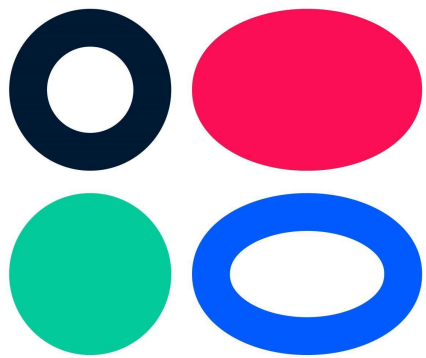
Deep Generative Models
Lecture 5

Roman Isachenko



Ozon Masters

Spring, 2021

Planar Flows

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

- $\boldsymbol{\theta} = \{\mathbf{u}, \mathbf{w}, b\}$;
- h is a smooth element-wise non-linearity.

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

The transformation is invertible, for example, if

$$h = \tanh; \quad h'(\mathbf{w}^T \mathbf{z} + b)\mathbf{u}^T \mathbf{w} \geq -1.$$

Sylvester flow: planar flow extension

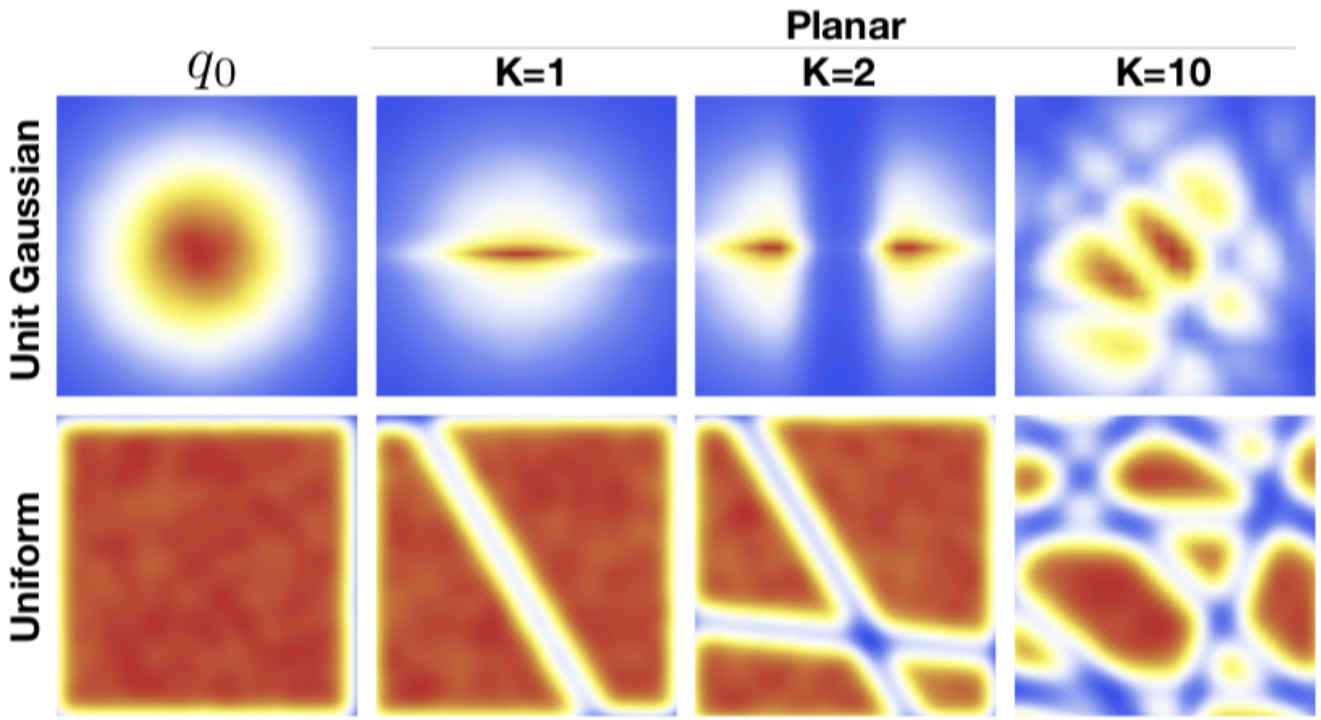
$$g(\mathbf{z}, \boldsymbol{\theta}) = \mathbf{z} + \mathbf{A}\, h(\mathbf{B}\mathbf{z} + \mathbf{b}).$$

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

Planar Flows

$$\mathbf{z}_K = g_1 \circ \cdots \circ g_K(\mathbf{z}); \quad g_k = g(\mathbf{z}_k, \boldsymbol{\theta}_k).$$

Expressiveness of planar flows



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

Jacobian structure

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 a determinant of a diagonal matrix?

$$\mathbf{z} = f(\mathbf{x}, \boldsymbol{\theta}) = (f_1(x_1, \boldsymbol{\theta}), \ldots, f_m(x_m, \boldsymbol{\theta})).$$

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

- What is a determinant of a triangular matrix?
  Let z_i depends only on $\mathbf{x}_{1:i}$ (or without loss of generality x_i depends on $\mathbf{z}_{1:i}$).
  What is the Jacobian of such a transformation?

NICE

Coupling layer

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

- $c : \mathbb{R}^d \to \mathbb{R}^k$ – coupling function (do not need to be invertible);
- $\tau : \mathbb{R}^{m-d} \times c(\mathbb{R}^d) \to \mathbb{R}^{m-d}$ – coupling law.
- $$\det\left(\frac{\partial \mathbf{z}}{\partial \mathbf{x}}\right) = \det\begin{pmatrix} \mathbf{I}_d & 0_{d \times m-d} \\ \frac{\partial \mathbf{z}_{d:m}}{\partial \mathbf{x}_{1:d}} & \frac{\partial \mathbf{z}_{d:m}}{\partial \mathbf{x}_{d:m}} \end{pmatrix} = \det\left(\frac{\partial \mathbf{z}_{d:m}}{\partial \mathbf{x}_{d:m}}\right)$$

Dinh L., Krueger D., Bengio Y. NICE: Non-linear Independent Components Estimation, 2014

NICE

Coupling layer

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

Coupling function $c(\cdot)$

Any complex function (without restrictions). For example, neural network.

Coupling law $\tau(\cdot, \cdot)$

- $\tau(x, c) = x + c$ – *additive*;
- $\tau(x, c) = x \odot c,\ c \neq 0$ – multiplicative;
- $\tau(x, c) = x \odot c_1 + c_2,\ c_1 \neq 0$ – affine.

To obtain more flexible class of dictributions, stack more coupling layers (with different ordering of components!).

Dinh L., Krueger D., Bengio Y. NICE: Non-linear Independent Components Estimation, 2014

NICE

Coupling layer

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

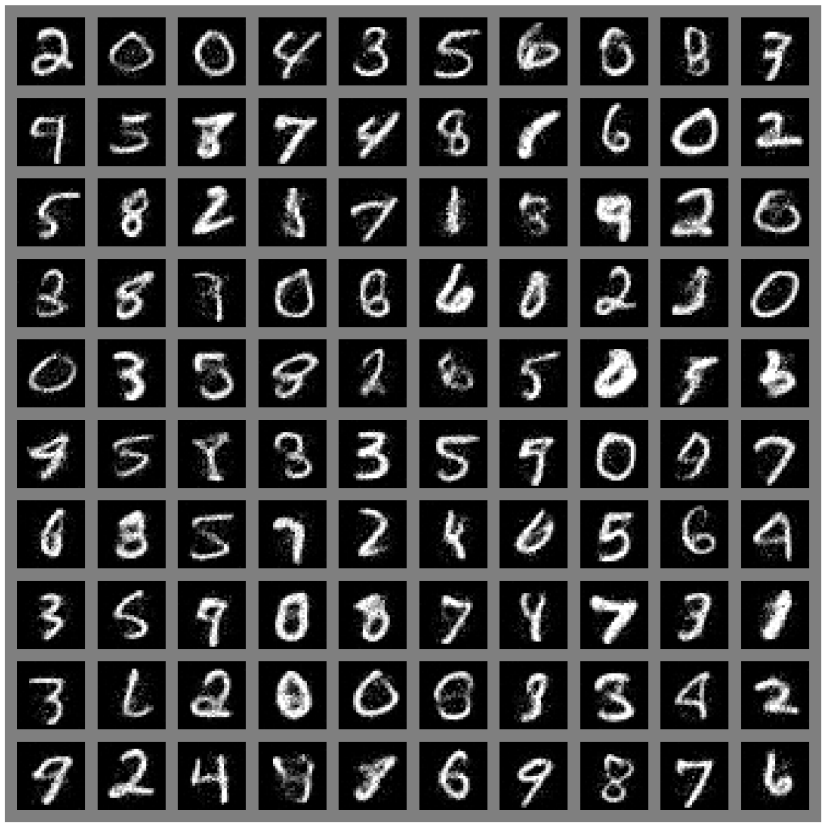
Jacobian

$$\det\left(\frac{\partial \mathbf{z}}{\partial \mathbf{x}}\right) = \det\begin{pmatrix} \mathbf{I}_d & 0_{d\times m-d} \\ \frac{\partial \mathbf{z}_{d:m}}{\partial \mathbf{x}_{1:d}} & \frac{\partial \mathbf{z}_{d:m}}{\partial \mathbf{x}_{d:m}} \end{pmatrix} = \det\left(\frac{\partial \mathbf{z}_{d:m}}{\partial \mathbf{x}_{d:m}}\right)$$

What is the Jacobian for the additive coupling law $\tau(x + c) = x + c$?
In this case the transformation is *volume preserving*.
The last layer is rescaling $z_i = s_i x_i$ ($x_i = z_i / s_i$).
What is the Jacobian of the last layer?

Dinh L., Krueger D., Bengio Y. NICE: Non-linear Independent Components Estimation, 2014

NICE



(a) Model trained on MNIST

(b) Model trained on TFD

Dinh L., Krueger D., Bengio Y. NICE: Non-linear Independent Components Estimation, 2014

RealNVP

Affine coupling law

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

$$\begin{cases} \mathbf{x}_{1:d} = \mathbf{z}_{1:d}; \\ \mathbf{x}_{d:m} = (\mathbf{z}_{d:m} - c_2(\mathbf{x}_{1:d}, \boldsymbol{\theta})) \odot \exp(-c_1(\mathbf{x}_{1:d}, \boldsymbol{\theta})). \end{cases}$$

Jacobian

$$\det\left(\frac{\partial \mathbf{z}}{\partial \mathbf{x}}\right) = \det\begin{pmatrix} \mathbf{I}_d & 0_{d\times m-d} \\ \frac{\partial \mathbf{z}_{d:m}}{\partial \mathbf{x}_{1:d}} & \frac{\partial \mathbf{z}_{d:m}}{\partial \mathbf{x}_{d:m}} \end{pmatrix} = \prod_{i=1}^{m-d} \exp(c_1(\mathbf{x}_{1:d}, \boldsymbol{\theta})_i).$$

Non-Volume Preserving.

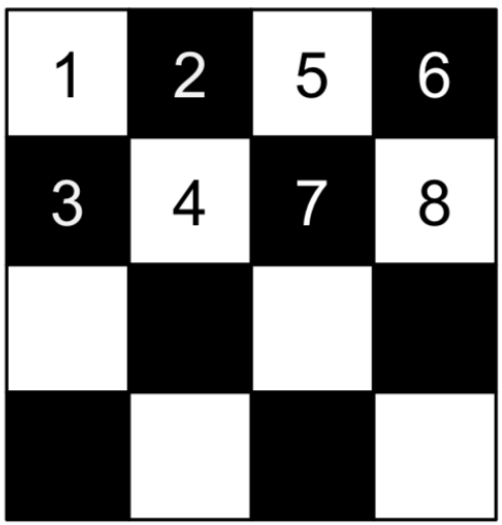
Dinh L., Sohl-Dickstein J., Bengio S. Density estimation using Real NVP, 2016

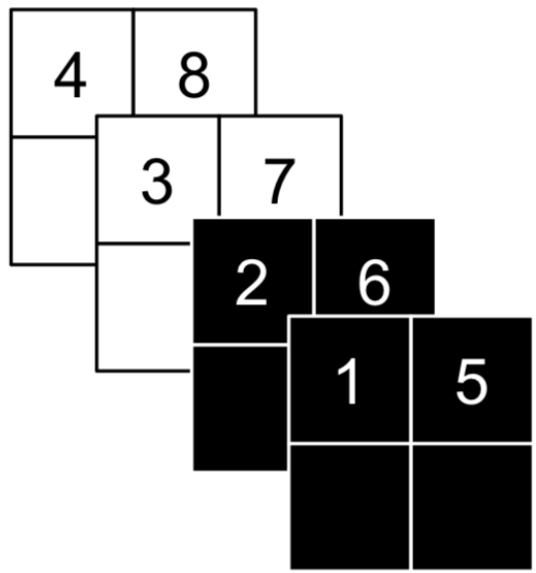
RealNVP

Affine coupling law

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

How to choose variable partitioning for images?

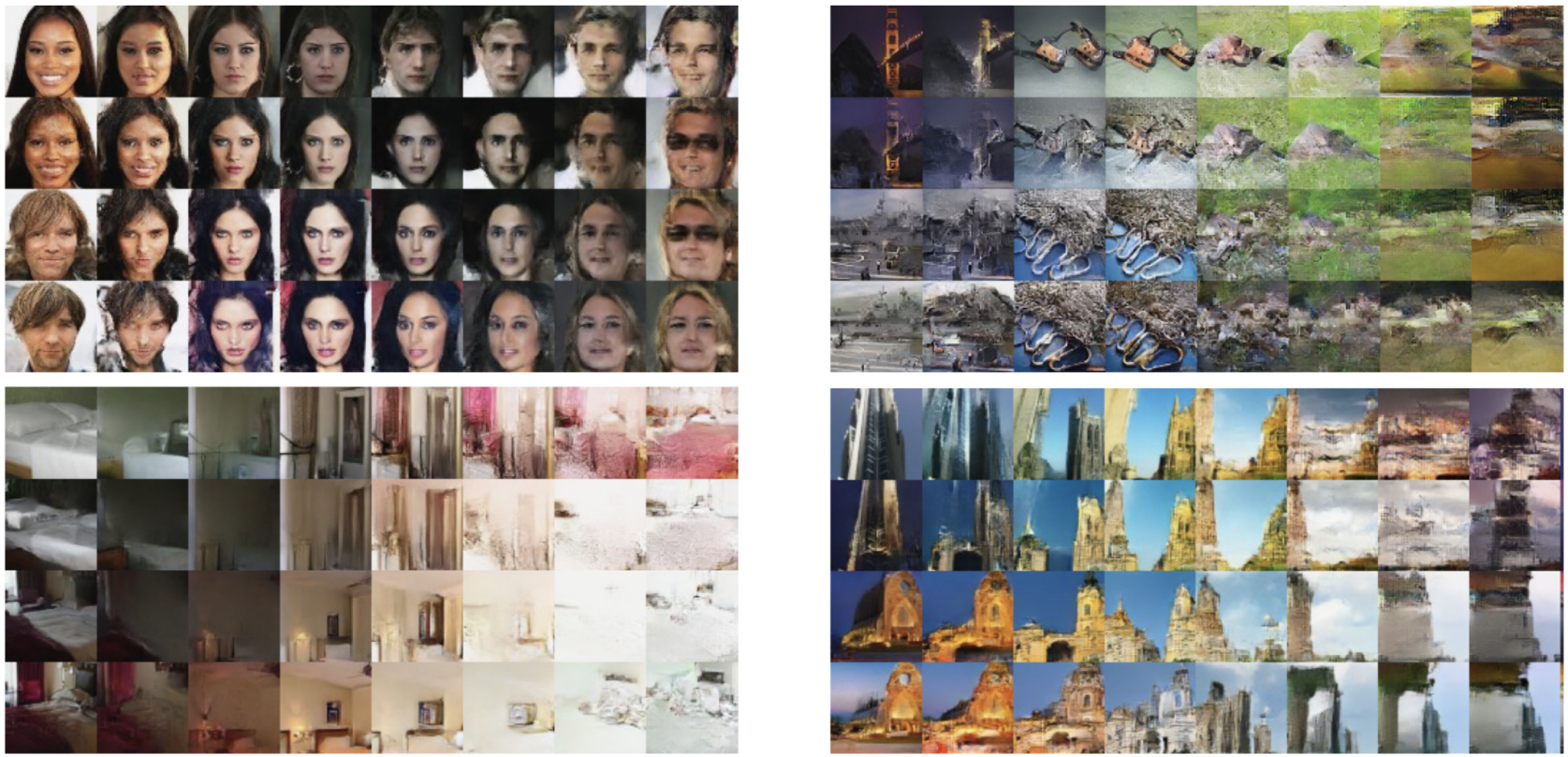




Masked convolutions are used to define ordering.

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

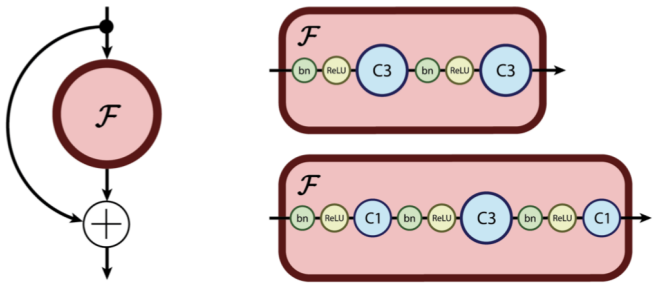
RealNVP



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

RevNets, 2017

- Modern neural networks are trained via backpropagation.
- Residual networks are state of the art in image classification.
- Backpropagation requires storing the network activations.



Problem

Storing the activations imposes an increasing memory burden. GPUs have limited memory capacity, leading to constraints often exceeded by state-of-the-art architectures (with thousand layers).

Gomez A. N. et al. The Reversible Residual Network: Backpropagation Without Storing Activations, 2017

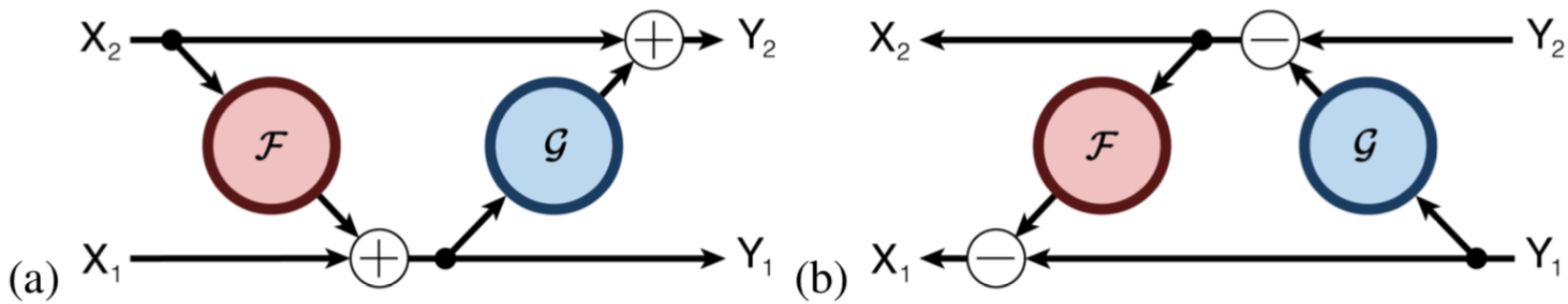
RevNets, 2017

NICE

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

RevNet

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



Gomez A. N. et al. The Reversible Residual Network: Backpropagation Without Storing Activations, 2017

RevNets, 2017

Architecture	CIFAR-10 [15]		CIFAR-100 [15]	
	ResNet	RevNet	ResNet	RevNet
32 (38)	**7.14%**	7.24%	29.95%	**28.96%**
110	**5.74%**	5.76%	26.44%	**25.40%**
164	5.24%	**5.17%**	**23.37%**	23.69%

- If the network contains non-reversible blocks (poolings, strides), activations for these blocks should be stored.
- To avoid storing activations in the modern frameworks, the backward pass should be manually redefined.

Gomez A. N. et al. The Reversible Residual Network: Backpropagation Without Storing Activations, 2017

i-RevNet, 2018

Hypothesis

The success of deep convolutional networks is based on progressively discarding uninformative variability about the input with respect to the problem at hand.

- It is difficult to recover images from their hidden representations.
- Information bottleneck principle: an optimal representation must reduce the MI between an input and its representation to reduce uninformative variability + maximize the MI between the output and its representation to preserve each class from collapsing onto other classes.

Jacobsen J. H., Smeulders A., Oyallon E. i-RevNet: Deep Invertible Networks, 2018

i-RevNet, 2018

Hypothesis

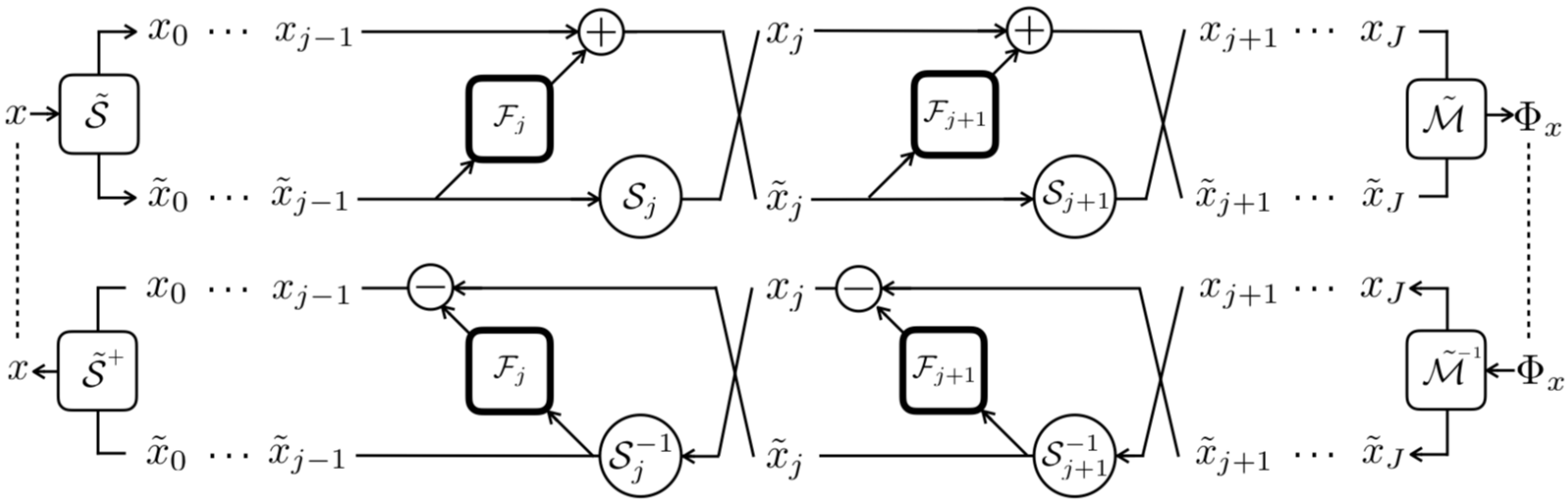
The success of deep convolutional networks is based on progressively discarding uninformative variability about the input with respect to the problem at hand.

Idea

Build a cascade of homeomorphic layers (i-RevNet), a network that can be fully inverted up to the final projection onto the classes, i.e. no information is discarded.

Jacobsen J. H., Smeulders A., Oyallon E. i-RevNet: Deep Invertible Networks, 2018

i-RevNet, 2018



Architecture	Injective	Bijective	Top-1 error	Parameters
ResNet	-	-	24.7	26M
RevNet	-	-	25.2	28M
i-RevNet (a)	yes	-	24.7	181M
i-RevNet (b)	yes	yes	26.7	29M

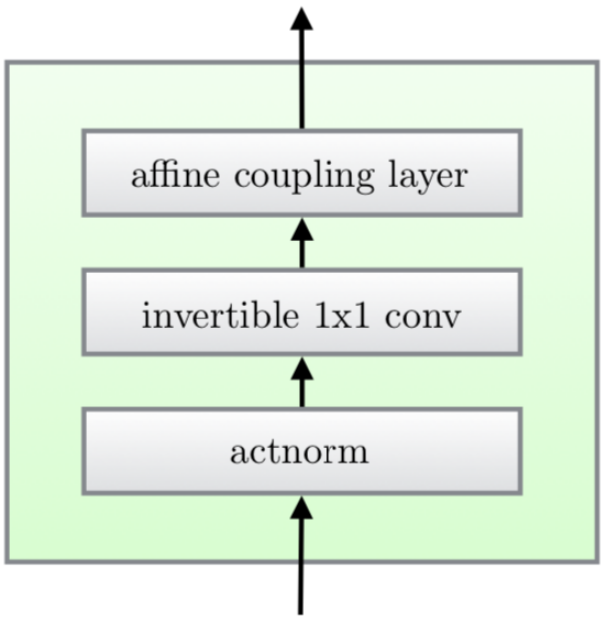
Jacobsen J. H., Smeulders A., Oyallon E. i-RevNet: Deep Invertible Networks, 2018

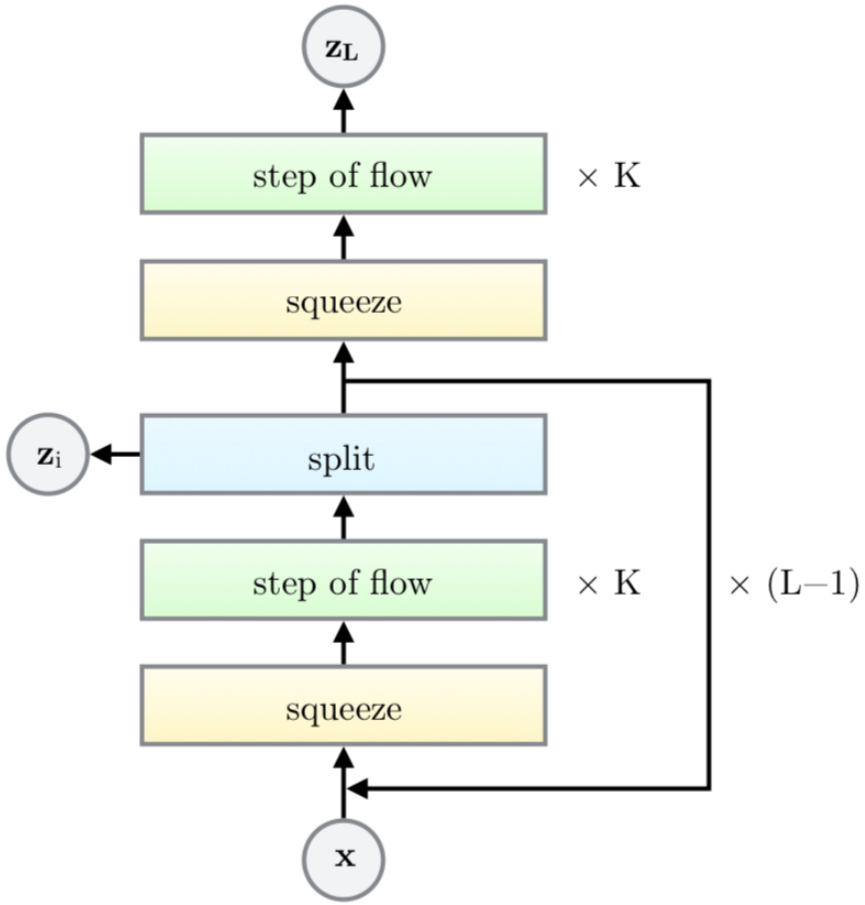
Glow, 2018

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

Glow, 2018

Model architecture





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

Glow, 2018

NICE

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

First step is **split** operator which decouples a 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 $O(c^3)$.

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

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)	$\mathbf{x}_a, \mathbf{x}_b = \texttt{split}(\mathbf{x})$ $(\log \mathbf{s}, \mathbf{t}) = \texttt{NN}(\mathbf{x}_b)$ $\mathbf{s} = \exp(\log \mathbf{s})$ $\mathbf{y}_a = \mathbf{s} \odot \mathbf{x}_a + \mathbf{t}$ $\mathbf{y}_b = \mathbf{x}_b$ $\mathbf{y} = \texttt{concat}(\mathbf{y}_a, \mathbf{y}_b)$	$\mathbf{y}_a, \mathbf{y}_b = \texttt{split}(\mathbf{y})$ $(\log \mathbf{s}, \mathbf{t}) = \texttt{NN}(\mathbf{y}_b)$ $\mathbf{s} = \exp(\log \mathbf{s})$ $\mathbf{x}_a = (\mathbf{y}_a - \mathbf{t})/\mathbf{s}$ $\mathbf{x}_b = \mathbf{y}_b$ $\mathbf{x} = \texttt{concat}(\mathbf{x}_a, \mathbf{x}_b)$	$\texttt{sum}(\log(\lvert\mathbf{s}\rvert))$

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

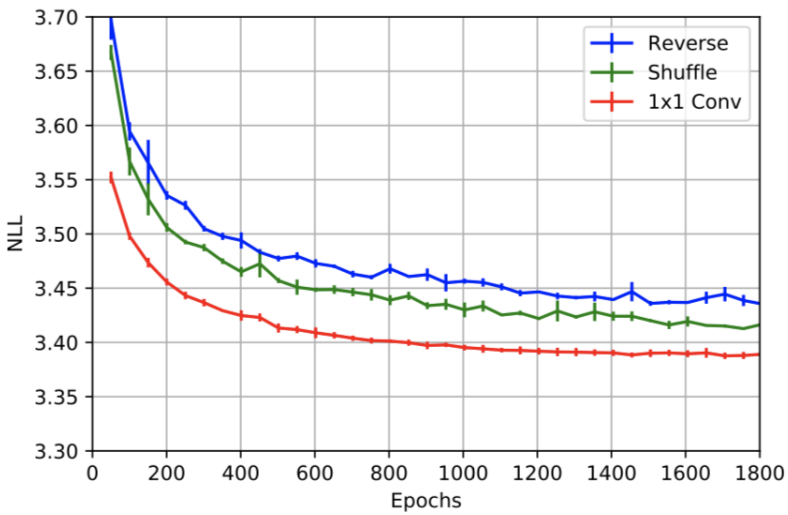
Glow, 2018

Invertible 1x1 conv

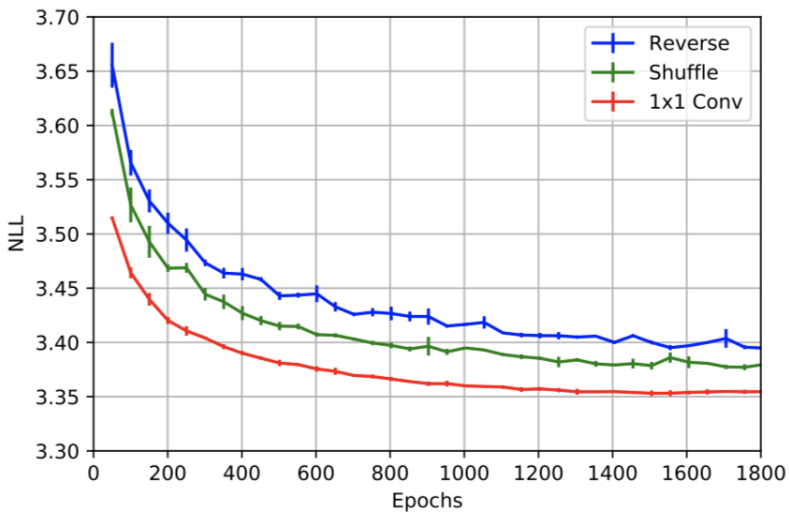
Cost to compute $\det(\mathbf{W})$ is $O(c^3)$. LU-decomposition reduces the cost to $O(c)$:

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

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.

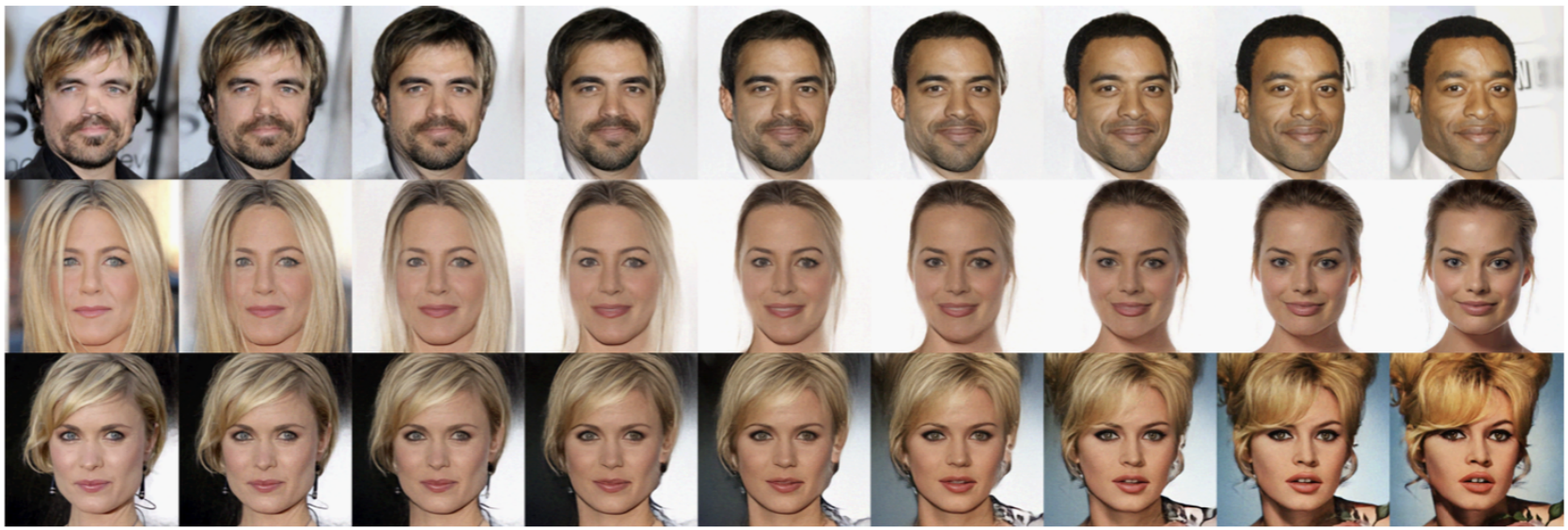


(b) Affine coupling.

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

Glow, 2018

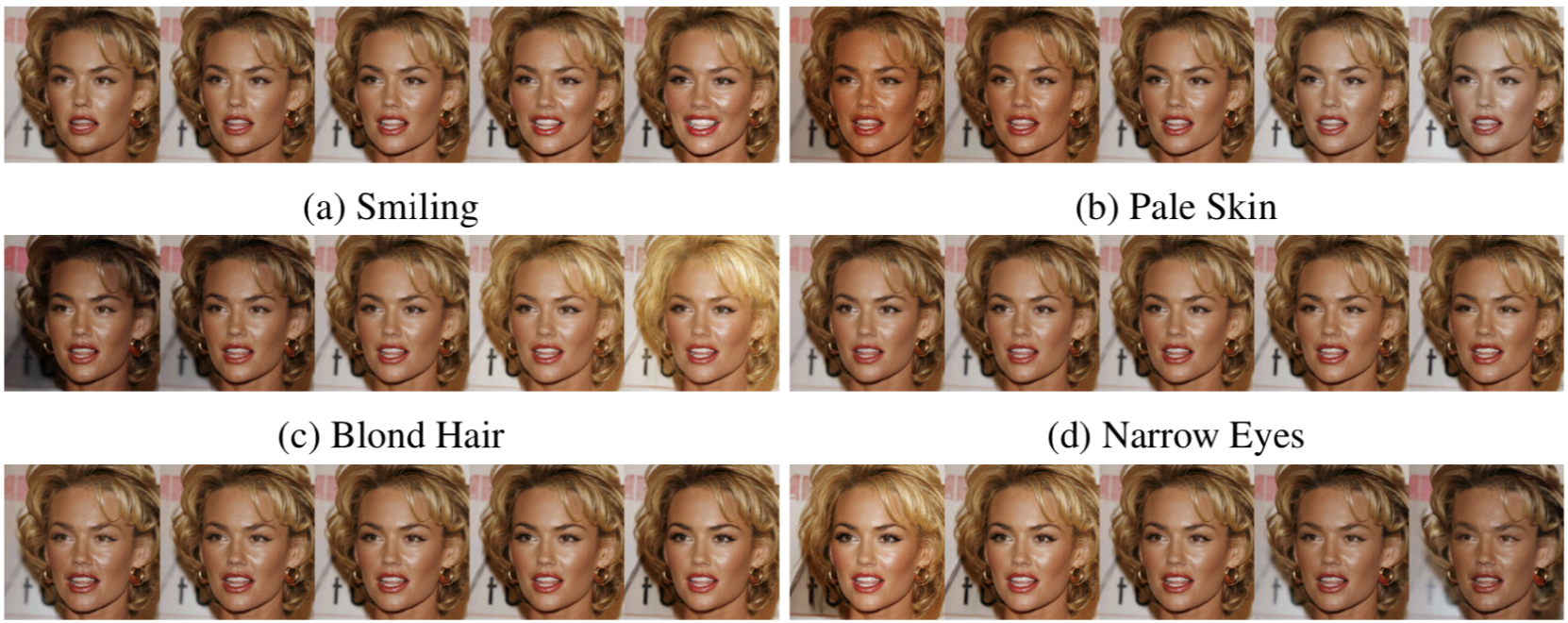
Face interpolation



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

Glow, 2018

Face attributes manipulation



(a) Smiling (b) Pale Skin

(c) Blond Hair (d) Narrow Eyes

(e) Young (f) Male

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

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.

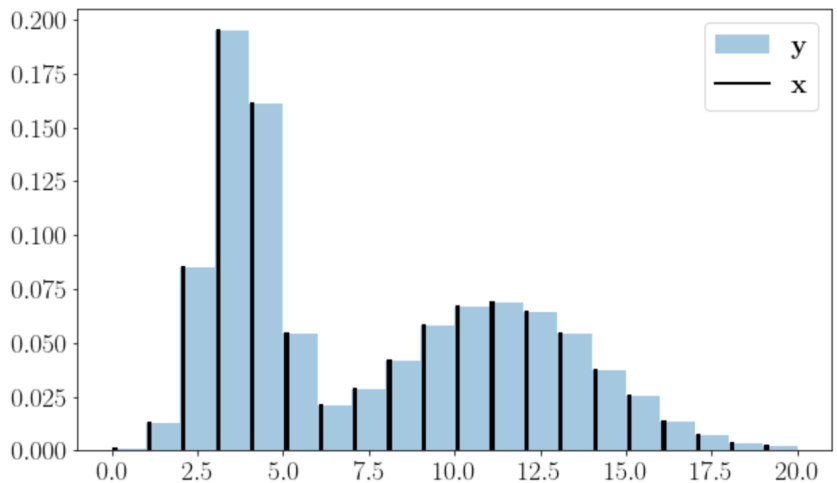
Dequantization

- 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 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:

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

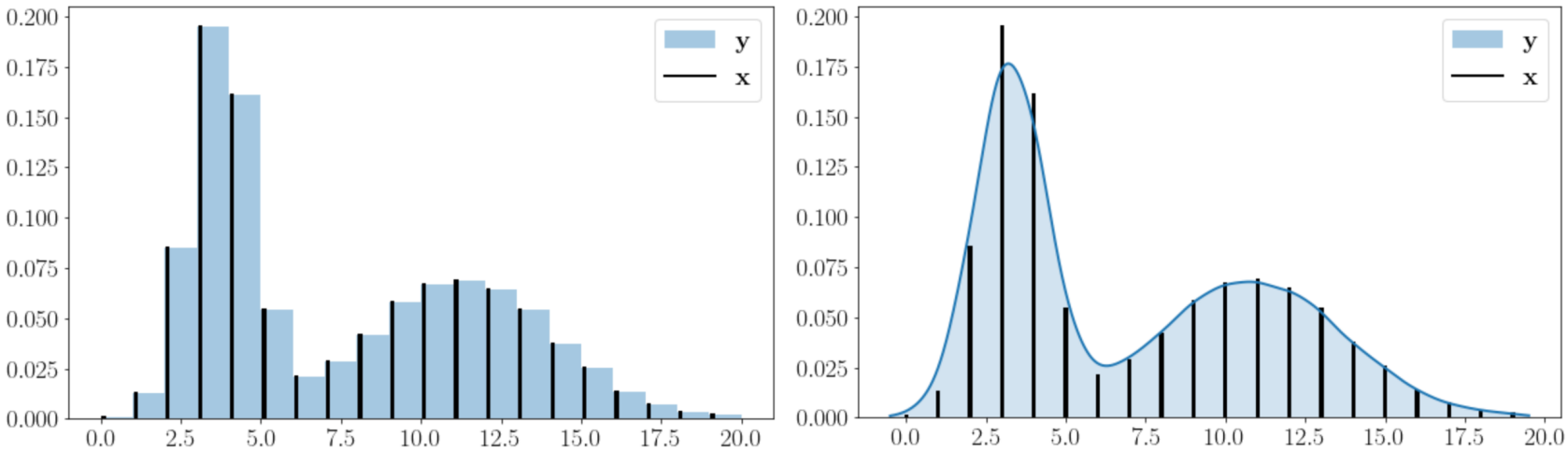
Thus, maximizing the log-likelihood of the continuous model on $\mathbf{y}$ cannot lead to the collapsing onto the discrete data (objective is bounded above by the log-likelihood of a discrete model).

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

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

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

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

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

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

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

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

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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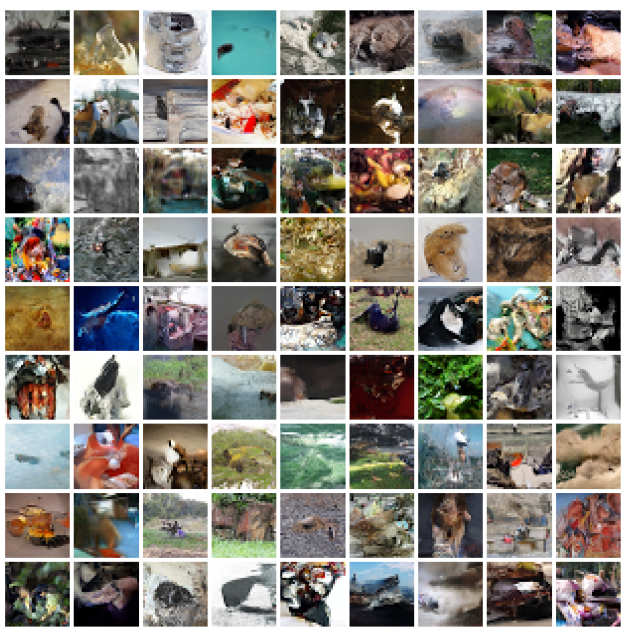
Flow++

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

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

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

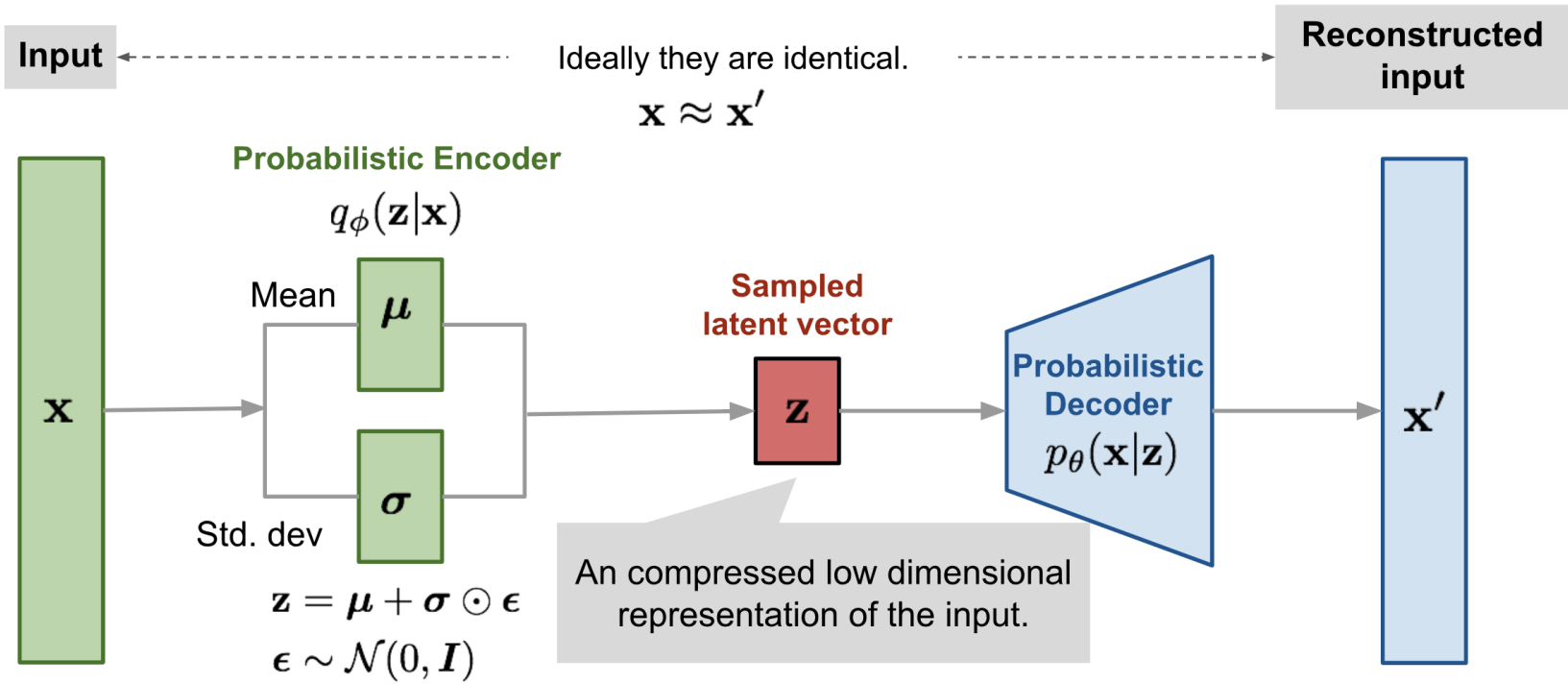


image credit:
https://lilianweng.github.io/lil-log/2018/08/12/from-autoencoder-to-beta-vae.html

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)

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

- 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 convert a simple base distribution to a compex 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

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

Here, $q(\mathbf{z}|\mathbf{x}, \phi)$ (which is a VAE encoder) plays a role of a base distribution.

$$\mathbf{z}_0 \xrightarrow{g_1} \mathbf{z}_1 \xrightarrow{g_2} \ldots \xrightarrow{g_K} \mathbf{z}_K, \quad \mathbf{z}_K = g(\mathbf{z}_0), \quad g = g_K \circ \cdots \circ g_1.$$

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

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

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

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 $q_K(\mathbf{z}_K|\mathbf{x}, \phi_*)$, $\phi_* = \{\phi, \phi_1, \ldots, \phi_K\}$ as a variational distribution.
Here ϕ – encoder parameters, $\{\phi\}_{k=1}^K$ – flow parameters.

ELBO objective

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

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

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

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

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

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 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

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

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: $\boldsymbol{\sigma} = \frac{1}{\hat{\boldsymbol{\sigma}}}; \quad \boldsymbol{\mu} = -\frac{\hat{\boldsymbol{\mu}}}{\hat{\boldsymbol{\sigma}}}.$

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

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

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

This process is **not** sequential.

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

Inverse autoregressive flow (IAF)

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

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

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

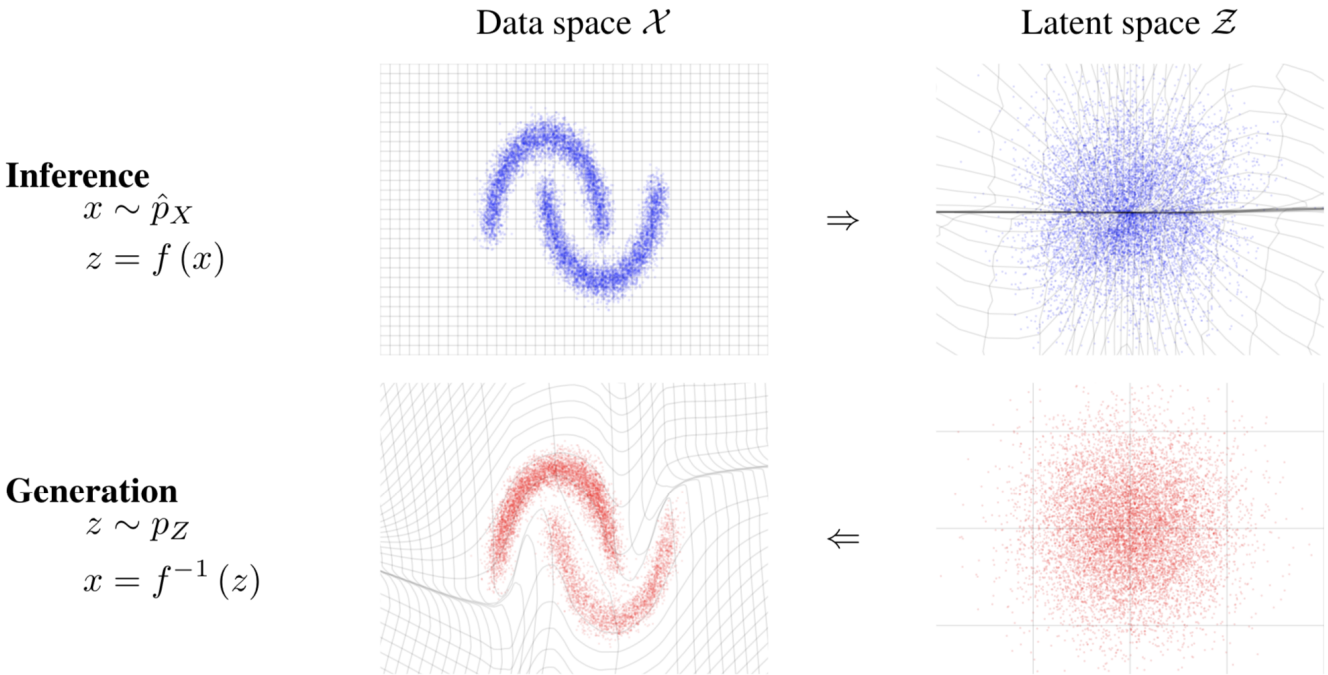
Inverse autoregressive flow use such inverted autoregressive model as a flow in VAE:

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

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

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

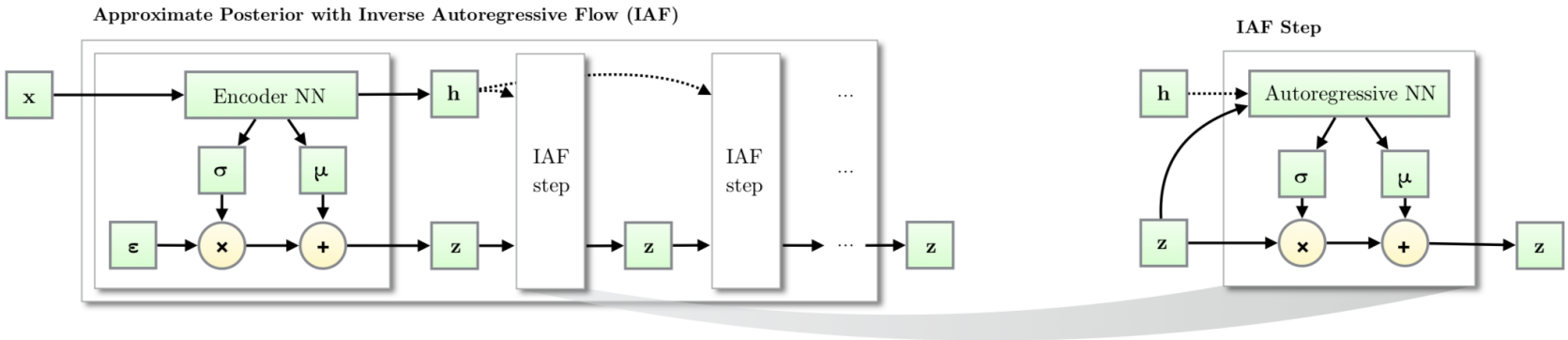
Flows

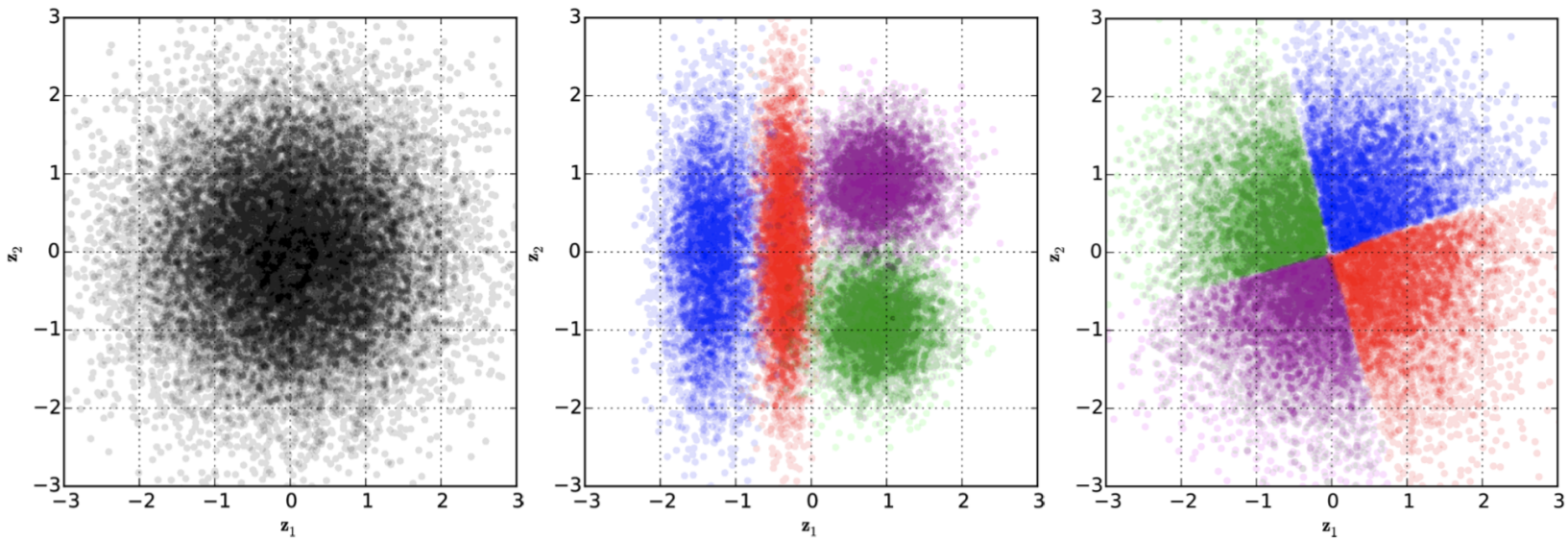


- Inference mode in autoregressive flows is used for density estimation tasks.
- Generation mode in autoregressive flows (IAF) is used for stochastic variational inference to get a more flexible posterior distribution.

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

Inverse autoregressive flow (IAF)





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

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

Summary

- Planar flows is a simple form of an invertible flow model (Sylvester flows are their extension). The NICE model is a more powerful type of flow.