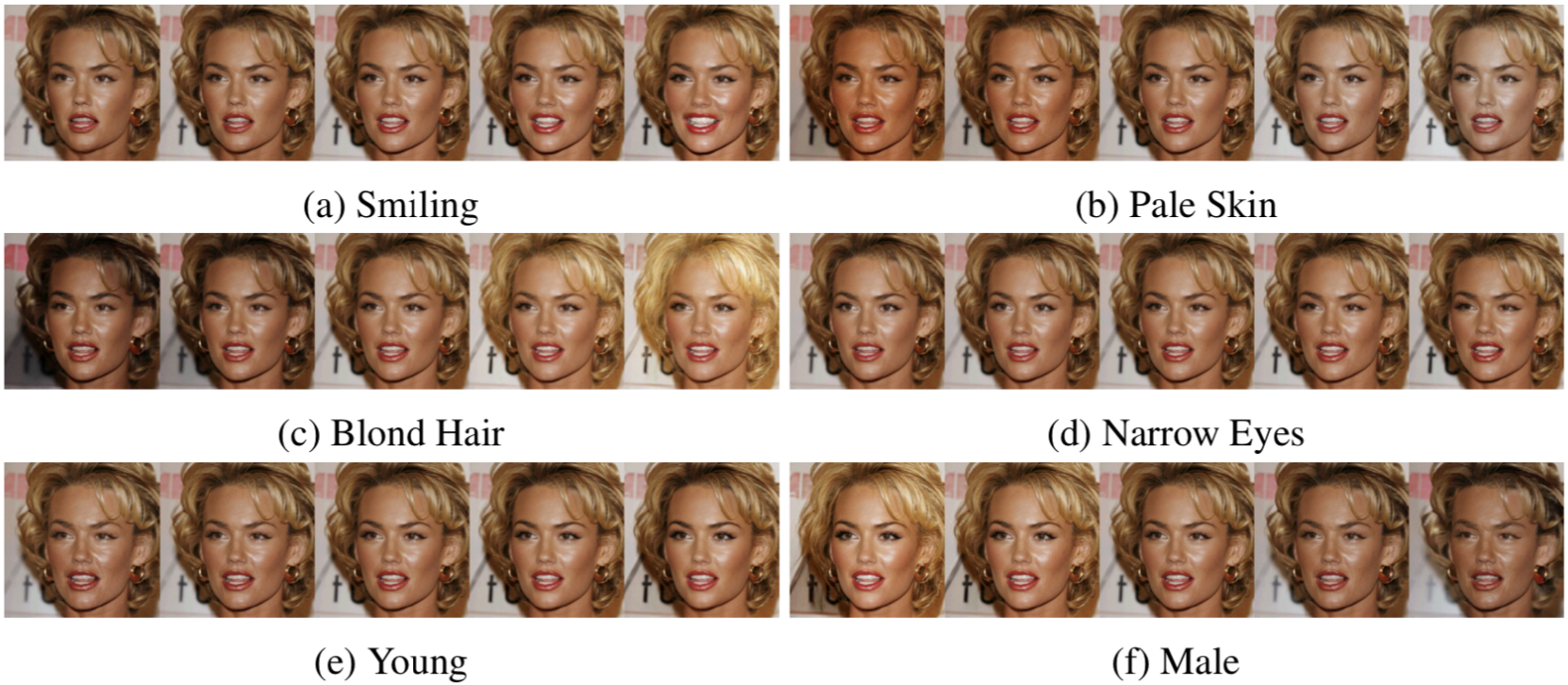
Glow, 2018

Face attributes manipulation



(a) Smiling (b) Pale Skin

(c) Blond Hair (d) Narrow Eyes

(e) Young (f) Male

https://arxiv.org/pdf/1807.03039.pdf

Summary

- Flows are generative models with tractable likelihood and latent representation.
- Flows transform simple distributions to the complex one via sequence of invertible transformations.
- The goal is to achieve tractable Jacobian for efficient learning and density estimation.

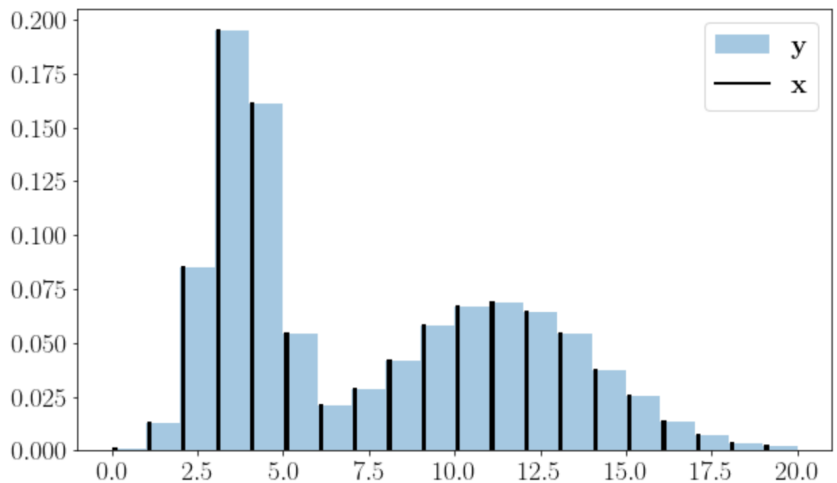
Dequantization

- Images are discrete data (pixels lies in the [0, 255] integer domain).
- Flow is a continuous model.

Fitting a continuous density model to discrete data, produces a degenerate solution with all probability mass on discrete values. How to convert discrete data distribution to the continuous one?

Uniform dequantization

$$\mathbf{y} = \mathbf{x} + \mathbf{u}, \quad \mathbf{u} \sim U[0, 1]$$



Uniform dequantization

Statement

Fitting continious 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 the log-likelihood for a discrete model:

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

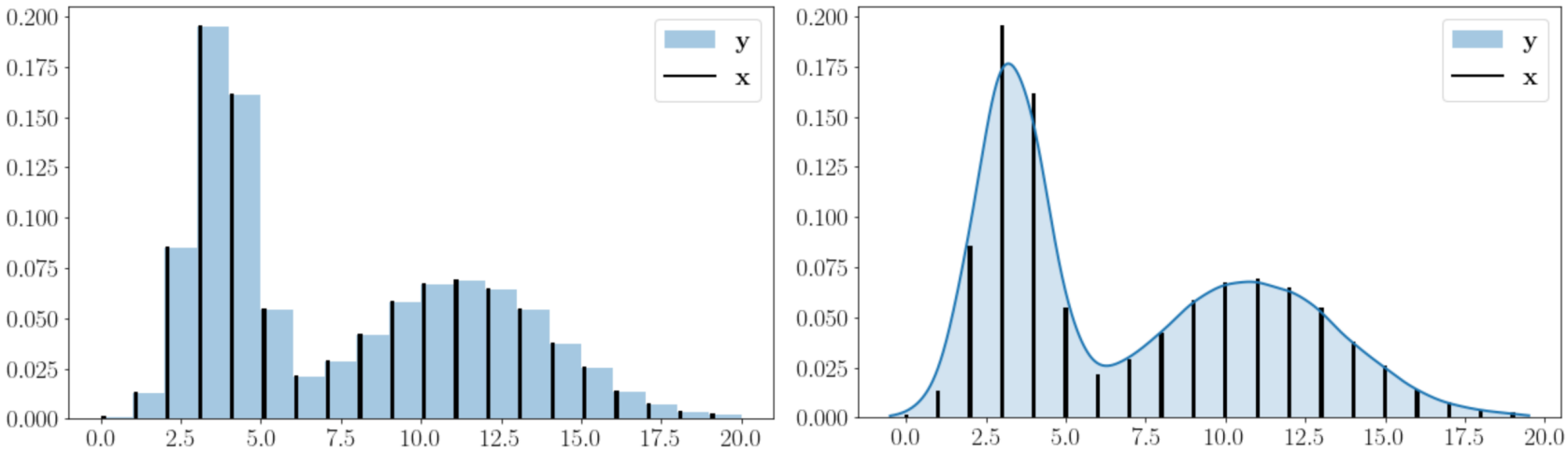
Thus, maximizing the log-likelihood of the continuous model on $\mathbf{y}$ cannot lead to the collapsing onto the discrete data (objective is bounded above by the log-likelihood of a discrete model).

Proof

$$\log p(\mathbf{Y}|\boldsymbol{\theta}) = \sum_{i=1}^{n} \log p(\mathbf{y}_i|\boldsymbol{\theta}) = \sum_{i=1}^{n} \int_{U[0,1]} \log p(\mathbf{x}_i + \mathbf{u}|\boldsymbol{\theta}) d\mathbf{u}$$

$$\leq \sum_{i=1}^{n} \log \int_{U[0,1]} p(\mathbf{x}_i + \mathbf{u}|\boldsymbol{\theta}) d\mathbf{u} = \sum_{i=1}^{n} \log P(\mathbf{x}_i|\boldsymbol{\theta}).$$

Variational dequantization



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

How to make 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

$$\log P(\mathbf{X}|\boldsymbol{\theta}) = \sum_{i=1}^{n} \log P(\mathbf{x}_i|\boldsymbol{\theta}) = \sum_{i=1}^{n} \left[\log \int q(\mathbf{u}|\mathbf{x}) \frac{p(\mathbf{x}+\mathbf{u}|\boldsymbol{\theta})}{q(\mathbf{u}|\mathbf{x})} d\mathbf{u} \right] \geq$$

$$\geq \sum_{i=1}^{n} \left[\int q(\mathbf{u}|\mathbf{x}) \log \frac{p(\mathbf{x}+\mathbf{u}|\boldsymbol{\theta})}{q(\mathbf{u}|\mathbf{x})} d\mathbf{u} \right] =$$

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

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https://arxiv.org/pdf/1902.00275.pdf

Flow++

Variational lower bound

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

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

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

Then

$$\log P(\mathbf{X}|\theta) \geq \sum_{i=1}^{n} \int \log \left(\frac{p(\mathbf{x} + h(\epsilon))}{p(\epsilon) \cdot \left| \det \frac{\partial h(\epsilon)}{\partial \epsilon} \right|^{-1}} \right) d\epsilon.$$

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https://arxiv.org/pdf/1902.00275.pdf

Flow++

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

If $p(\mathbf{x} + \mathbf{u}|\boldsymbol{\theta})$ is also a flow model, it is straightforward to calculate stochastic gradient of this ELBO.
Note: 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.

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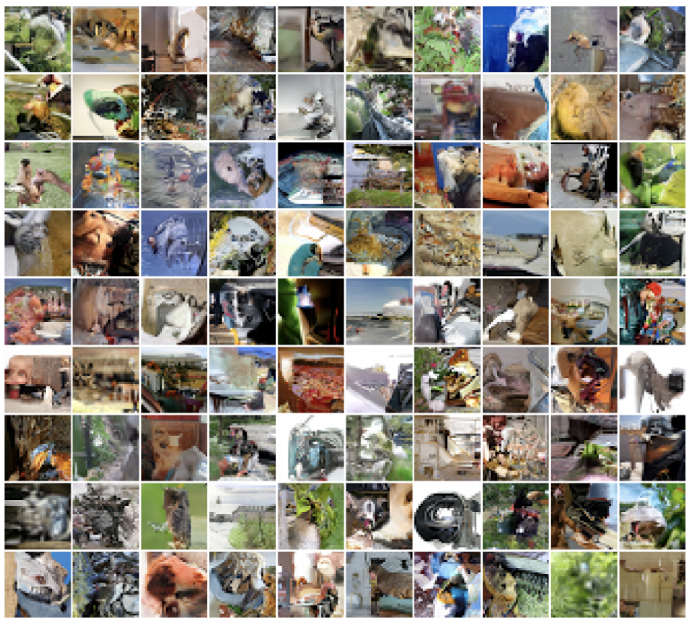
https://arxiv.org/pdf/1902.00275.pdf

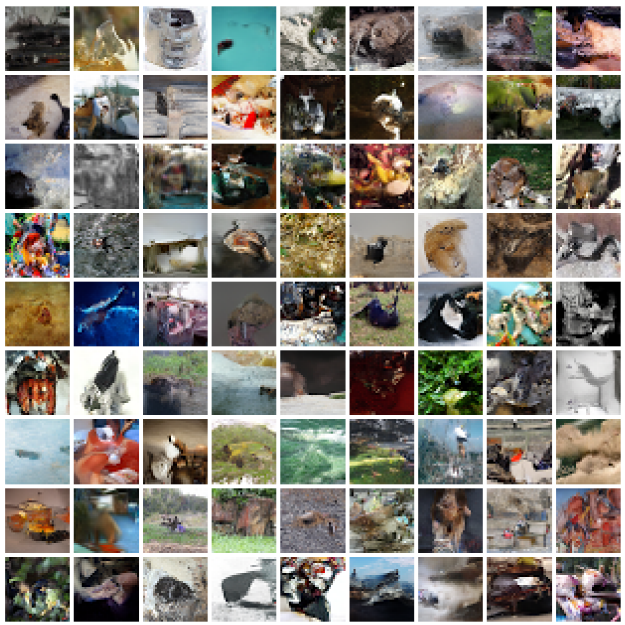
Flow++

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++

https://arxiv.org/pdf/1902.00275.pdf

Likelihood-based models

Exact likelihood evaluation

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

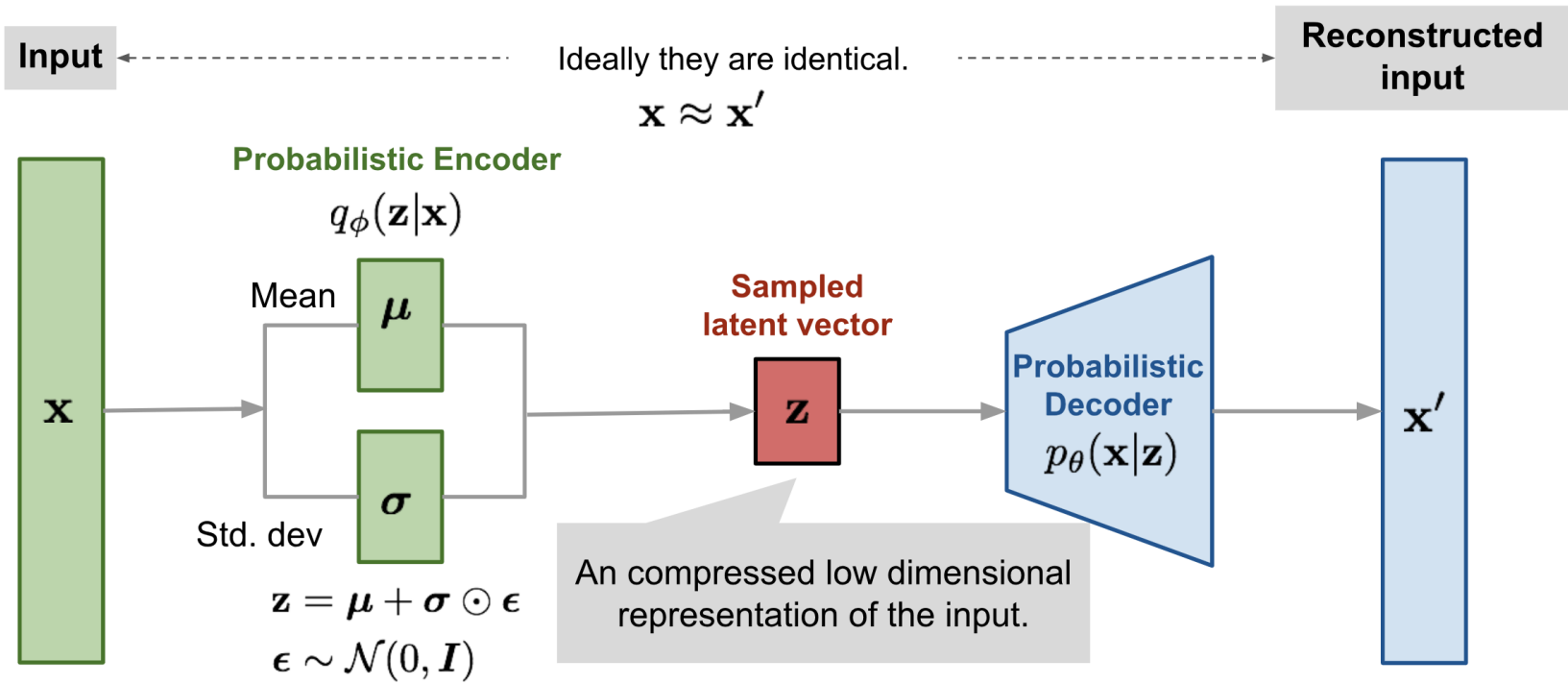
Approximate likelihood evaluation

- Latent variable models (VAE).

What are the pros and cons of each of them?

VAE recap

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



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)

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

- Loose lower bound

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

Variational posterior

We wish $KL(q(\mathbf{z}|\mathbf{x}, \phi)||p(\mathbf{z}|\mathbf{x}, \theta)) = 0$.
(In this case the lower bound is tight $p(\mathbf{x}|\theta) = \mathcal{L}(q, \theta)$).

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 transform simple base distribution to compex one using invertible transformation with simple Jacobian.

How to use flows in VAE?

Flows in VAE

Apply the sequence of transformations to the random variables

$$\mathbf{z}_0 \sim q_0(\mathbf{z}|\mathbf{x}, \phi) = \mathcal{N}(\mathbf{z}|\boldsymbol{\mu}_\phi(\mathbf{x}), \boldsymbol{\sigma}^2_\phi(\mathbf{x})).$$

Here, $q_0(\mathbf{z}|\mathbf{x}, \phi)$ plays the role of a base distribution.

$$\mathbf{z}_0 \xrightarrow{g_1} \mathbf{z}_1 \xrightarrow{g_2} \ldots \xrightarrow{g_K} \mathbf{z}_K.$$

Each g_k is a flow transformation (e.g. planar, radial, coupling layer).

$$\log q_K(\mathbf{z}_K) = \log q_0(\mathbf{z}_0) - \sum_{k=1}^{K} \log \left| \det \left(\frac{\partial g_k(\mathbf{z}_{k-1})}{\partial \mathbf{z}_{k-1}} \right) \right|.$$

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https://arxiv.org/pdf/1505.05770.pdf

Flows in VAE

$$\log q_K(\mathbf{z}_K) = \log q_0(\mathbf{z}_0) - \sum_{k=1}^{K} \log \left| \det \left(\frac{\partial g_k(\mathbf{z}_{k-1})}{\partial \mathbf{z}_{k-1}} \right) \right|.$$

Now the variational posterior is $q_K(\mathbf{z}_K|\mathbf{x}, \phi)$.

$$\begin{aligned}
\mathcal{L}(\phi, \theta) &= \mathbb{E}_{q_K(\mathbf{z}_K|\mathbf{x},\phi)} \log \frac{p(\mathbf{x}, \mathbf{z}_K|\theta)}{q_K(\mathbf{z}_K|\mathbf{x}, \phi)} \\
&= \mathbb{E}_{q_K(\mathbf{z}_K|\mathbf{x},\phi)} \left[\log p(\mathbf{x}, \mathbf{z}_K|\theta) - \log q_K(\mathbf{z}_K|\mathbf{x}, \phi) \right] \\
&= \mathbb{E}_{q_0(\mathbf{z}_0|\mathbf{x},\phi)} \left[\log p(\mathbf{x}, \mathbf{z}_K|\theta) - \log q_K(\mathbf{z}_K|\mathbf{x}, \phi) \right] \\
&= \mathbb{E}_{q_0(\mathbf{z}_0|\mathbf{x},\phi)} \Bigg[\log p(\mathbf{x}, \mathbf{z}_K|\theta) - \log q_0(\mathbf{z}_0|\mathbf{x}, \phi) - \\
&\quad - \sum_{k=1}^{K} \log \left| \det \left(\frac{\partial g_k(\mathbf{z}_{k-1})}{\partial \mathbf{z}_{k-1}} \right) \right| \Bigg].
\end{aligned}$$

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https://arxiv.org/pdf/1505.05770.pdf

Gaussian autoregressive model

Consider autoregressive model

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

with conditionals

$$p(x_i|\mathbf{x}_{1:i-1}, \boldsymbol{\theta}) = \mathcal{N}\left(\hat{\mu}_i(\mathbf{x}_{1:i-1}), \hat{\sigma}_i^2(\mathbf{x}_{1:i-1})\right).$$

Sampling

$$x_i = \hat{\sigma}_i(\mathbf{x}_{1:i-1}) \cdot z_i + \hat{\mu}_i(\mathbf{x}_{1:i-1}), \quad z_i \sim \mathcal{N}(0, 1).$$

Sampling from autoregressive model is sequential.
Note that we could interpret this sampling as a transormation $\mathbf{x} = g(\mathbf{z}, \boldsymbol{\theta})$, where $\mathbf{z}$ comes from base distribution $\mathcal{N}(0, 1)$.

Gaussian autoregressive model

Sampling

$$x_i = \hat{\sigma}_i(\mathbf{x}_{1:i-1}) \cdot z_i + \hat{\mu}_i(\mathbf{x}_{1:i-1}), \quad z_i \sim \mathcal{N}(0, 1).$$

Jacobian

$$\log \left| \det \left(\frac{\partial f(\mathbf{x}, \boldsymbol{\theta})}{\partial \mathbf{x}} \right) \right| = -\log \left| \det \left(\frac{\partial g(\mathbf{z}, \boldsymbol{\theta})}{\partial \mathbf{z}} \right) \right| = -\sum_{i=1}^{m} \log \hat{\sigma}_i(\mathbf{x}_{1:i-1}).$$

Inverse transform

$$z_i = (x_i - \hat{\mu}_i(\mathbf{x}_{1:i-1})) \cdot \frac{1}{\hat{\sigma}_i(\mathbf{x}_{1:i-1})}.$$

We get an autoregressive model with tractable (triangular) Jacobian, which is easily invertible. It is a flow!

Inverse autoregressive flow (IAF)

Gaussian autoregressive model ($\mathbf{z} \to \mathbf{x}$)

$$x_i = \hat{\sigma}_i(\mathbf{x}_{1:i-1}) \cdot z_i + \hat{\mu}_i(\mathbf{x}_{1:i-1}).$$

$$z_i = (x_i - \hat{\mu}_i(\mathbf{x}_{1:i-1})) \cdot \frac{1}{\hat{\sigma}_i(\mathbf{x}_{1:i-1})}.$$

This process is sequential.
Let use the following reparametrization: $\hat{\boldsymbol{\sigma}} = \frac{1}{\boldsymbol{\sigma}}; \quad \hat{\boldsymbol{\mu}} = -\frac{\boldsymbol{\mu}}{\boldsymbol{\sigma}}.$

Inverse transform ($\mathbf{x} \to \mathbf{z}$)

$$z_i = \boldsymbol{\sigma}_i(\mathbf{x}_{1:i-1}) \cdot x_i + \boldsymbol{\mu}_i(\mathbf{x}_{1:i-1}).$$

$$x_i = (z_i - \boldsymbol{\mu}_i(\mathbf{x}_{1:i-1})) \cdot \frac{1}{\boldsymbol{\sigma}_i(\mathbf{x}_{1:i-1})}.$$

This process is **not** sequential.

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https://arxiv.org/pdf/1606.04934.pdf

Inverse autoregressive flow (IAF)

Inverse transform ($\mathbf{x} \to \mathbf{z}$)

$$z_i = \boldsymbol{\sigma}_i(\mathbf{x}_{1:i-1}) \cdot x_i + \boldsymbol{\mu}_i(\mathbf{x}_{1:i-1}).$$

$$x_i = (z_i - \boldsymbol{\mu}_i(\mathbf{x}_{1:i-1})) \cdot \frac{1}{\boldsymbol{\sigma}_i(\mathbf{x}_{1:i-1})}.$$

Inverse autoregressive flow use such inverted autoregressive model as a flow in VAE:

$$\mathbf{z}_0 = \boldsymbol{\sigma}_0(\mathbf{x}) \cdot \boldsymbol{\epsilon} + \boldsymbol{\mu}_0(\mathbf{x}), \quad \boldsymbol{\epsilon} \sim \mathcal{N}(0, 1); \quad (q_0(\mathbf{z}_0|\mathbf{x}, \boldsymbol{\phi}))$$

$$\mathbf{z}_k = \boldsymbol{\sigma}_k(\mathbf{z}_{k-1}) \cdot \mathbf{z}_{t-1} + \boldsymbol{\mu}_k(\mathbf{z}_{k-1}), \quad k \geq 1 \quad (q_k(\mathbf{z}_k|\mathbf{x}, \boldsymbol{\phi})).$$

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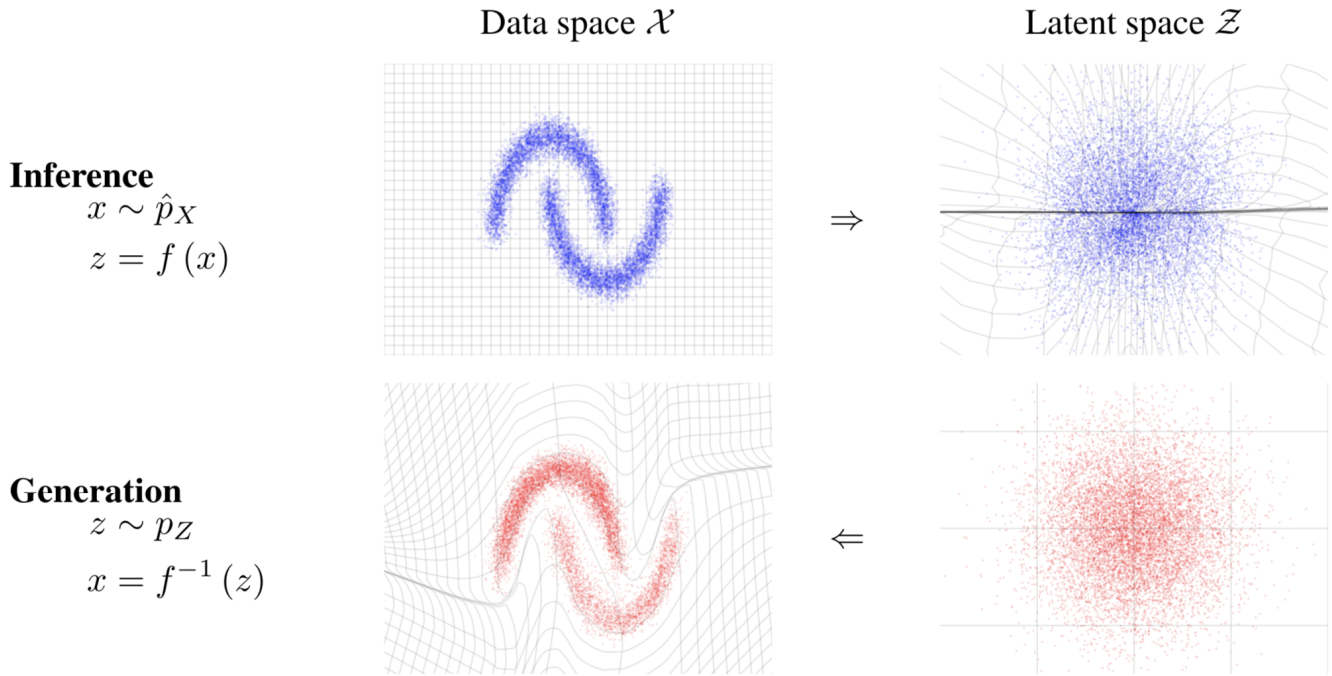
Flows



- Inference mode in autoregressive flows is used for density estimation task.
- Generation mode in autoregressive flows (IAF) is used for stochastic variational inference to get more flexible posterior distribution.

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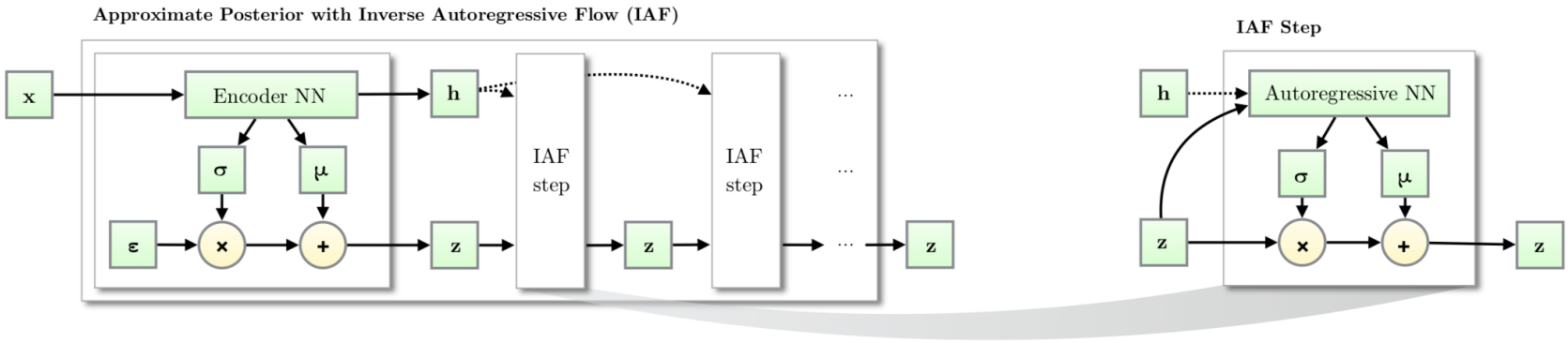
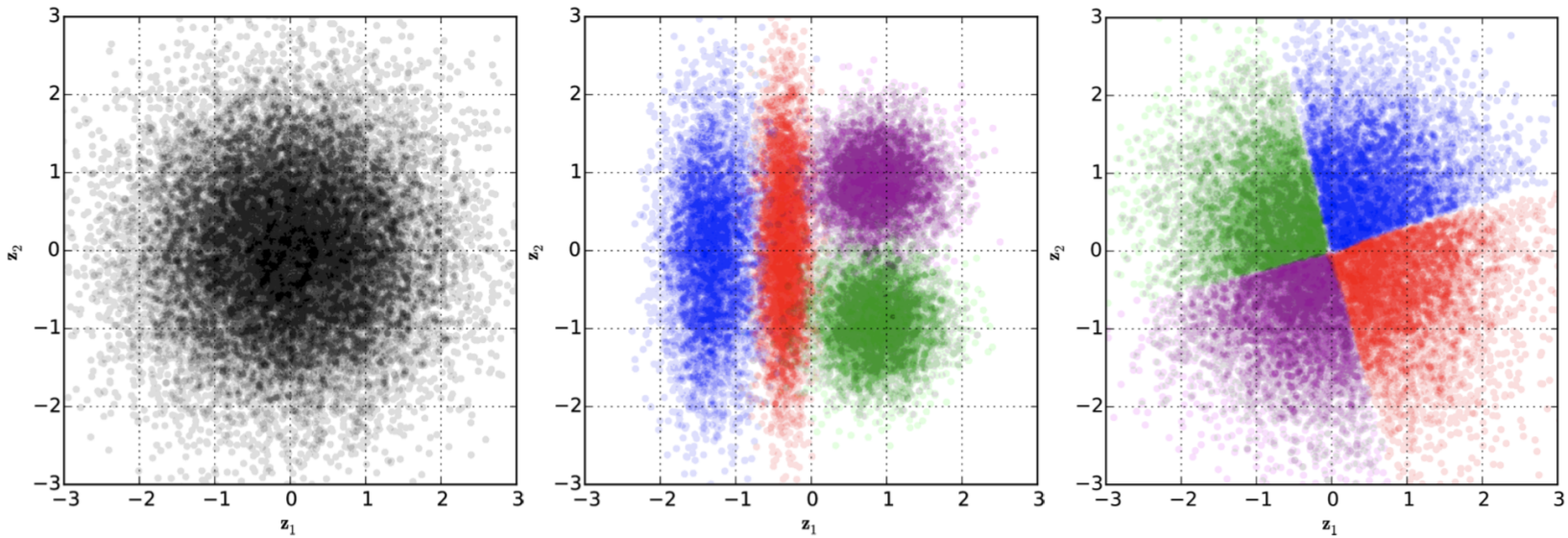
https://arxiv.org/pdf/1605.08803.pdf

Inverse autoregressive flow (IAF)





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

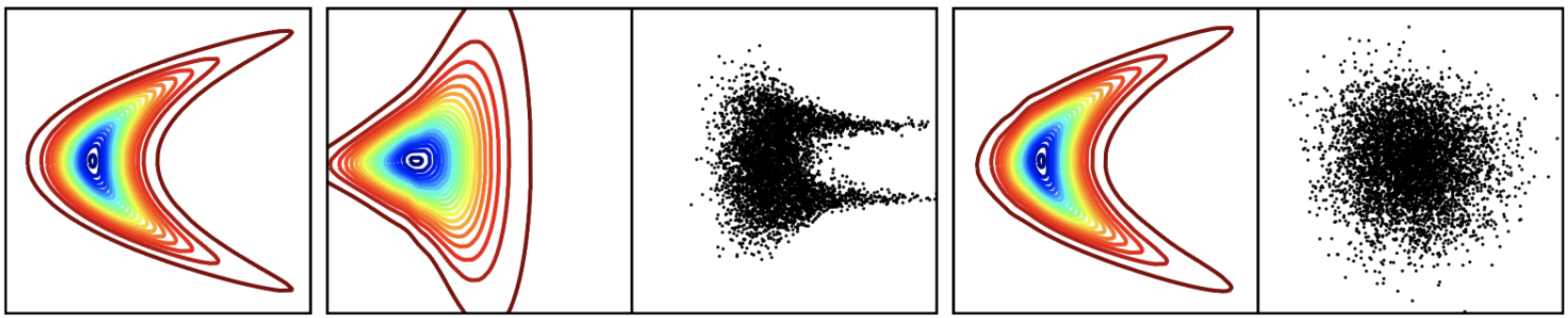
https://arxiv.org/pdf/1606.04934.pdf

Masked autoregressive flow (MAF)

Gaussian autoregressive model

$$p(\mathbf{x}|\boldsymbol{\theta}) = \prod_{i=1}^{m} p(x_i|\mathbf{x}_{1:i-1}, \boldsymbol{\theta}) = \prod_{i=1}^{m} \mathcal{N}\left(x_i|\mu_i(\mathbf{x}_{1:i-1}), \sigma_i^2(\mathbf{x}_{1:i-1})\right).$$

We could use MADE (masked autoencoder) as conditional model. The sampling order could be crucial.



(a) Target density (b) MADE with Gaussian conditionals (c) MAF with 5 layers

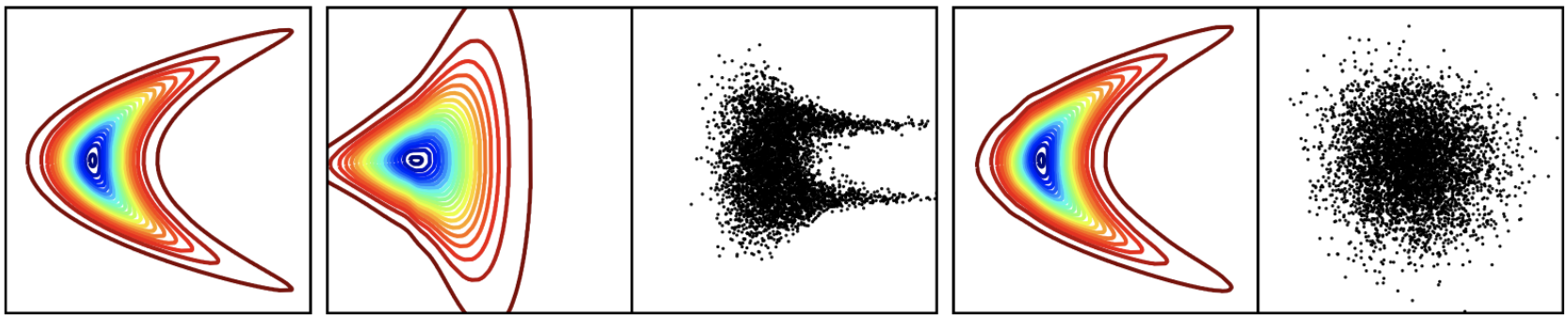
Samples from the base distribution could be an indicator of how good the flow was fitted.

https://arxiv.org/pdf/1705.07057.pdf

Masked autoregressive flow (MAF)

Gaussian autoregressive model

$$p(\mathbf{x}|\boldsymbol{\theta}) = \prod_{i=1}^{m} p(x_i|\mathbf{x}_{1:i-1}, \boldsymbol{\theta}) = \prod_{i=1}^{m} \mathcal{N}\left(x_i|\mu_i(\mathbf{x}_{1:i-1}), \sigma_i^2(\mathbf{x}_{1:i-1})\right) .$$



(a) Target density (b) MADE with Gaussian conditionals (c) MAF with 5 layers

MAF is just a stacked MADE model.

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https://arxiv.org/pdf/1705.07057.pdf

MAF vs IAF

Sampling and inverse transform in MAF

$$x_i = \hat{\sigma}_i(\mathbf{x}_{1:i-1}) \cdot z_i + \hat{\mu}_i(\mathbf{x}_{1:i-1}).$$

$$z_i = (x_i - \hat{\mu}_i(\mathbf{x}_{1:i-1})) \cdot \frac{1}{\hat{\sigma}_i(\mathbf{x}_{1:i-1})}.$$

- Sampling is slow (sequential).
- Density estimation is fast.

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MAF vs IAF

Theorem

Training a MAF with maximum likelihood corresponds to fitting an implicit IAF with stochastic variational inference where the posterior is taken to be the base density:

$$\max_{\boldsymbol{\theta}} p(\mathbf{X}|\boldsymbol{\theta}) \quad \Leftrightarrow \quad \min_{\boldsymbol{\theta}} KL\left(p(\mathbf{z}|\boldsymbol{\theta})||\pi(\mathbf{z})\right)$$

(Here, $\pi(\mathbf{z})$ is a base distribution, $\pi(\mathbf{x})$ is a data distribution).

Proof

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

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

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

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MAF vs IAF

Proof (continued)

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

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

Unbiased estimator is MLE:

$$\mathbb{E}_{\pi(\mathbf{x})} \log p(\mathbf{x}|\boldsymbol{\theta}) = \sum_{i=1}^{n} \log p(\mathbf{x}_i|\boldsymbol{\theta}).$$

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https://arxiv.org/pdf/1705.07057.pdf

MAF vs IAF vs RealNVP

MAF

$$\mathbf{x} = \hat{\sigma}(\mathbf{x}) \odot \mathbf{z} + \hat{\mu}(\mathbf{x}).$$

- Calculating the density $p(\mathbf{x}|\theta)$ - 1 pass.
- Sampling - m passes.

IAF

$$\mathbf{x} = \sigma(\mathbf{z}) \odot \mathbf{z} + \mu(\mathbf{z}).$$

- Calculating the density $p(\mathbf{x}|\theta)$ - m passes.
- Sampling - 1 pass.

RealNVP

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

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https://arxiv.org/pdf/1705.07057.pdf

MAF vs IAF vs RealNVP

RealNVP

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

- Calculating the density $p(\mathbf{x}|\boldsymbol{\theta})$ - 1 pass.
- Sampling - 1 pass.

RealNVP is a special case of MAF and IAF:

MAF

$$\begin{cases} \hat{\mu}_i = \hat{\sigma}_i = 0,\ i = 1, \ldots, d; \\ \hat{\mu}_i, \hat{\sigma}_i - \text{functions of } \mathbf{x}_{1:d},\ i = d+1, \ldots, m. \end{cases}$$

IAF

$$\begin{cases} \mu_i = \sigma_i = 0,\ i = 1, \ldots, d; \\ \mu_i, \sigma_i - \text{functions of } \mathbf{z}_{1:d},\ i = d+1, \ldots, m. \end{cases}$$

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https://arxiv.org/pdf/1705.07057.pdf

References

- **Glow:** Better Reversible Generative Models
  https://arxiv.org/abs/1807.03039
  Summary: Extension of RealNVP. Suggests 1x1 reversible convolutions instead of reversing channel ordering. 1x1 conv is square matrix which could be easily be inversed. Compares 1x1 conv with reversing and fixed shuffling.
- **Flow++:** Improving Flow-Based Generative Models with Variational Dequantization and Architecture Design
  https://arxiv.org/abs/1902.00275
  Summary: Flow model which investigates the dequantization of discrete probability distribution. Derives ELBO objective with variational noise dequantization distribution.
- **IAF**: Improving Variational Inference with Inverse Autoregressive Flow
  https://arxiv.org/abs/1606.04934
  Summary: Introduce inverse autoregressive flow (IAF). Models each autoregressive conditional as gaussian with autoregressive means and covariances. Inverse transformation allows to parallelize sampling.
- **MAF**: Masked Autoregressive Flow for Density Estimation
  https://arxiv.org/pdf/1705.07057.pdf
  Summary: Similar to IAF. Give comprehensive overview with link to IAF and RealNVP. MAF is suitable for density estimation, IAF as a recognition network.