

Deep Generative Models

Lecture 5

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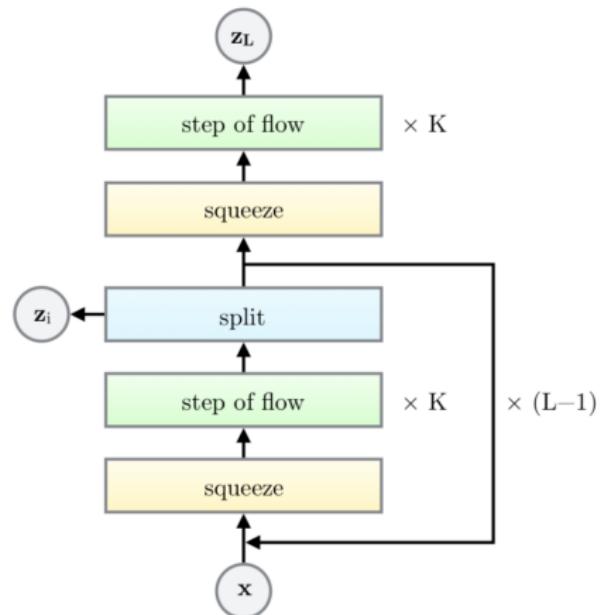
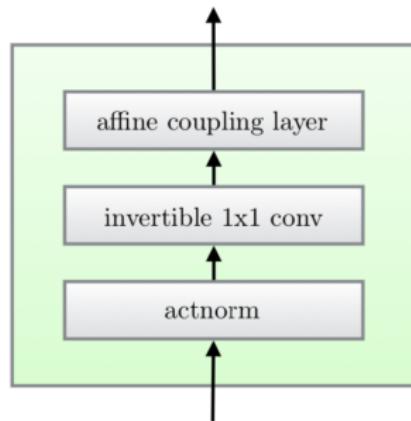
Ozon Masters

2021

Glow, 2018



Model architecture



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 **split** operator which decouples a variable into 2 subparts (usually channel-wise). The order of decoupling should be manually changed between layers.

Could we use more general operator?

Let's 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 $O(c^3)$.

Glow, 2018

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

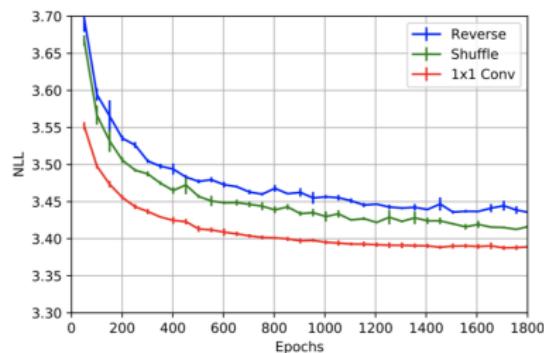
<https://arxiv.org/pdf/1807.03039.pdf>

Invertible 1×1 conv

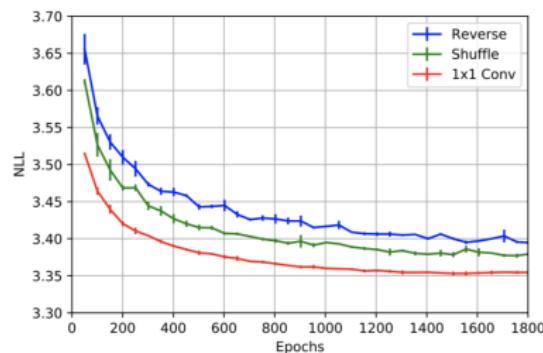
Cost to compute $\det(\mathbf{W})$ is $O(c^3)$. LU-decomposition reduces the cost to $O(c)$:

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

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.

Glow, 2018

Face interpolation



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

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 into the complex ones via sequences of invertible transformations.
- ▶ The goal is to achieve tractable Jacobian for efficient learning and density estimation.

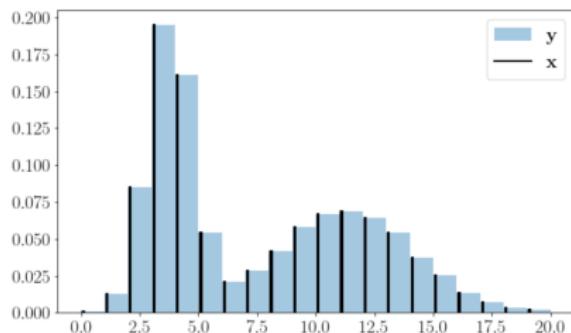
Dequantization

- ▶ 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 continuous model $p(\mathbf{y}|\theta)$ 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:

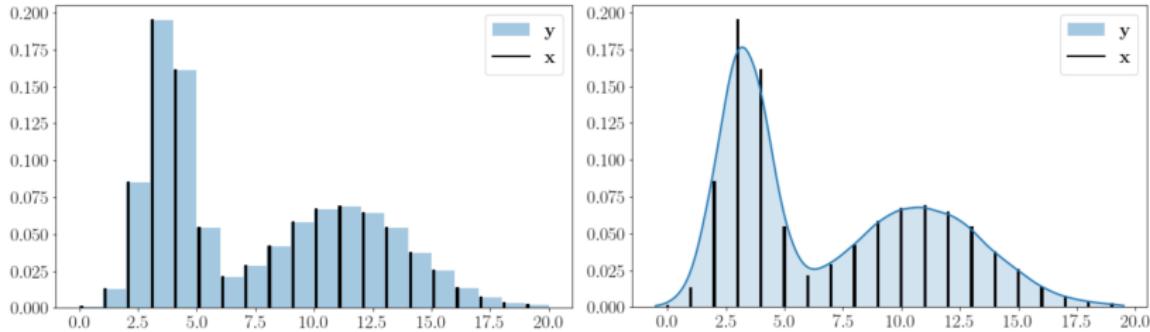
$$P(\mathbf{x}|\theta) = \int_{U[0,1]} p(\mathbf{x} + \mathbf{u}|\theta) d\mathbf{u}$$

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

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

Variational dequantization



- ▶ $p(y|\theta)$ assign uniform density to unit hypercubes $x + U[0, 1]$ (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

$$\begin{aligned}\log P(\mathbf{X}|\theta) &= \sum_{i=1}^n \log P(\mathbf{x}_i|\theta) = \sum_{i=1}^n \left[\log \int q(\mathbf{u}|\mathbf{x}) \frac{p(\mathbf{x} + \mathbf{u}|\theta)}{q(\mathbf{u}|\mathbf{x})} d\mathbf{u} \right] \geq \\ &\geq \sum_{i=1}^n \left[\int q(\mathbf{u}|\mathbf{x}) \log \frac{p(\mathbf{x} + \mathbf{u}|\theta)}{q(\mathbf{u}|\mathbf{x})} d\mathbf{u} \right] = \\ &= \int q(\mathbf{U}|\mathbf{X}) \log \frac{p(\mathbf{X} + \mathbf{U}|\theta)}{q(\mathbf{U}|\mathbf{X})} d\mathbf{U} = \mathcal{L}(q, \theta).\end{aligned}$$

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

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

Flow++

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

If $p(\mathbf{x} + \mathbf{u}|\theta)$ 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 $\log P(\mathbf{X}|\theta)$ and the derived ELBO is

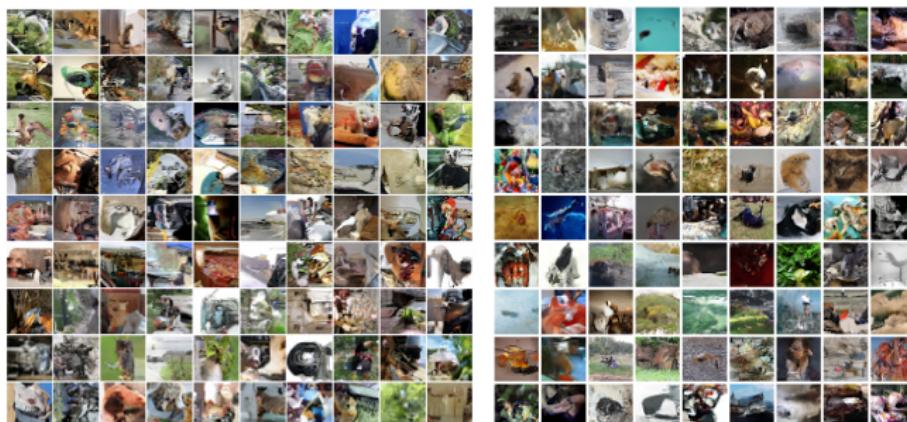
$$KL(q(\mathbf{U}|\mathbf{X}) || p(\mathbf{U}|\mathbf{X})).$$

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 .

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++

Likelihood-based models

Exact likelihood evaluation

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

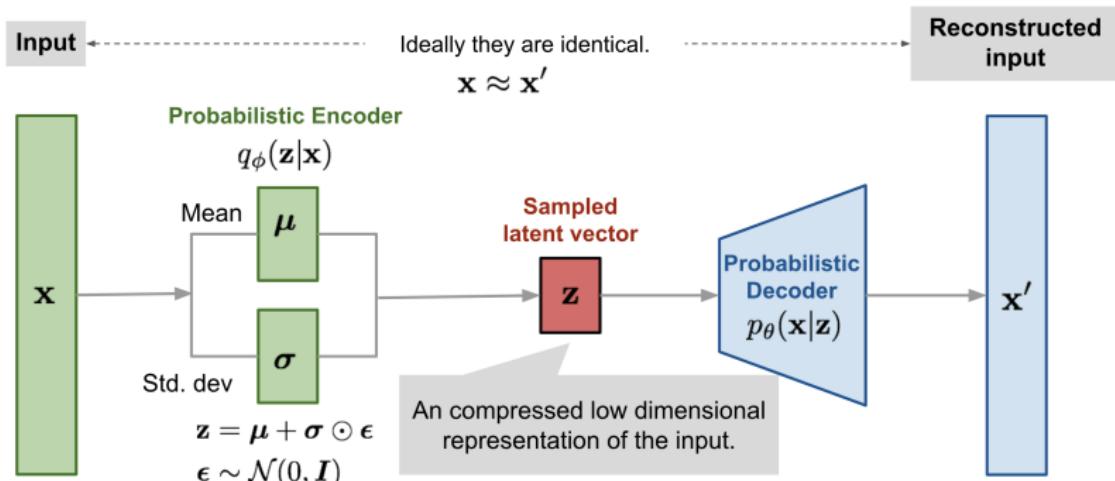
Approximate likelihood evaluation

- ▶ Latent variable models (VAE).

What are the pros and cons of each of them?

VAE recap

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



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

VAE limitations

- ▶ Poor variational posterior distribution (encoder)

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

- ▶ Poor prior distribution

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

- ▶ Poor probabilistic model (decoder)

$$p(\mathbf{x}|\mathbf{z}, \theta) = \mathcal{N}(\mathbf{x}|\mu_\theta(\mathbf{z}), \sigma_\theta^2(\mathbf{z})).$$

- ▶ Loose lower bound

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

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

Apply a sequence of transformations to the random variables

$$\mathbf{z}_0 \sim q(\mathbf{z}|\mathbf{x}, \phi) = \mathcal{N}(\mathbf{z}|\mu_\phi(\mathbf{x}), \sigma_\phi^2(\mathbf{x})).$$

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, radial, coupling layer) parameterized by ϕ_k .

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

Flows in VAE

Flow model in latent space

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

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, $\{\phi\}_{k=1}^K$ – flow parameters.

ELBO objective

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

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

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

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

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

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 transformation $\mathbf{x} = g(\mathbf{z}, \boldsymbol{\theta})$, 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

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

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 ($\mathbf{z} \rightarrow \mathbf{x}$)

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

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

This process is sequential.

Let use the following reparametrization: $\sigma = \frac{1}{\hat{\sigma}}$; $\mu = -\frac{\hat{\mu}}{\hat{\sigma}}$.

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

$$z_i = \sigma_i(\mathbf{x}_{1:i-1}) \cdot x_i + \mu_i(\mathbf{x}_{1:i-1}).$$

$$x_i = (z_i - \mu_i(\mathbf{x}_{1:i-1})) \cdot \frac{1}{\sigma_i(\mathbf{x}_{1:i-1})}.$$

This process is **not** sequential.

Inverse autoregressive flow (IAF)

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

$$z_i = \sigma_i(\mathbf{x}_{1:i-1}) \cdot x_i + \mu_i(\mathbf{x}_{1:i-1}).$$

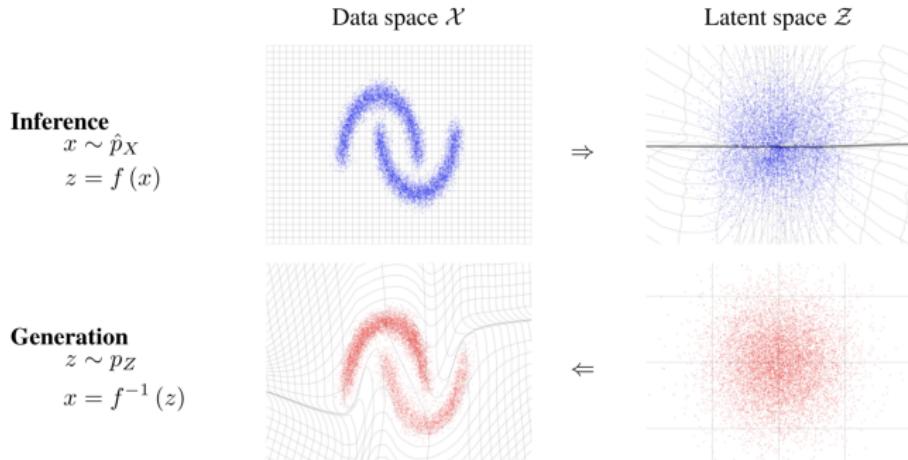
$$x_i = (z_i - \mu_i(\mathbf{x}_{1:i-1})) \cdot \frac{1}{\sigma_i(\mathbf{x}_{1:i-1})}.$$

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

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

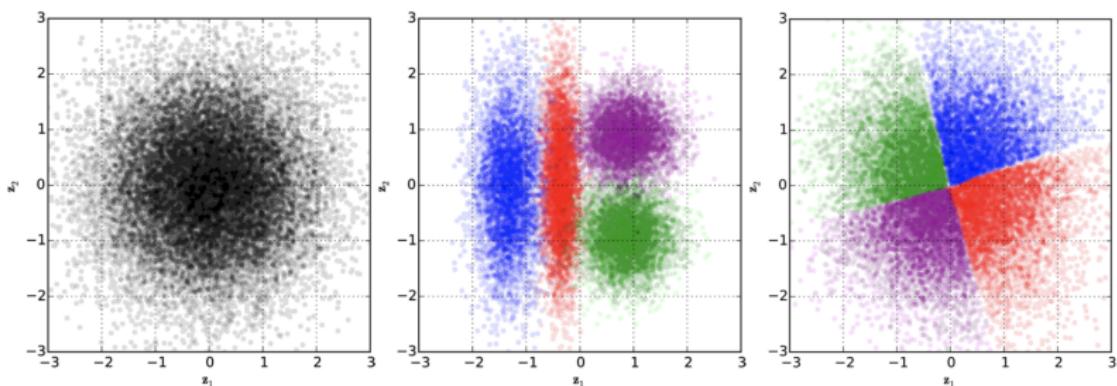
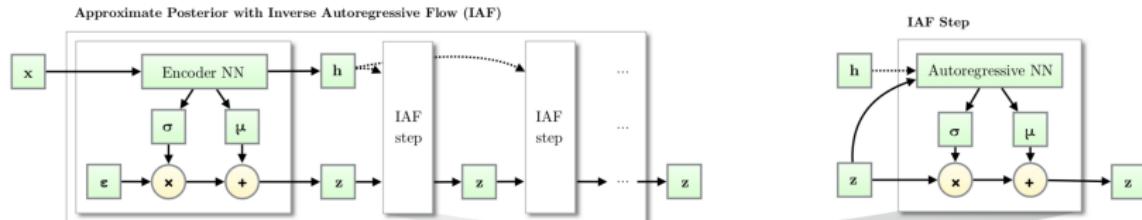
$$\mathbf{z}_k = \boldsymbol{\sigma}_k(\mathbf{z}_{k-1}) \cdot \mathbf{z}_{k-1} + \boldsymbol{\mu}_k(\mathbf{z}_{k-1}), \quad k \geq 1; \quad \sim q_k(\mathbf{z}_k | \mathbf{x}, \phi, \{\phi_j\}_{j=1}^k).$$

Flows



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

Inverse autoregressive flow (IAF)



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 inverted. 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.
- ▶ Variational Inference with Normalizing Flows
<https://arxiv.org/abs/1505.05770>
Summary: Propose to use normalizing flows in variational inference. Discuss finite and infinitesimal flows. Uses invertible flows: planar, radial. Comparison with NICE.
- ▶ **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.