# Deep Generative Models

Lecture 5

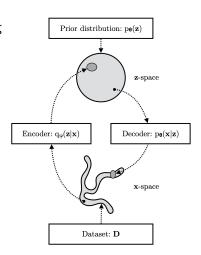
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# Variational autoencoder (VAE)

- ▶ VAE learns stochastic mapping between **x**-space, from  $\pi(\mathbf{x})$ , and a latent **z**-space, with simple distribution.
- The generative model learns distribution  $p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta}) = p(\mathbf{z})p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})$ , with a prior distribution  $p(\mathbf{z})$ , and a stochastic decoder  $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})$ .
- The stochastic encoder  $q(\mathbf{z}|\mathbf{x}, \phi)$  (inference model), approximates the true but intractable posterior  $p(\mathbf{z}|\mathbf{x}, \theta)$ .



## LVM

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

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

## Autoregressive decoder

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

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

# Decoder weakening

- 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.

## KL annealing

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

Start training with  $\beta=$  0, increase it until  $\beta=$  1 during training.

#### Free bits

Ensure the use of less than  $\lambda$  bits of information:

$$\mathcal{L}(q, \theta, \lambda) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x})} \log p(\mathbf{x}|\mathbf{z}, \theta) - \max(\lambda, \mathsf{KL}(q(\mathbf{z}|\mathbf{x})||p(\mathbf{z}))).$$

This results in  $KL(q(\mathbf{z}|\mathbf{x})||p(\mathbf{z})) \geq \lambda$ .

## VAE objective

$$\log p(\mathbf{x}|oldsymbol{ heta}) \geq \mathcal{L}(q,oldsymbol{ heta}) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x})} \log rac{p(\mathbf{x},\mathbf{z}|oldsymbol{ heta})}{q(\mathbf{z}|\mathbf{x})} 
ightarrow \max_{q,oldsymbol{ heta}}$$

## **IWAE** objective

$$\mathcal{L}_{\mathcal{K}}(q, oldsymbol{ heta}) = \mathbb{E}_{\mathsf{z}_1, ..., \mathsf{z}_{\mathcal{K}} \sim q(\mathsf{z}|\mathsf{x})} \log \left( rac{1}{\mathcal{K}} \sum_{k=1}^{\mathcal{K}} rac{p(\mathsf{x}, \mathsf{z}_k | oldsymbol{ heta})}{q(\mathsf{z}_k | \mathsf{x})} 
ight) 
ightarrow \max_{q, oldsymbol{ heta}}.$$

#### Theorem

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

# Outline

# Likelihood-based models so far...

## Autoregressive models

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

- tractable likelihood,
- no inferred latent factors.

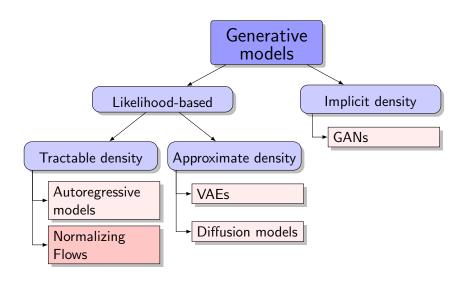
#### Latent variable models

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

- latent feature representation,
- intractable likelihood.

How to build model with latent variables and tractable likelihood?

# Generative models zoo



# Normalizing flows prerequisites

# Change of variable theorem

Let  $\mathbf{x}$  be a random variable with density function  $p(\mathbf{x})$  and  $f: \mathbb{R}^m \to \mathbb{R}^m$  is a differentiable, invertible function (diffeomorphism). If  $\mathbf{z} = f(\mathbf{x})$ ,  $\mathbf{x} = f^{-1}(\mathbf{z}) = g(\mathbf{z})$ , then

$$\begin{aligned} & p(\mathbf{x}) = p(\mathbf{z}) \left| \det \left( \frac{\partial \mathbf{z}}{\partial \mathbf{x}} \right) \right| = p(f(\mathbf{x})) \left| \det \left( \frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} \right) \right| \\ & p(\mathbf{z}) = p(\mathbf{x}) \left| \det \left( \frac{\partial \mathbf{x}}{\partial \mathbf{z}} \right) \right| = p(g(\mathbf{z})) \left| \det \left( \frac{\partial g(\mathbf{z})}{\partial \mathbf{z}} \right) \right|. \end{aligned}$$

#### Inverse function theorem

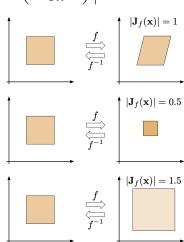
If function f is invertible and Jacobian is continuous and non-singular, then

$$\left| \det \left( \frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} \right) \right| = \left| \det \left( \frac{\partial g^{-1}(\mathbf{x})}{\partial \mathbf{x}} \right) \right| = \left| \det \left( \frac{\partial g(\mathbf{z})}{\partial \mathbf{z}} \right) \right|^{-1}$$

# Jacobian-determinant

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

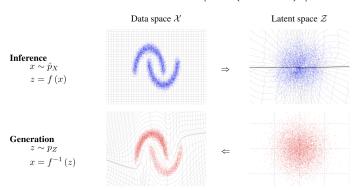
- **x** and **z** have the same dimensionality  $(\mathbb{R}^m)$ .
- $f(\mathbf{x}, \boldsymbol{\theta})$  could be parametric function.
- Determinant of Jacobian  $\mathbf{J} = \frac{\partial f(\mathbf{x}, \boldsymbol{\theta})}{\partial \mathbf{x}}$  shows how the volume changes under the transorfmation.



# Fitting flows

# MLE problem

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



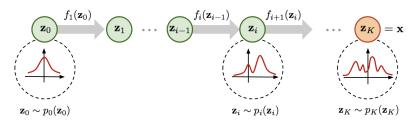
Dinh L., Sohl-Dickstein J., Bengio S. Density estimation using Real NVP, 2016

# Composition of flows

#### **Theorem**

Diffeomorphisms are **composable** (If  $\{f_k\}_{k=1}^K$  satisfy conditions of the change of variable theorem, then  $\mathbf{z} = f(\mathbf{x}) = f_K \circ \cdots \circ f_1(\mathbf{x})$  also satisfies it).

$$\begin{aligned} p(\mathbf{x}) &= p(f(\mathbf{x})) \left| \det \left( \frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} \right) \right| = p(f(\mathbf{x})) \left| \det \left( \frac{\partial f_K \circ \cdots \circ f_1(\mathbf{x})}{\partial \mathbf{x}} \right) \right| = \\ &= p(f(\mathbf{x})) \left| \det \left( \frac{\partial f_K}{\partial f_{K-1}} \cdots \frac{\partial f_1}{\partial \mathbf{x}} \right) \right| = p(f(\mathbf{x})) \prod_{k=1}^K \left| \det \left( \frac{\partial f_k}{\partial f_{k-1}} \right) \right| \end{aligned}$$



## **Flows**

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

#### Definition

Normalizing flow is a *differentiable, invertible* mapping from data  $\mathbf{x}$  to the noise  $\mathbf{z}$ .

- Normalizing means that the inverse flow takes samples from  $p(\mathbf{x})$  and normalizes them into samples from density  $p(\mathbf{z})$ .
- **Flow** refers to the trajectory followed by samples from  $p(\mathbf{z})$  as they are transformed by the sequence of transformations

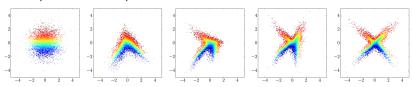
$$\mathbf{z} = f_K \circ \cdots \circ f_1(\mathbf{x}); \quad \mathbf{x} = f_1^{-1} \circ \cdots \circ f_K^{-1}(\mathbf{z}) = g_1 \circ \cdots \circ g_K(\mathbf{z})$$

$$p(\mathbf{x}) = p(f_K \circ \cdots \circ f_1(\mathbf{x})) \left| \det \left( \frac{\partial f_K \circ \cdots \circ f_1(\mathbf{x})}{\partial \mathbf{x}} \right) \right| =$$

$$= p(f_K \circ \cdots \circ f_1(\mathbf{x})) \prod_{K=1}^{K} \left| \det \left( \frac{\partial \mathbf{f}_k}{\partial \mathbf{f}_{k-1}} \right) \right|.$$

## Flows

## Example of a 4-step flow



#### Flow likelihood

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

What is the complexity of the determinant computation?

#### What we want

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

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

## Forward KL vs Reverse KL

#### Forward KL

$$\begin{aligned} \mathsf{KL}(\pi||p) &= \int \pi(\mathbf{x}) \log \frac{\pi(\mathbf{x})}{p(\mathbf{x}|\boldsymbol{\theta})} d\mathbf{x} \\ &= -\mathbb{E}_{\pi(\mathbf{x})} \log p(\mathbf{x}|\boldsymbol{\theta}) + \mathsf{const} \to \min_{\boldsymbol{\theta}} \end{aligned}$$

Maximum likelihood estimation is equivalent to minimization of the Monte-Carlo estimation of forward KL.

#### Forward KL for flow model

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

- ▶ We need to be able to compute  $f(\mathbf{x}, \theta)$  and its Jacobian.
- ▶ We need to be able to compute the density p(z).
- We don't need to think about computing the function  $g(\mathbf{z}, \theta) = f^{-1}(\mathbf{z}, \theta)$  until we want to sample from the flow.

# Forward KL vs Reverse KL

Reverse KL

$$KL(p||\pi) = \int p(\mathbf{x}|\theta) \log \frac{p(\mathbf{x}|\theta)}{\pi(\mathbf{x})} d\mathbf{x}$$
$$= \mathbb{E}_{p(\mathbf{x}|\theta)} [\log p(\mathbf{x}|\theta) - \log \pi(\mathbf{x})] \to \min_{\theta}$$

Reverse KL for flow model

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

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

- ▶ We need to be able to compute  $g(\mathbf{z}, \theta)$  and its Jacobian.
- We need to be able to sample from the density p(z) (do not need to evaluate it).
- ▶ We don't need to think about computing the function  $f(\mathbf{x}, \boldsymbol{\theta})$ .

# Flow KL duality

#### **Theorem**

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

$$\mathop{\arg\min}_{\boldsymbol{\theta}} \mathit{KL}(\pi(\mathbf{x})||p(\mathbf{x}|\boldsymbol{\theta})) = \mathop{\arg\min}_{\boldsymbol{\theta}} \mathit{KL}(p(\mathbf{z}|\boldsymbol{\theta})||p(\mathbf{z})).$$

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

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

# Flow KL duality

#### **Theorem**

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$$\mathop{\arg\min}_{\boldsymbol{\theta}} \mathit{KL}(\pi(\mathbf{x})||p(\mathbf{x}|\boldsymbol{\theta})) = \mathop{\arg\min}_{\boldsymbol{\theta}} \mathit{KL}(p(\mathbf{z}|\boldsymbol{\theta})||p(\mathbf{z})).$$

## Proof

$$\begin{split} & \mathsf{KL}\left(p(\mathbf{z}|\boldsymbol{\theta})||\pi(\mathbf{z})\right) = \mathbb{E}_{p(\mathbf{z}|\boldsymbol{\theta})} \big[\log p(\mathbf{z}|\boldsymbol{\theta}) - \log p(\mathbf{z})\big] = \\ & = \mathbb{E}_{p(\mathbf{z}|\boldsymbol{\theta})} \left[\log \pi(g(\mathbf{z},\boldsymbol{\theta})) + \log \left|\det \left(\frac{\partial g(\mathbf{z},\boldsymbol{\theta})}{\partial \mathbf{z}}\right)\right| - \log p(\mathbf{z})\right] = \\ & = \mathbb{E}_{\pi(\mathbf{x})} \left[\log \pi(\mathbf{x}) - \log \left|\det \left(\frac{\partial f(\mathbf{x},\boldsymbol{\theta})}{\partial \mathbf{x}}\right)\right| - \log p(f(\mathbf{x},\boldsymbol{\theta}))\right] = \\ & = \mathbb{E}_{\pi(\mathbf{x})} \big[\log \pi(\mathbf{x}) - \log p(\mathbf{x}|\boldsymbol{\theta})\big] = \mathsf{KL}(\pi(\mathbf{x})||p(\mathbf{x}|\boldsymbol{\theta})). \end{split}$$

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

## Jacobian structure

# Flow log-likelihood

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

The main challenge is a determinant of the Jacobian.

What is a det of Jacobian in the following cases?

- 1. Consider a linear layer z = Wx.
- 2. Let **z** be a permutation of **x**.
- 3. Let  $z_i$  depend only on  $\mathbf{x}_i$ .

$$\log \left| \det \left( \frac{\partial f(\mathbf{x}, \boldsymbol{\theta})}{\partial \mathbf{x}} \right) \right| = \log \left| \prod_{i=1}^m f_i'(x_i, \boldsymbol{\theta}) \right| = \sum_{i=1}^m \log \left| f_i'(x_i, \boldsymbol{\theta}) \right|.$$

4. Let  $z_i$  depend only on  $\mathbf{x}_{1:i}$  (autoregressive dependency).

## Residual Flows

#### Matrix determinant lemma

$$\det\left(\mathbf{I}_m + \mathbf{V}\mathbf{W}^T\right) = \det(\mathbf{I}_d + \mathbf{W}^T\mathbf{V}), \quad ext{where } \mathbf{V}, \mathbf{W} \in \mathbb{R}^{m imes d}.$$

## Planar flow

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

Here  $\theta = \{\mathbf{u}, \mathbf{w}, b\}$ ,  $\sigma(\cdot)$  is a smooth element-wise non-linearity.

$$\left| \det \left( \frac{\partial g(\mathbf{z}, \boldsymbol{\theta})}{\partial \mathbf{z}} \right) \right| = \left| \det \left( \mathbf{I} + \sigma'(\mathbf{w}^T \mathbf{z} + b) \mathbf{w} \mathbf{u}^T \right) \right| = \left| 1 + \sigma'(\mathbf{w}^T \mathbf{z} + b) \mathbf{w}^T \mathbf{u} \right|$$

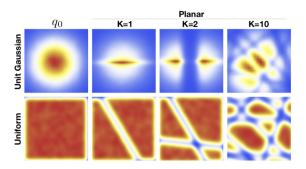
The transformation is invertible, for example, if

$$\sigma = \tanh$$
:  $\sigma'(\mathbf{w}^T \mathbf{z} + b) \mathbf{u}^T \mathbf{w} > -1$ .

## Residual Flows

# Expressiveness of planar flows

$$\mathbf{z}_K = g_1 \circ \cdots \circ g_K(\mathbf{z}); \quad g_k = g(\mathbf{z}_k, \boldsymbol{\theta}_k) = \mathbf{z}_k + \mathbf{u}_k \, \sigma(\mathbf{w}_k^T \mathbf{z}_k + b_k).$$



# Sylvester flow: planar flow extension

$$g(\mathbf{z}, \boldsymbol{\theta}) = \mathbf{z} + \mathbf{V} \, \sigma(\mathbf{W}^T \mathbf{z} + \mathbf{b}).$$

Rezende D. J., Mohamed S. Variational Inference with Normalizing Flows, 2015 Berg R. et al. Sylvester normalizing flows for variational inference, 2018

## Linear flows

#### RealNVP

$$\begin{cases} \mathbf{z}_{1:d} = \mathbf{x}_{1:d}; \\ \mathbf{z}_{d:m} = \tau(\mathbf{x}_{d:m}, c(\mathbf{x}_{1:d})); \end{cases} \Leftrightarrow \begin{cases} \mathbf{x}_{1:d} = \mathbf{z}_{1:d}; \\ \mathbf{x}_{d:m} = \tau^{-1}(\mathbf{z}_{d:m}, c(\mathbf{z}_{1:d})). \end{cases}$$

- First step is a **split** operator which decouples a variable into 2 subparts: **x**<sub>1</sub> and **x**<sub>2</sub> (usualy channel-wise).
- We should permute components between different layers.

$$z = Wx$$
,  $W \in \mathbb{R}^{m \times m}$ 

In general, we need  $O(m^3)$  to invert matrix.

## Invertibility

- ▶ Diagonal matrix O(m).
- ▶ Triangular matrix  $O(m^2)$ .
- It is impossible to parametrize all invertible matrices.

## Linear flows

$$z = Wx$$
,  $W \in \mathbb{R}^{m \times m}$ 

# Matrix decompositions

► LU-decomposition

$$W = PLU$$
,

where P is a permutation matrix, L is lower triangular with positive diagonal, U is upper triangular with positive diagonal.

QR-decomposition

$$W = QR$$

where  $\mathbf{Q}$  is an orthogonal matrix,  $\mathbf{R}$  is an upper triangular matrix with positive diagonal.

Kingma D. P., Dhariwal P. Glow: Generative Flow with Invertible 1x1 Convolutions, 2018

Hoogeboom E., Van Den Berg R., and Welling M. Emerging convolutions for generative normalizing flows, 2019

# Glow samples



Kingma D. P., Dhariwal P. Glow: Generative Flow with Invertible 1x1 Convolutions, 2018

# Summary

- ► Flow models transform a simple base distribution to a complex one via a sequence of invertible transformations with tractable Jacobian.
- Flow models have a tractable likelihood that is given by the change of variable theorem.
- Flows could be fitted using forward and reverse KL minimization. We will consider each of the scenarios later in the course.
- ▶ Planar and Sylvester flows are residual flows which use matrix determinant lemma.
- ► Linear flows try to parametrize set of invertible matrices via matrix decompositions.