Deep Generative Models
Lecture 4

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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?

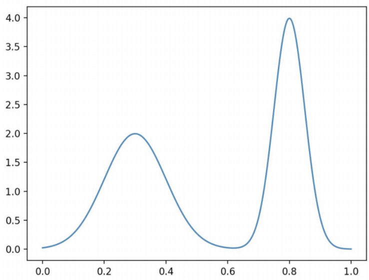
Flows intuition

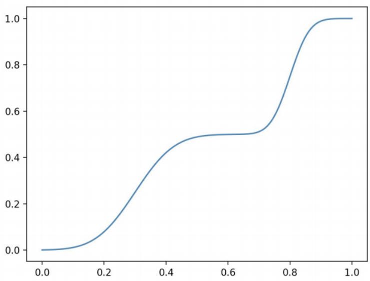
Let X be a random variable with density $p_X(x)$. Then

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

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,
- $\mathbf{z} = f(\mathbf{x})$, $\mathbf{x} = f^{-1}(\mathbf{z}) = g(\mathbf{z})$.

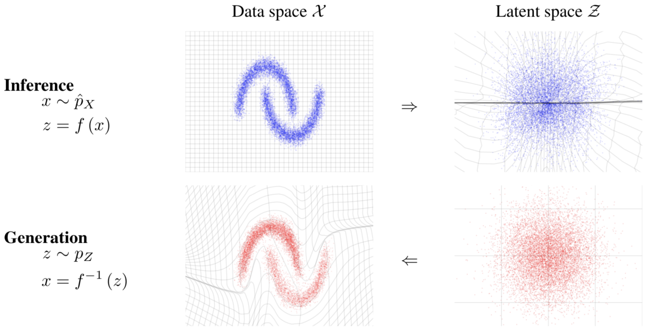
Then

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

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



- Latent representation is given by $\mathbf{z} = f(\mathbf{x}, \boldsymbol{\theta})$.
- 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 $\mathbf{x} = f^{-1}(\mathbf{z}, \boldsymbol{\theta}) = g(\mathbf{z}, \boldsymbol{\theta})$.

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).

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

What we will get in the case $\mathbf{z} = f(\mathbf{x}) = f_n \circ \dots \circ f_1(\mathbf{x})$?

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

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

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

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

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 is the computational comprexity of computing the determinant?

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

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

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

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

The transformation is invertible if (just one of example)

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

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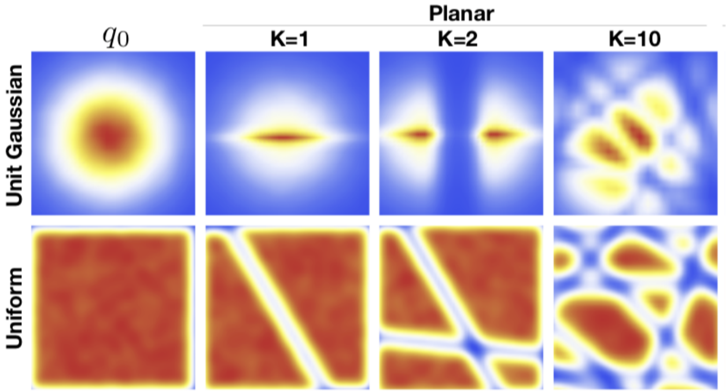
https://arxiv.org/pdf/1505.05770.pdf

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?

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

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

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

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

NICE, 2014

Coupling layer

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

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?

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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.

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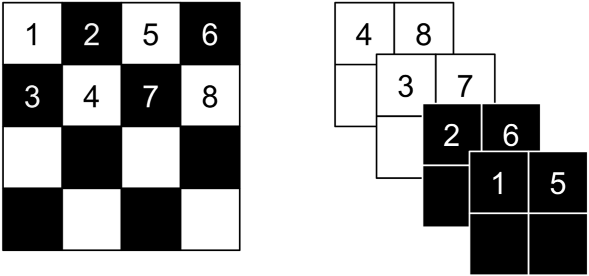
https://arxiv.org/pdf/1605.08803.pdf

RealNVP, 2016



Masked convolutions are used to define ordering.

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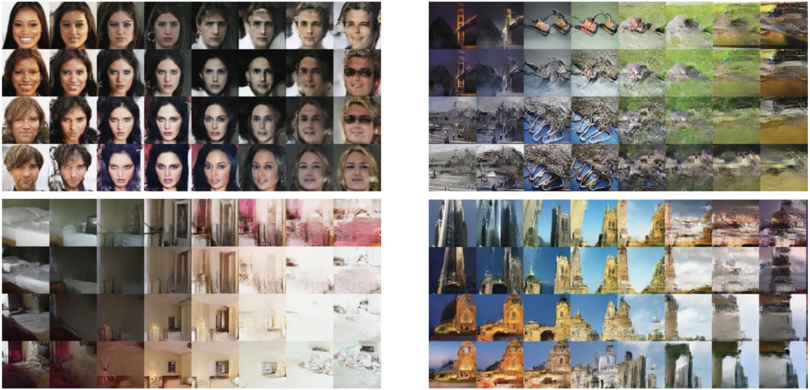
https://arxiv.org/pdf/1605.08803.pdf

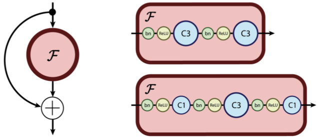
RealNVP, 2016



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).

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

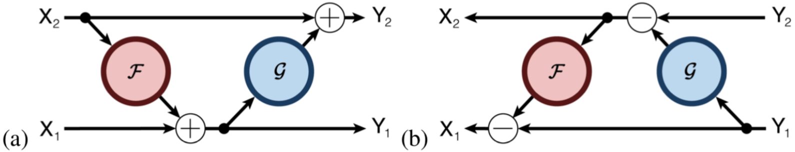
RevNets, 2017

NICE

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

RevNet

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



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.

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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.

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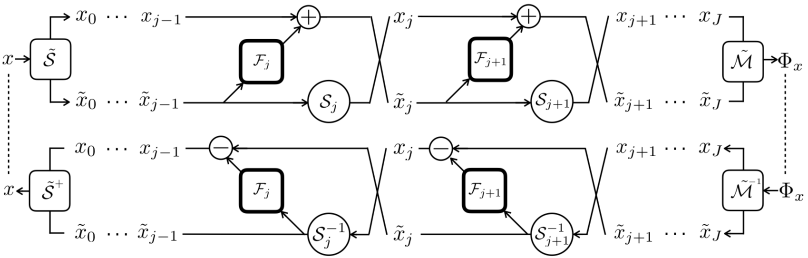
https://arxiv.org/pdf/1802.07088.pdf

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

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.