Deep Generative Models
Lecture 4

Roman Isachenko

Moscow Institute of Physics and Technology

2020

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?

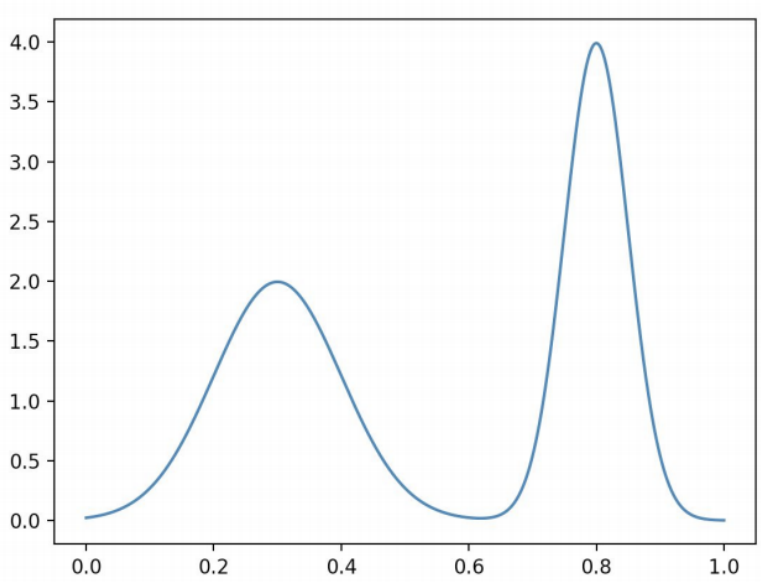
Flows intuition

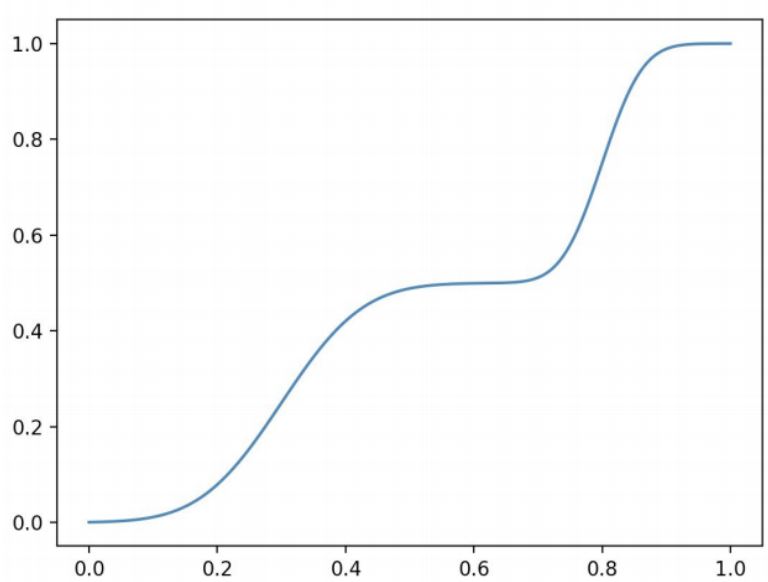
Let X be a random variable with density $p_X(x)$. Then

$$Z = F(X) = \int_{-\infty}^{x} p(t)dt \sim U[0, 1].$$

Hence

$$Z \sim U[0, 1]; \quad X = F^{-1}(Z) \quad X \sim p(x).$$





https://sites.google.com/view/berkeley-cs294-158-sp19/home

Change of variables

Theorem

Let

- $\mathbf{x}$ is a random variable,
- $f : \mathbb{R}^m \to \mathbb{R}^m$ is a differentiable, invertible function,
- $\mathbf{z} = f(\mathbf{x})$, $\mathbf{x} = f^{-1}(\mathbf{z}) = g(\mathbf{z})$.

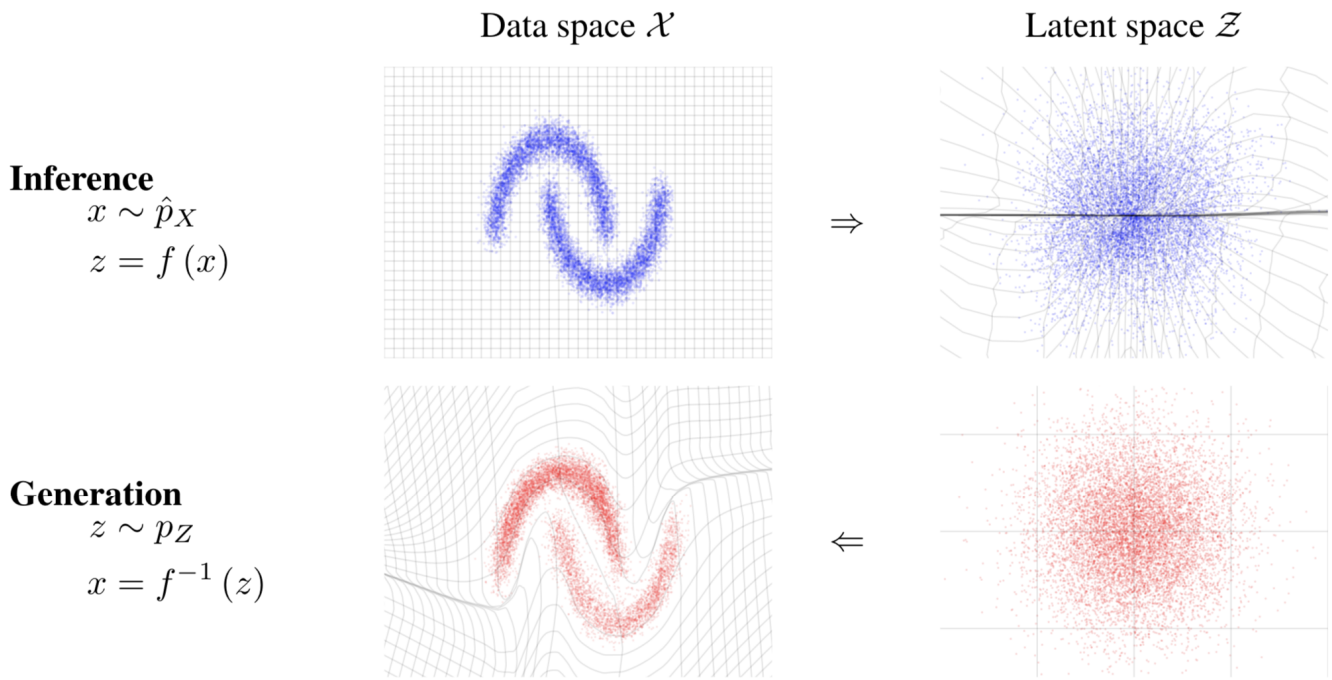
Then

$$p(\mathbf{x}) = p(\mathbf{z}) \left| \det \left(\frac{\partial \mathbf{z}}{\partial \mathbf{x}} \right) \right| = p(f(\mathbf{x})) \left| \det \left(\frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} \right) \right|.$$

Note

- $\mathbf{x}$ and $\mathbf{z}$ have the same dimensionality;
- $\left| \det \left(\frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} \right) \right| = \left| \det \left(\frac{\partial g^{-1}(\mathbf{x})}{\partial \mathbf{x}} \right) \right| = \left| \det \left(\frac{\partial g(\mathbf{z})}{\partial \mathbf{z}} \right) \right|^{-1}$;
- $f(\mathbf{x}, \boldsymbol{\theta})$ could be parametric.

Flows



- Likelihood is given by $\mathbf{z} = f(\mathbf{x}, \boldsymbol{\theta})$ and change of variables.
- Sampling of $\mathbf{x}$ is performed by sampling from a base distribution $p(\mathbf{z})$ and applying $\mathbf{x} = f^{-1}(\mathbf{z}, \boldsymbol{\theta}) = g(\mathbf{z}, \boldsymbol{\theta})$.
- Latent representation is given by $\mathbf{z} = f(\mathbf{x}, \boldsymbol{\theta})$.

---

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

Fitting flows

MLE problem

$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} p(\mathbf{X}|\boldsymbol{\theta}) = \arg\max_{\boldsymbol{\theta}} \prod_{i=1}^{n} p(\mathbf{x}_i|\boldsymbol{\theta}) = \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \log p(\mathbf{x}_i|\boldsymbol{\theta}).$$

Challenge

$p(\mathbf{x}|\boldsymbol{\theta})$ could be intractable.

Fitting flow to solve MLE

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

Stacking flows

Let $\mathbf{z} = f(\mathbf{x}) = f_2 \circ f_1(\mathbf{x})$ and f_1, f_2 satisfy conditions of change of variable theorem (differentiable and invertible).

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

$$= p(f(\mathbf{x})) \left| \det \left(\frac{\partial f_2 \circ f_1(\mathbf{x})}{\partial \mathbf{x}} \right) \right| = p(f(\mathbf{x})) \left| \det \left(\frac{\partial \mathbf{f}_2}{\partial \mathbf{f}_1} \cdot \frac{\partial \mathbf{f}_1}{\partial \mathbf{x}} \right) \right| =$$

$$= p(f(\mathbf{x})) \left| \det \left(\frac{\partial \mathbf{f}_2}{\partial \mathbf{f}_1} \right) \right| \cdot \left| \det \left(\frac{\partial \mathbf{f}_1}{\partial \mathbf{x}} \right) \right|$$

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 - convert data distribution to *noise*.
- Flow - sequence of such mapping is also a flow

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

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

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

Flows

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

What we want

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

Planar Flows, 2015

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

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

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

The transformation is invertible if (just one of example)

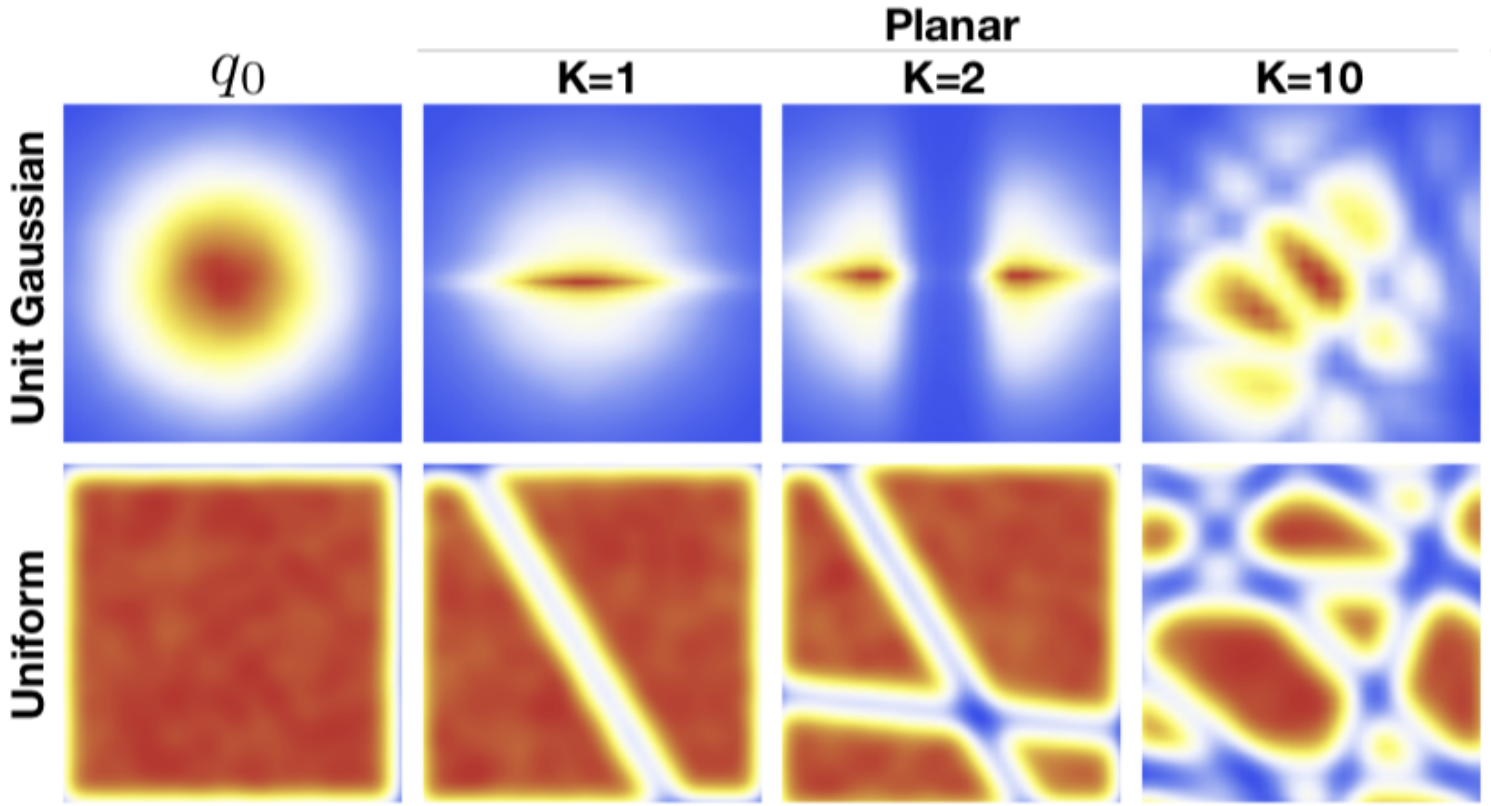
$$h = \tanh; \quad h'(\mathbf{w}^T\mathbf{z} + b)\mathbf{u}^T\mathbf{w} \geq -1.$$

---

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

Planar Flows, 2015

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



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

Jacobian structure

- What is the 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 the 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 inverse of such transformations?

NICE, 2014

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;
- $\tau : \mathbb{R}^{m-d} \times c(\mathbb{R}^d) \to \mathbb{R}^{m-d}$ – coupling law.
- $$\det\left(\frac{\partial \mathbf{z}}{\partial \mathbf{x}}\right) = \det\begin{pmatrix} \mathbf{I}_d & 0_{d\times m-d} \\ \frac{\partial \mathbf{z}_{d:m}}{\partial \mathbf{x}_{1:d}} & \frac{\partial \mathbf{z}_{d:m}}{\partial \mathbf{x}_{d:m}} \end{pmatrix} = \det\left(\frac{\partial \mathbf{z}_{d:m}}{\partial \mathbf{x}_{d:m}}\right)$$

---

https://arxiv.org/pdf/1410.8516.pdf

NICE, 2014

Coupling layer

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

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!).

https://arxiv.org/pdf/1410.8516.pdf

NICE, 2014

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

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:

$$z_i = s_i x_i; \quad x_i = z_i / s_i.$$

What is the Jacobian of the last layer?

---

https://arxiv.org/pdf/1410.8516.pdf

NICE, 2014

(a) Model trained on MNIST

(b) Model trained on TFD

---

https://arxiv.org/pdf/1410.8516.pdf

RealNVP, 2016

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

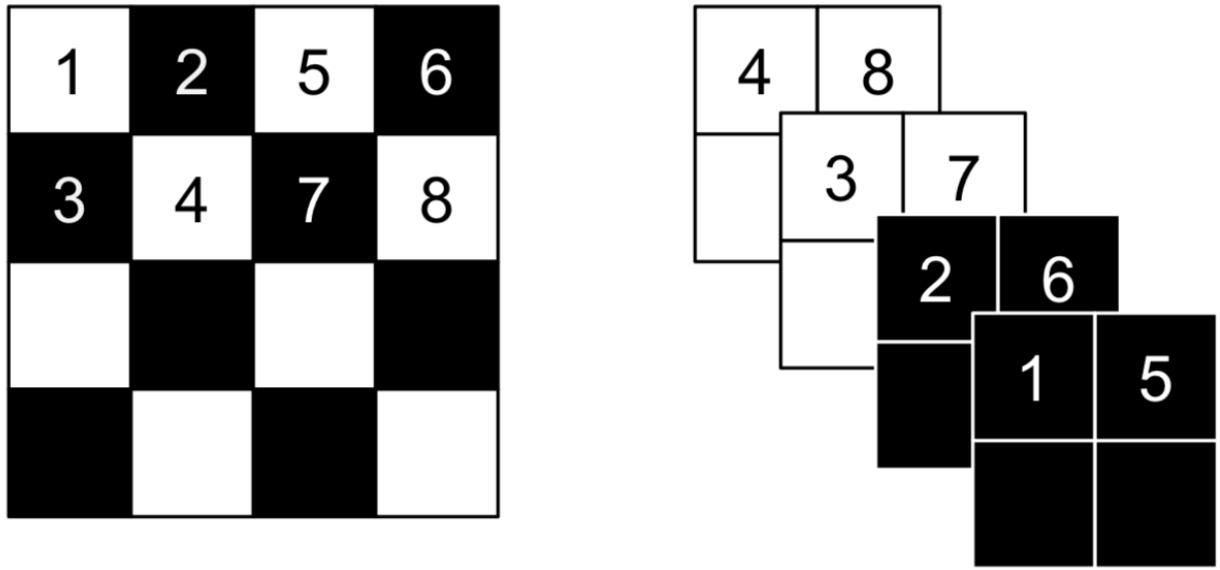
$$\det\left(\frac{\partial \mathbf{z}}{\partial \mathbf{x}}\right) = \det\begin{pmatrix} \mathbf{I}_d & 0_{d\times m-d} \\ \frac{\partial \mathbf{z}_{d:m}}{\partial \mathbf{x}_{1:d}} & \frac{\partial \mathbf{z}_{d:m}}{\partial \mathbf{x}_{d:m}} \end{pmatrix} = \prod_{i=1}^{m-d} \exp(c_1(\mathbf{x}_{1:d},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

Non-Volume Preserving.

---

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

RealNVP, 2016

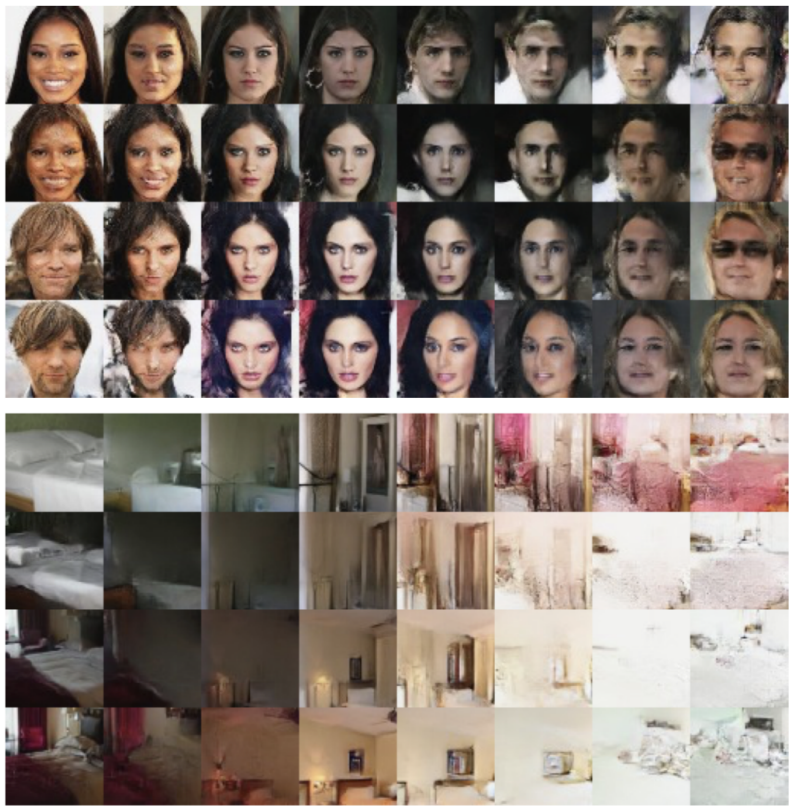


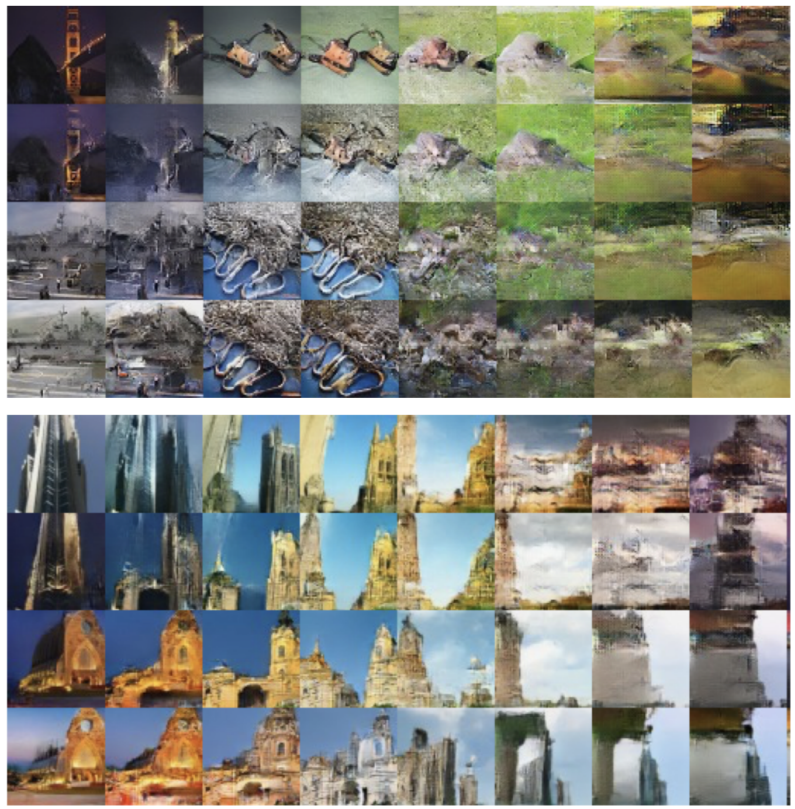
Masked convolutions are used to define ordering.

---

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

RealNVP, 2016

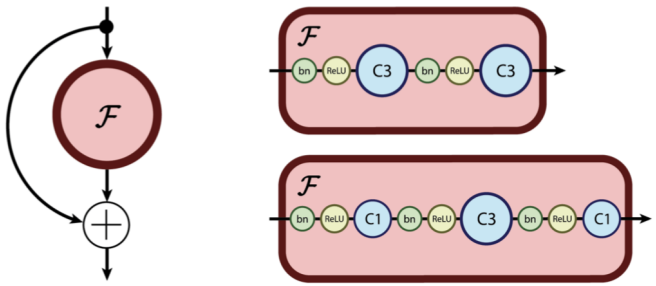




https://arxiv.org/pdf/1605.08803.pdf

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).

---

https://arxiv.org/pdf/1707.04585.pdf

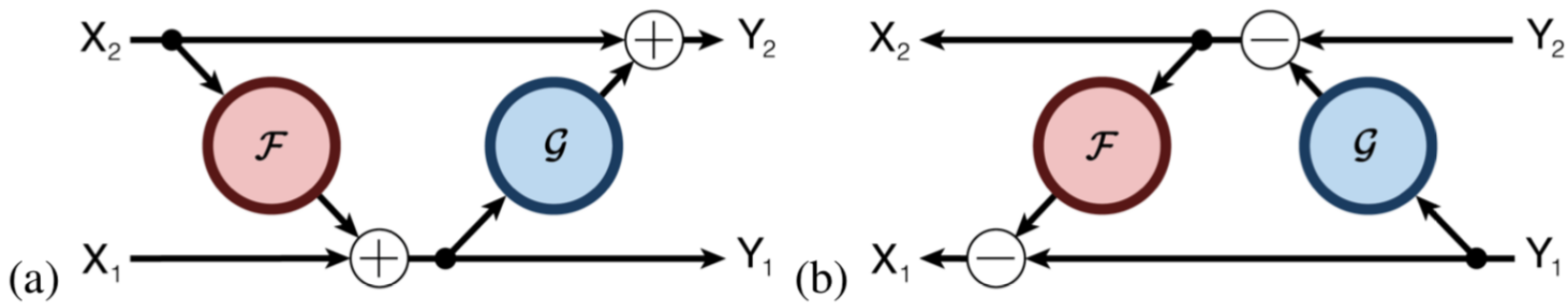
RevNets, 2017

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

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



https://arxiv.org/pdf/1707.04585.pdf

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 this blocks should be stored.
- To avoid storing activations in the modern frameworks, the backward pass should be manually redefined.

---

https://arxiv.org/pdf/1707.04585.pdf

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 of recovering 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.

---

https://arxiv.org/pdf/1802.07088.pdf

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.

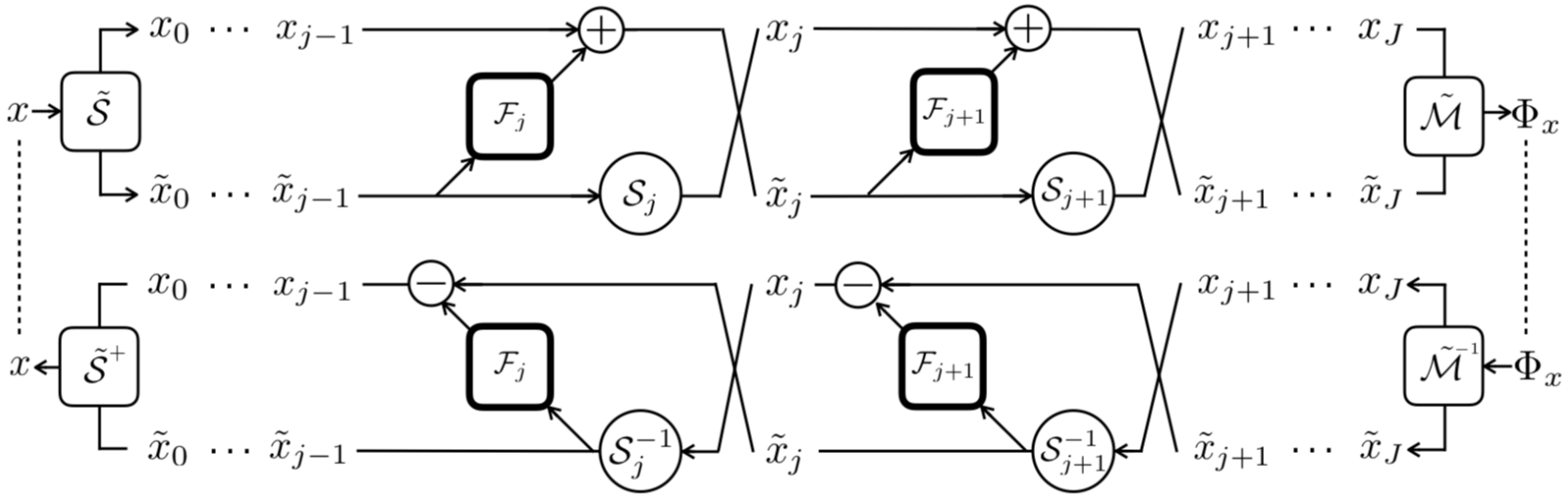
Idea

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.

---

https://arxiv.org/pdf/1802.07088.pdf

i-RevNet, 2018



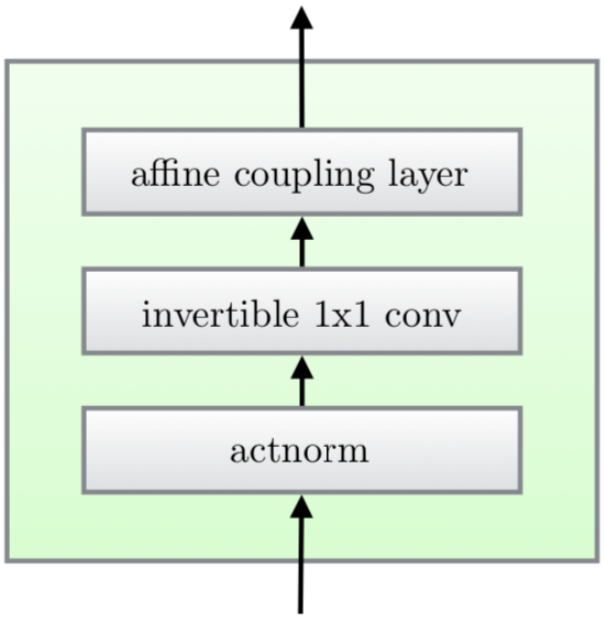
Architecture	Injective	Bijective	Top-1 error	Parameters
ResNet	-	-	24.7	26M
RevNet	-	-	25.2	28M
i-RevNet (a)	yes	-	24.7	181M
i-RevNet (b)	yes	yes	26.7	29M

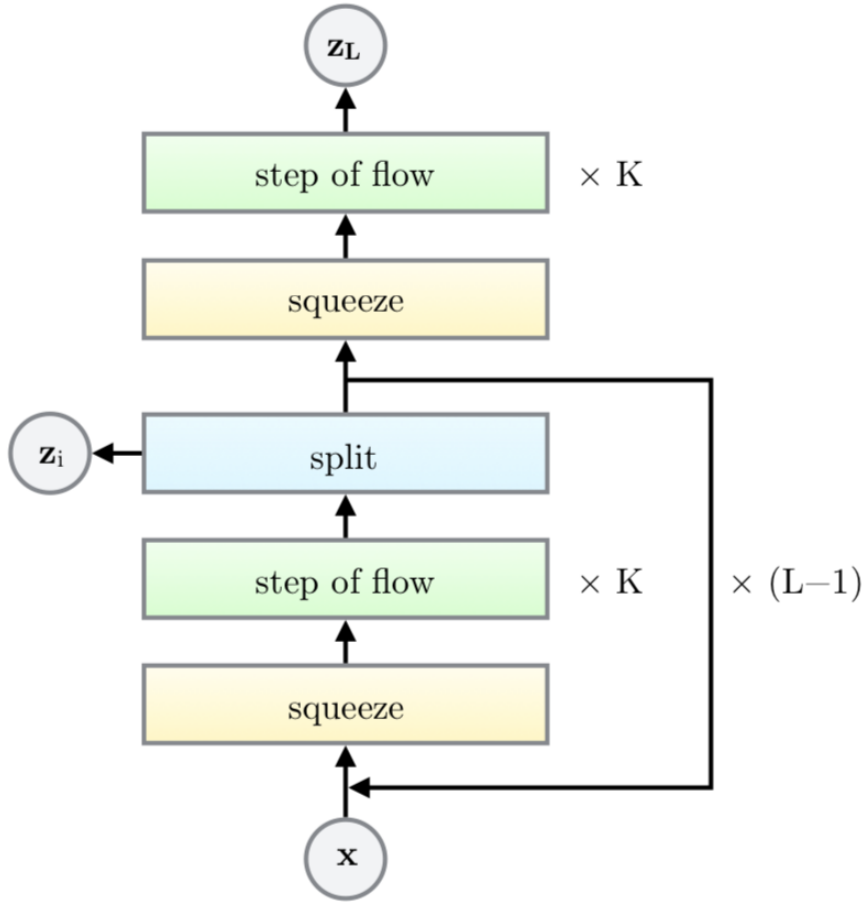
https://arxiv.org/pdf/1802.07088.pdf

Glow, 2018

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

Glow, 2018





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

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

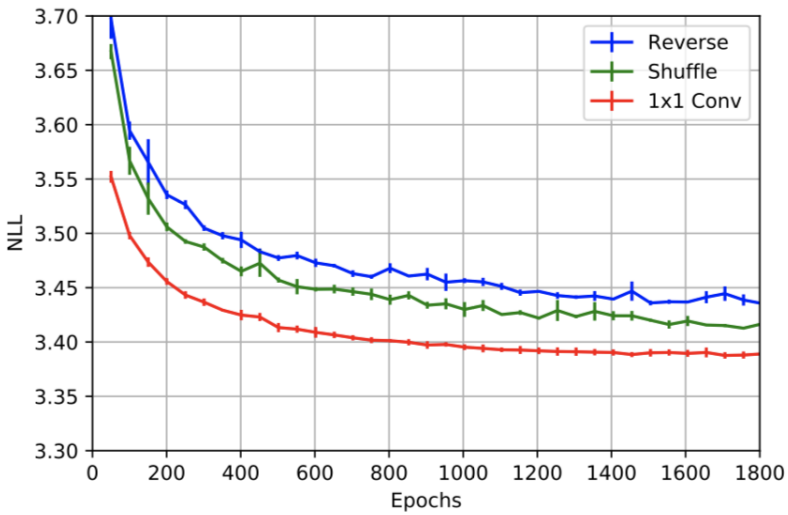
Glow, 2018

Invertible 1x1 conv

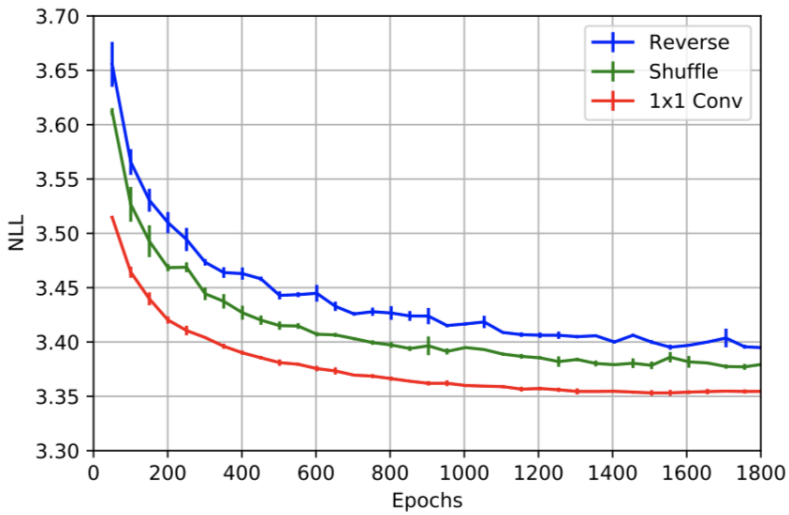
Cost to compute $\det(\mathbf{W})$ is $O(c^3)$.

LU-decomposition reduces the cost to $O(c)$:

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



(a) Additive coupling.



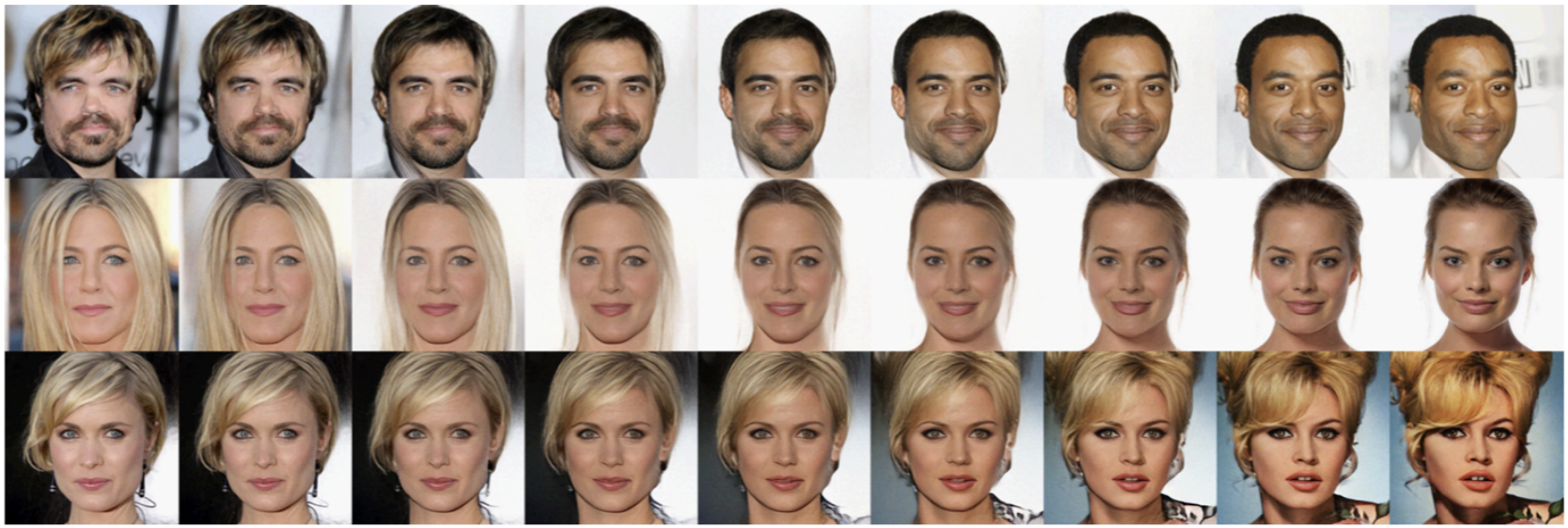
(b) Affine coupling.

---

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

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

References

- **NICE**: Non-linear Independent Components Estimation
  https://arxiv.org/abs/1410.8516
  Summary: Uses flows to model complex high-dimensional densities. Introduce the ways to compute determinant of Jacobian in a simple way. Triangular Jacobian, coupling layers, factorized 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.
- **RealNVP**: Density estimation using Real NVP
  https://arxiv.org/pdf/1605.08803.pdf
  Summary: Authors of NICE. The same idea and architecture, more practical. Lots of experiments and images. Coupling layers with checkerboard and channel-wise permutations.
- **RevNet:** The Reversible Residual Network: Backpropagation Without Storing Activations
  https://arxiv.org/abs/1707.04585
  Summary: RevNet allows not to store network activations. Each layer's activations can be computed from the next layer's activations. RevNets are composed of a series of reversible blocks. Could enable training larger and more powerful networks with limited computational resources.
- **i-RevNet:** Deep Invertible Networks
  https://arxiv.org/abs/1802.07088
  Summary: Invertible reversible networks. Remove noninvertible blocks (max-pooling, strides) from RevNets. Loss of information is not a necessary condition to learn representations that generalize well on hard problems, such as ImageNet.
- **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.