Deep Generative Models
Lecture 4

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Bayesian framework

Bayes theorem

$$p(\mathbf{t}|\mathbf{x}) = \frac{p(\mathbf{x}|\mathbf{t})p(\mathbf{t})}{p(\mathbf{x})} = \frac{p(\mathbf{x}|\mathbf{t})p(\mathbf{t})}{\int p(\mathbf{x}|\mathbf{t})p(\mathbf{t})d\mathbf{t}}$$

- $\mathbf{x}$ – observed variables, $\mathbf{t}$ – unobserved variables (latent variables/parameters);
- $p(\mathbf{x}|\mathbf{t})$ – likelihood;
- $p(\mathbf{x}) = \int p(\mathbf{x}|\mathbf{t})p(\mathbf{t})d\mathbf{t}$ – evidence;
- $p(\mathbf{t})$ – prior distribution, $p(\mathbf{t}|\mathbf{x})$ – posterior distribution.

Meaning

We have unobserved variables $\mathbf{t}$ and some prior knowledge about them $p(\mathbf{t})$. Then, the data $\mathbf{x}$ has been observed. Posterior distribution $p(\mathbf{t}|\mathbf{x})$ summarizes the knoweldge after the obbservations.

Variational Lower Bound

We are given the set of objects $\mathbf{X} = \{\mathbf{x}_i\}_{i=1}^n$. The goal is to perform bayesian inference on the unobserved variables $\mathbf{T} = \{\mathbf{t}_i\}_{i=1}^n$.

Evidence Lower Bound (ELBO)

$$\log p(\mathbf{X}) = \log \frac{p(\mathbf{X}, \mathbf{T})}{p(\mathbf{T}|\mathbf{X})} =$$
$$= \int q(\mathbf{T}) \log \frac{p(\mathbf{X}, \mathbf{T})}{p(\mathbf{T}|\mathbf{X})} d\mathbf{T} = \int q(\mathbf{T}) \log \frac{p(\mathbf{X}, \mathbf{T}) q(\mathbf{T})}{p(\mathbf{T}|\mathbf{X}) q(\mathbf{T})} d\mathbf{T} =$$
$$= \int q(\mathbf{T}) \log \frac{p(\mathbf{X}, \mathbf{T})}{q(\mathbf{T})} d\mathbf{T} + \int q(\mathbf{T}) \log \frac{q(\mathbf{T})}{p(\mathbf{T}|\mathbf{X})} d\mathbf{T} =$$
$$= \mathcal{L}(q) + KL(q(\mathbf{T}) || p(\mathbf{T}|\mathbf{X})) \geq \mathcal{L}(q).$$

We would like to maximize lower bound $\mathcal{L}(q)$.

Mean field approximation

Independence assumption

$$q(\mathbf{T}) = \prod_{i=1}^{k} q_i(\mathbf{T}_i), \quad \mathbf{T} = [\mathbf{T}_1, \dots, \mathbf{T}_k],\ \mathbf{T}_j = \{\mathbf{t}_{ij}\}_{i=1}^{n},\ \mathbf{t}_i = \{\mathbf{T}_{ij}\}_{j=1}^{k}.$$

Block coordinate optimization of ELBO for $q_j(\mathbf{T}_j)$

$$\mathcal{L}(q) = \int q(\mathbf{T}) \log \frac{p(\mathbf{X}, \mathbf{T})}{q(\mathbf{T})} d\mathbf{T} = \int \left[\prod_{i=1}^{k} q_i(\mathbf{T}_i)\right] \log \frac{p(\mathbf{X}, \mathbf{T})}{\left[\prod_{i=1}^{k} q_i(\mathbf{T}_i)\right]} \prod_{i=1}^{k} d\mathbf{T}_i =$$

$$= \int \left[\prod_{i=1}^{k} q_i\right] \log p(\mathbf{X}, \mathbf{T}) \prod_{i=1}^{k} d\mathbf{T}_i - \sum_{i=1}^{k} \int \left[\prod_{j=1}^{k} q_j\right] \log q_i \prod_{j=1}^{k} d\mathbf{T}_j =$$

$$= \int q_j \left[\int \log p(\mathbf{X}, \mathbf{T}) \prod_{i \neq j} q_i d\mathbf{T}_i\right] d\mathbf{T}_j -$$

$$- \int q_j \log q_j d\mathbf{T}_j + \text{const}(q_j) \to \max_{q_j}$$

Mean field approximation

Block coordinate optimization of ELBO for $q_j(\mathbf{T}_j)$

$$\mathcal{L}(q) = \int q_j \left[\int \log p(\mathbf{X}, \mathbf{T}) \prod_{i \neq j} q_i d\mathbf{T}_i \right] d\mathbf{T}_j - \int q_j \log q_j d\mathbf{T}_j + \text{const}(q_j) =$$

$$= \int q_j \log \hat{p}(\mathbf{X}, \mathbf{T}_j) d\mathbf{T}_j - \int q_j \log q_j d\mathbf{T}_j + \text{const}(q_j) \to \max_{q_j}.$$

Here we introduce

$$\log \hat{p}(\mathbf{X}, \mathbf{T}_j) = \int \log p(\mathbf{X}, \mathbf{T}) \prod_{i \neq j} q_i d\mathbf{T}_i = \mathbb{E}_{i \neq j} \log p(\mathbf{X}, \mathbf{T}) + \text{const}(q_j)$$

Final ELBO derivation for $q_j(\mathbf{T}_j)$

$$\mathcal{L}(q) = \int q_j(\mathbf{T}_j) \log \hat{p}(\mathbf{X}, \mathbf{T}_j) d\mathbf{T}_j - \int q_j(\mathbf{T}_j) \log q_j(\mathbf{T}_j) d\mathbf{T}_j + \text{const}(q_j) =$$

$$\int q_j(\mathbf{T}_j) \log \frac{\hat{p}(\mathbf{X}, \mathbf{T}_j)}{q_j(\mathbf{T}_j)} d\mathbf{T}_j + \text{const}(q_j) =$$

$$= -KL(q_j(\mathbf{T}_j) || \hat{p}(\mathbf{X}, \mathbf{T}_j)) + \text{const}(q_j) \to \max_{q_j}.$$

Mean field approximation

Independence assumption

$$q(\mathbf{T}) = \prod_{i=1}^{k} q_i(\mathbf{T}_i), \quad \mathbf{T} = [\mathbf{T}_1, \dots, \mathbf{T}_k], \quad \mathbf{T}_j = \{\mathbf{t}_{ij}\}_{i=1}^{n}.$$

ELBO

$$\mathcal{L}(q) = -KL(q_j(\mathbf{T}_j) || \hat{p}(\mathbf{X}, \mathbf{T}_j)) + \mathrm{const}(q_j) \to \max_{q_j}.$$

Solution

$$q_j(\mathbf{T}_j) = \mathrm{const} \cdot \hat{p}(\mathbf{X}, \mathbf{T}_j)$$

$$\log \hat{p}(\mathbf{X}, \mathbf{T}_j) = \mathbb{E}_{i \neq j} \log p(\mathbf{X}, \mathbf{T}) + \mathrm{const}$$

$$\log q_j(\mathbf{T}_j) = \mathbb{E}_{i \neq j} \log p(\mathbf{X}, \mathbf{T}) + \mathrm{const}$$

Mean field approximation

ELBO

$$\mathcal{L}(q) = -KL(q_j(\mathbf{T}_j)||\hat{p}(\mathbf{X}, \mathbf{T}_j)) + \text{const}(q_j) \to \max_{q_j}.$$

Solution

$$\log q_j(\mathbf{T}_j) = \mathbb{E}_{i \neq j} \log p(\mathbf{X}, \mathbf{T}) + \text{const}$$

Let assume

- $\mathbf{T} = [\mathbf{T}_1, \mathbf{T}_2] = [\mathbf{Z}, \boldsymbol{\theta}]$, $q(\mathbf{T}) = q(\mathbf{T}_1) \cdot q(\mathbf{T}_2) = q(\mathbf{Z}) \cdot q(\boldsymbol{\theta})$.
- restrict the class of probability distribution for $\boldsymbol{\theta}$ to Dirac delta functions:
  $$q_2 = q(\mathbf{T}_2) = q(\boldsymbol{\theta}) = \delta(\boldsymbol{\theta} - \boldsymbol{\theta}^*).$$
  Under the restrictions the exact solution for q_2 is not reached (KL could be greater than 0).

Mean field approximation

General solution

$$\log q_j(\mathbf{T}_j) = \mathbb{E}_{i \neq j} \log p(\mathbf{X}, \mathbf{T}) + \text{const}$$

Solution for $q_1 = q(\mathbf{Z})$

$$\log q(\mathbf{Z}) = \int q(\boldsymbol{\theta}) \log p(\mathbf{X}, \mathbf{Z}, \boldsymbol{\theta}) d\boldsymbol{\theta} + \text{const} =$$

$$= \int \delta(\boldsymbol{\theta} - \boldsymbol{\theta}^*) \log p(\mathbf{X}, \mathbf{Z}, \boldsymbol{\theta}) d\boldsymbol{\theta} + \text{const} =$$

$$= \log p(\mathbf{Z} | \mathbf{X}, \boldsymbol{\theta}^*) + \text{const}.$$

EM-algorithm (E-step)

$$q(\mathbf{Z}) = \arg\max_q \mathcal{L}(q, \boldsymbol{\theta}^*) = \arg\min_q KL(q || p) = p(\mathbf{Z} | \mathbf{X}, \boldsymbol{\theta}^*).$$

Mean field approximation

ELBO

$$\mathcal{L}(q) = -KL(q_j(\mathbf{T}_j)||\hat{p}(\mathbf{X}, \mathbf{T}_j)) + \text{const}(q_j) \to \max_{q_j}.$$

ELBO maximization w.r.t. $q_2 = q(\boldsymbol{\theta}) = \delta(\boldsymbol{\theta} - \boldsymbol{\theta}^*)$

$$\begin{aligned}
\mathcal{L}(q_1, q_2) &= -KL(q(\boldsymbol{\theta})||\hat{p}(\mathbf{X}, \boldsymbol{\theta})) + \text{const}(\boldsymbol{\theta}^*) \\
&= \int q(\boldsymbol{\theta}) \log \frac{\hat{p}(\mathbf{X}, \boldsymbol{\theta})}{q(\boldsymbol{\theta})} d\boldsymbol{\theta} + \text{const}(\boldsymbol{\theta}^*) \\
&= \int q(\boldsymbol{\theta}) \log \hat{p}(\mathbf{X}, \boldsymbol{\theta}) d\boldsymbol{\theta} - \int q(\boldsymbol{\theta}) \log q(\boldsymbol{\theta}) d\boldsymbol{\theta} + \text{const}(\boldsymbol{\theta}^*) \\
&= \int \delta(\boldsymbol{\theta} - \boldsymbol{\theta}^*) \log \hat{p}(\mathbf{X}, \boldsymbol{\theta}) d\boldsymbol{\theta} + \text{const}(\boldsymbol{\theta}^*) \to \max_{\boldsymbol{\theta}^*}
\end{aligned}$$

Mean field approximation

ELBO maximization w.r.t. $q_2 = q(\boldsymbol{\theta}) = \delta(\boldsymbol{\theta} - \boldsymbol{\theta}^*)$

$$\mathcal{L}(q_1, q_2) = \int \delta(\boldsymbol{\theta} - \boldsymbol{\theta}^*) \log \hat{p}(\mathbf{X}, \boldsymbol{\theta}) d\boldsymbol{\theta} + \text{const} = \log \hat{p}(\mathbf{X}, \boldsymbol{\theta}^*) + \text{const}$$

$$= \mathbb{E}_{i \neq j} \log p(\mathbf{X}, \mathbf{T}) + \text{const} = \mathbb{E}_{q_1} \log p(\mathbf{X}, \mathbf{Z}, \boldsymbol{\theta}^*) + \text{const}$$

$$= \int q(\mathbf{Z}) \log p(\mathbf{X}, \mathbf{Z} | \boldsymbol{\theta}^*) d\mathbf{Z} + \log p(\boldsymbol{\theta}^*) + \text{const} \to \max_{\boldsymbol{\theta}^*}$$

EM-algorithm (M-step)

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

$$= \int q(\mathbf{Z}) \log p(\mathbf{X}, \mathbf{Z} | \boldsymbol{\theta}) d\mathbf{Z} + \text{const} \to \max_{\boldsymbol{\theta}}$$

Mean field approximation

Solution

$$\log q_j(\mathbf{T}_j) = \mathbb{E}_{i \neq j} \log p(\mathbf{X}, \mathbf{T}) + \text{const}$$

EM algorithm (special case)

- Initialize $\boldsymbol{\theta}^*$;
- E-step

$$q(\mathbf{Z}) = \arg\max_q \mathcal{L}(q, \boldsymbol{\theta}^*) = \arg\min_q KL(q||p) = p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}^*);$$

- M-step

$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} \mathcal{L}(q, \boldsymbol{\theta});$$

- Repeat E-step and M-step until convergence.

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

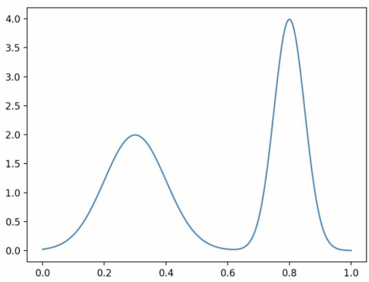
Let ξ be a random variable with density $p(\xi)$. Then

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

$$P(\eta < y) = P(F(\xi) < y) = P(\xi < F^{-1}(y)) = F(F^{-1}(y)) = y$$

Hence

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



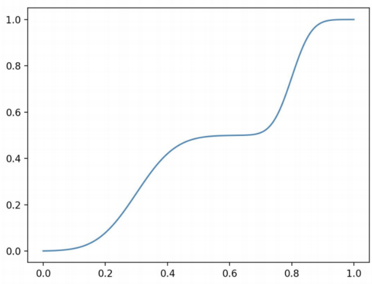


image credit: https://sites.google.com/view/berkeley-cs294-158-sp19/home

Flows intuition

- Let $\mathbf{z} \sim p(\mathbf{z})$ is a random variable with base distribution $p(\mathbf{z}) = U[0,1]^m$.
- Let $\mathbf{x} \sim p(\mathbf{x})$ is a random variable with complex distribution $p(\mathbf{x})$ and cdf $F(\mathbf{x})$.
- Then noise variable $\mathbf{z}$ could be transformed to $\mathbf{x}$ using inverse cdf F^{-1} ($\mathbf{x} = F^{-1}(\mathbf{z})$).

How to transform random variable $\mathbf{z}$ which have distribution different from uniform to $\mathbf{x}$?

- Let $\mathbf{z} \sim p(\mathbf{z})$ is a random variable with base distribution $p(\mathbf{z})$ and cdf $G(\mathbf{z})$.
- Then $\mathbf{z}_0 = G(\mathbf{z})$ has base distribution $p(\mathbf{z}_0) = U[0,1]^m$.
- Let $\mathbf{x} \sim p(\mathbf{x})$ is a random variable with complex distribution $p(\mathbf{x})$ and cdf $F(\mathbf{x})$.
- Then noise variable $\mathbf{z}$ could be transformed to $\mathbf{x}$ using cdf G and inverse cdf F^{-1} ($\mathbf{x} = F^{-1}(\mathbf{z}_0) = F^{-1}(G(\mathbf{z}))$).

Change of variables

Theorem

Let

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

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 (lies in $\mathbb{R}^m$);
- $\left| \det \left(\frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} \right) \right| = \left| \det \left(\frac{\partial g^{-1}(\mathbf{x})}{\partial \mathbf{x}} \right) \right| = \left| \det \left(\frac{\partial g(\mathbf{z})}{\partial \mathbf{z}} \right) \right|^{-1}$;
- $f(\mathbf{x}, \boldsymbol{\theta})$ could be parametric function.

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

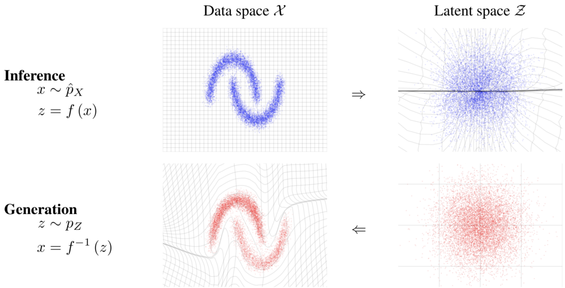
$p(\mathbf{x}|\boldsymbol{\theta})$ could be intractable.

Fitting flow to solve MLE

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

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

Flows



Computational requirement

- Evaluating model density $p(\mathbf{x}|\boldsymbol{\theta})$, we requires computing the transformation $\mathbf{z} = f(\mathbf{x}, \boldsymbol{\theta})$ and its Jacobian determinant $\left|\det\left(\frac{\partial f(\mathbf{x},\boldsymbol{\theta})}{\partial \mathbf{x}}\right)\right|$, and evaluating the density $p(\mathbf{z})$.
- Sampling $\mathbf{x}$ from the model requires the ability to sample from $p(\mathbf{z})$ and to compute the transformation $\mathbf{x} = g(\mathbf{z}, \boldsymbol{\theta}) = f^{-1}(\mathbf{z}, \boldsymbol{\theta})$.

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

Composition of flows

Theorem

Diffeomorphisms are **composable** (If Let f_1, f_2 satisfy conditions of the change of variable theorem (differentiable and invertible), then $\mathbf{z} = f(\mathbf{x}) = f_2 \circ f_1(\mathbf{x})$ also satisfy it).

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

What will we 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 **x** to the noise **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 that samples from $p(\mathbf{z})$ follow 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

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

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 $p(\mathbf{z})$;
- Efficient inversion of $f(\mathbf{x}, \boldsymbol{\theta})$.

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.

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

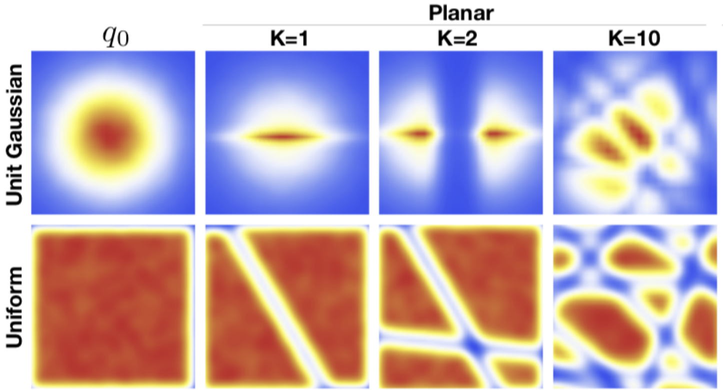
The transformation is invertible if (just one of example)

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

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

Planar Flows

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



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

Jacobian structure

- What is a 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 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 inverse 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;
- $\tau : \mathbb{R}^{m-d} \times c(\mathbb{R}^d) \to \mathbb{R}^{m-d}$ – 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

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

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!).

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

NICE

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

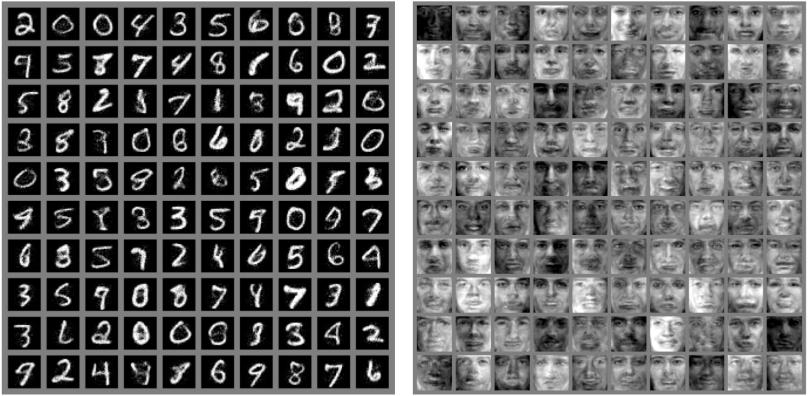
What is the Jacobian for the additive coupling law
$\tau(x + c) = x + c$?
In this case the transformation is *volume preserving*.
The last layer is rescaling:

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

What is the Jacobian of the last layer?

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

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

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

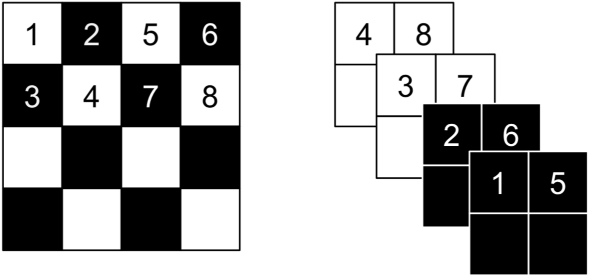
Jacobian

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

Non-Volume Preserving.

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

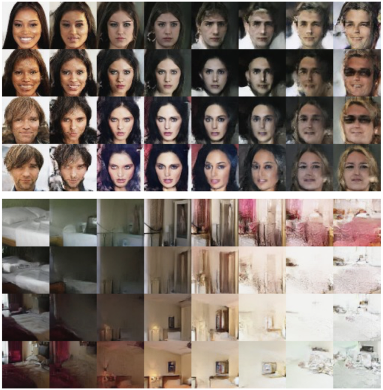
RealNVP

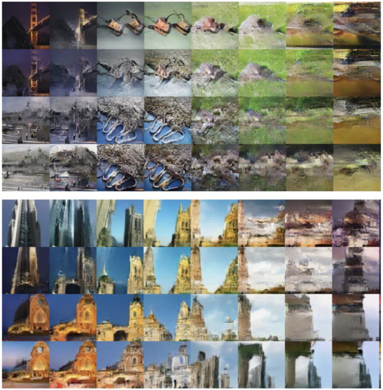


Masked convolutions are used to define ordering.

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

RealNVP

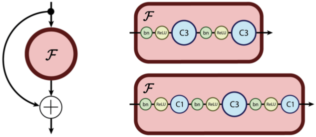




Dinh L., Sohl-Dickstein J., Bengio S. Density estimation using Real NVP, 2016

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

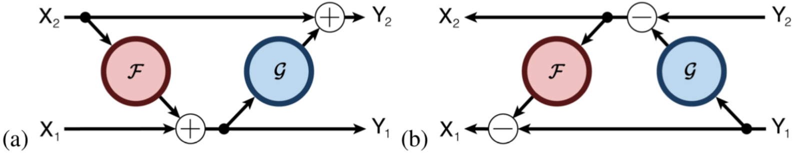
RevNets, 2017

NICE

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

RevNet

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



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

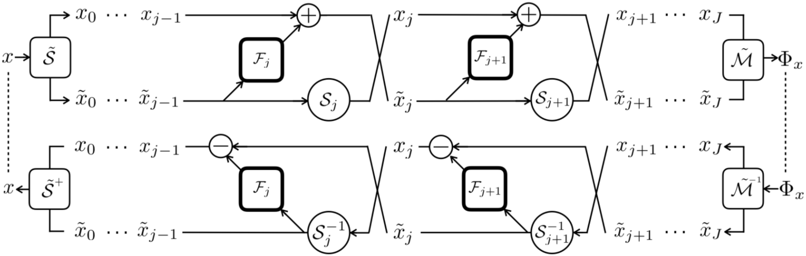
The success of deep convolutional networks is based on progressively discarding uninformative variability about the input with respect to the problem at hand.

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

Summary