Normalising Flows

Philip Schulz
https://vitutorial.github.io
https://github.com/vitutorial/VITutorial

The Case of Pictures

Have you modeled pixels as Gaussian variables? Do we really believe that the pixels follow a Gaussian distribution?

The case of Word Embeddings

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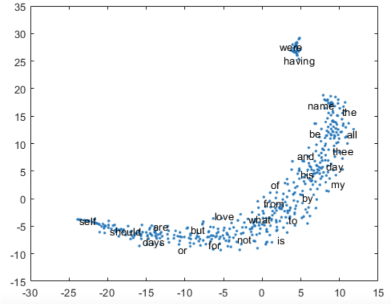

Figure: https://it.mathworks.com/help/textanalytics/ref/trainwordembedding.html

Posterior Approximations

We often use exponential families to approximate posteriors. Thus we assume unimodal posteriors. Is that realistic?

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Counter example

Gaussian mixture model

Recap: Change Of Variable

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The Jacobian matrix $J_{\mathcal{T}}(x)$ of $\mathcal{T}$
assessed at x is the matrix of partial derivatives

$$J_{ij} = \frac{\partial y_i}{\partial x_j}$$

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Inverse function theorem

$$J_{\mathcal{T}^{-1}}(y) = \left(J_{\mathcal{T}}(x)\right)^{-1}$$

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Express the density of a variable Y in terms of the density of a variable X. Assume that a differentiable, invertible mapping $h : \mathcal{X} \to \mathcal{Y}$ exists.

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The Challenge

The mapping h (or its inverse) needs to be defined.

Normalising Flows

Approach

Let's learn the transformation h (or its inverse).

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Problem

If we want to express $p(y)$ in terms of $p(x)$, we need to provide $|\det J_{h^{-1}}(y)|$ **in the forward pass**. But that's hard!

We are going to devise ways to get $|\det J_{h^{-1}}(y)|$.

Normalising Flows

Core Idea

Decompose mapping $h : \mathcal{X} \to \mathcal{Y}$ into

$$h = h_1 \circ h_2 \circ \ldots \circ h_K \ .$$

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$$h^{-1} = h_K^{-1} \circ h_{K-1}^{-1} \circ \ldots \circ h_1^{-1}$$
$$p_X(x) = p_Y(y) \left| \det J_{h_1} \left(y^{(1)}\right) \right| \left| \det J_{h_2} \left(y^{(2)}\right) \right| \ldots \left| \det J_{h_K} (x) \right|$$

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$$p_Y(y) = p_X(x) \left| \det J_{h_K^{-1}} \left(y^{(K-1)}\right) \right| \left| \det J_{h_{K-1}^{-1}} \left(y^{(K-2)}\right) \right| \ldots \left| \det J_{h_1^{-1}} (y) \right|$$

Normalising Flows

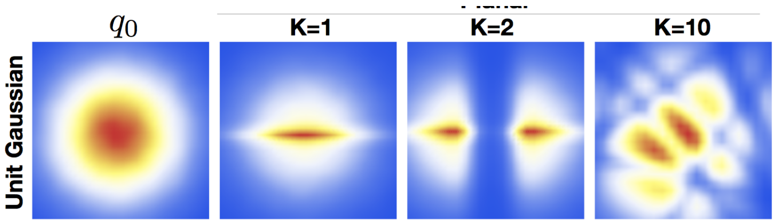

Figure: Taken from Rezende and Mohamed (2015)

Inverse Autoregressive Flows: Density Estimation

Setting

Our data x has unknown continuous density $p(x)$. We can therefore not handcraft a likelihood.

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$$\begin{aligned} p_X(x) &= p_\epsilon(\epsilon)\left|\det J_h(x)\right| \\ &= p_\epsilon(\epsilon)\left|\det J_{h_1}\left(\epsilon^{(1)}\right)\right|\left|\det J_{h_2}\left(\epsilon^{(2)}\right)\right|\ldots\left|\det J_{h_K}(x)\right| \end{aligned}$$

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&= p_\epsilon(h_1(\epsilon^{(1)}))\left|\det J_{h_1}\left(\epsilon^{(1)}\right)\right| \dots \left|\det J_{h_K}\left(x\right)\right|
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2-step Flow

$$p_X(x) = p_\epsilon(\overbrace{\epsilon}^{\epsilon^{(0)}})\left|\det J_{h_1}\left(\epsilon^{(1)}\right)\right|\left|\det J_{h_2}(x)\right|$$

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The transformations h_1 and h_2 are learned by backprop (while still being invertible). The determinants need to be computed analytically.

Designing a Transformation

Assume: $x = (x_1, x_2, \ldots x_M)$. Then factorise the density according to the chain rule.

$$\log p(x|\theta) = \sum_{j=1}^{M} \log p(x_j|x_{<j}\theta)$$

Next assume an invertible mapping $h(x_j) = \epsilon_j$.

Simple Mapping

$$h(x) = \epsilon$$
$$h^{-1}(\epsilon) = x$$

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Flow Mapping

$$h_1 \circ h_2 \circ \ldots \circ h_K(x) = \epsilon$$
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Designing a Transformation

MADE (Germain et al., 2015)

An autoregressive network that takes constant time. Its connectivity matrix is lower-triangular.

$$\begin{bmatrix} 0 & 0 & \cdots & 0 & 0 \\ 1 & 0 & \cdots & 0 & 0 \\ 1 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \cdots & \vdots & \vdots \\ 1 & 1 & \cdots & 1 & 0 \end{bmatrix}$$

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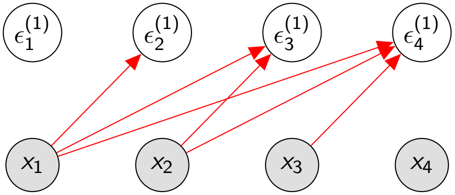

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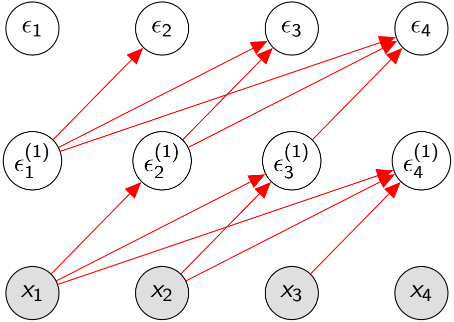

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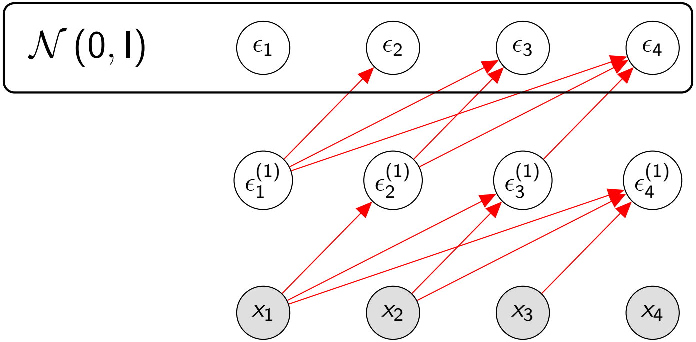

Designing a Transformation

We use a MADE $g_\theta^{(2)}$ to predict the parameters of the first transformation: $\begin{bmatrix}\mu_j & \sigma_j\end{bmatrix} = g_\theta^{(2)}(x_{<j})$. Then we apply the first transformation.

$$\epsilon_j^{(1)} = h_2(x)_j \ = \frac{x_j - \mu(x_{<j})}{\sigma(x_{<j})}$$

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$$J_{h_2}(x) = \mathrm{I}\,\sigma^{-1} + J_{\frac{-\mu}{\sigma}}(x)$$

Designing a Transformation

Define $\alpha_{lj} = \frac{d}{dx_l}\frac{-\mu_j}{\sigma_j}$.

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$$\begin{bmatrix} \sigma_{11}^{-1} & 0 & \cdots & 0 & 0 \\ 0 & \sigma_{22}^{-1} & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \cdots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & \sigma_{mm}^{-1} \end{bmatrix}$$

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Designing a Transformation

Simple Jacobian Determinant

$$\left|\det J_{h_2}(x)\right| = \prod_{j=1}^{M} \sigma_j^{-1}$$

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In practice we work with the log-likelihood.

$$\log\left|\det J_{h_2}(x)\right| = -\sum_{j=1}^{M} \log \sigma_j$$

2-step Flow

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\begin{aligned}
p_X(x) &= p_\epsilon(\epsilon)\left|\det J_{h_1}\left(\epsilon^{(1)}\right)\right|\left|\det J_{h_2}(x)\right| \\
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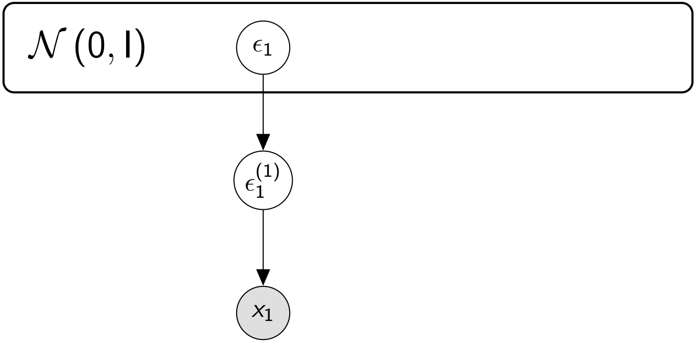
Intermediate Summary

- NFs map transform complex distributions to simpler ones (or vice versa)
- Use in density estimation for complex distributions
- Jacobian needs to be carefully designed
- Sampling is slow because sequential

Sampling From the Flow



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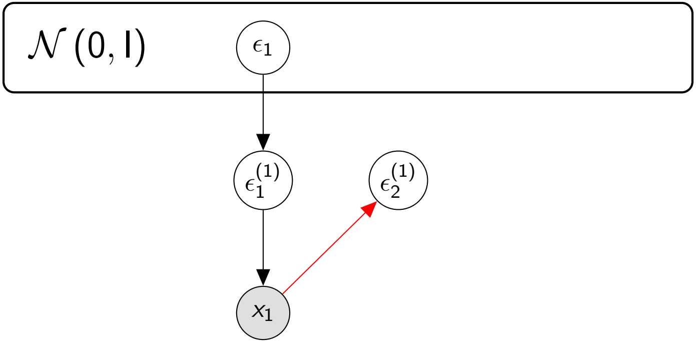

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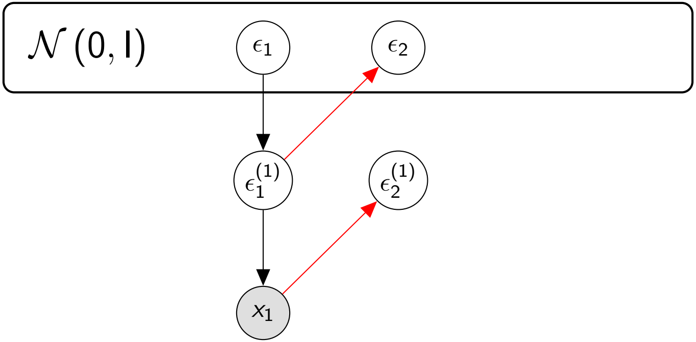

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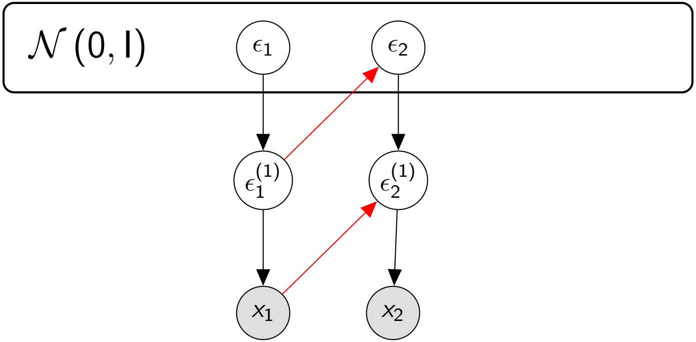

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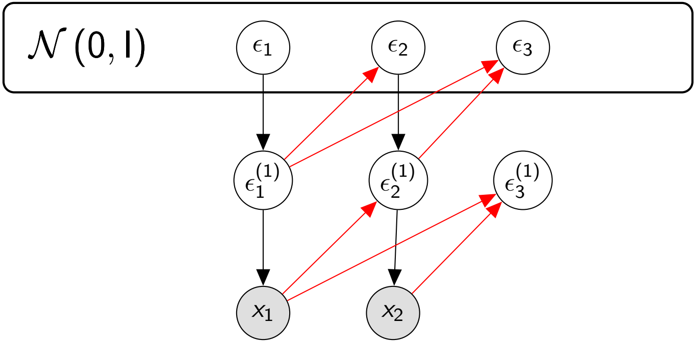

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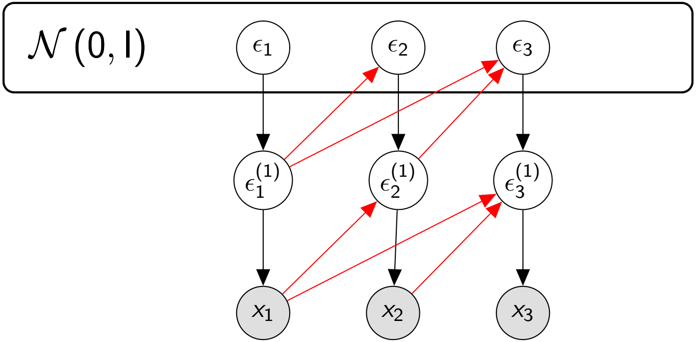

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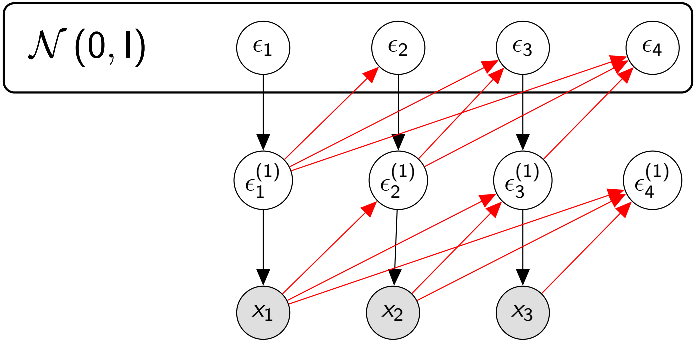

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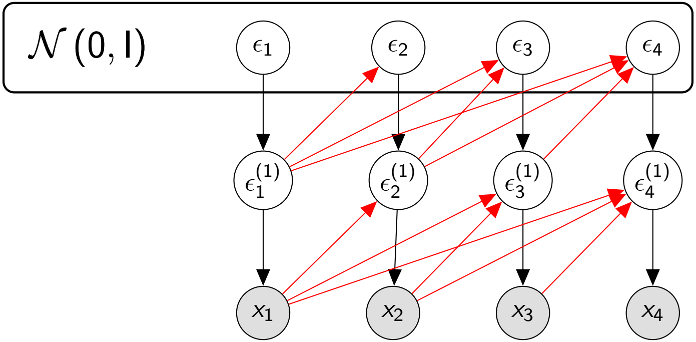

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Goal

We want a complex, multimodal approximate posterior $q(z|x)$.

Inverse Autoregressive Flow: Inference

$$
\begin{aligned}
\text{ELBO} &= -\,\text{KL}\left(q(z|x) \;||\; p(z|x)\right) \\
&= \mathbb{E}_{q(z|\lambda)}\left[\log p(x|z)\right] - \text{KL}\left(q(z|\lambda)) \;||\; p(z)\right) \\
&= \underbrace{\mathbb{E}_{q(\epsilon)}\left[\log p(x|h^{-1}(\epsilon))\right]}_{\text{sample } z} - \underbrace{\text{KL}\left(q(z|\lambda) \;||\; p(z)\right)}_{\text{assess density}}
\end{aligned}
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Simple Mapping

$$
\begin{aligned}
h(z) &= \epsilon \text{ s.t. } \epsilon \perp \lambda \\
h^{-1}(\epsilon) &= z
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Normalising Flows: Inference

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2-step Flow

$$q_Z(z^{(2)}) = q_\epsilon(\epsilon)\left|\det J_{h_1^{-1}}\left(z^{(1)}\right)\right|\left|\det J_{h_2^{-1}}\left(z^{(2)}\right)\right|$$

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\begin{aligned}
q_Z(z^{(2)}) &= q_\epsilon(\epsilon)\left|\det J_{h_1^{-1}}\left(z^{(1)}\right)\right|\left|\det J_{h_2^{-1}}\left(z^{(2)}\right)\right| \\
&= q_\epsilon(\epsilon)\left|\det J_{h_1^{-1}}\left(h_1^{-1}(\epsilon)\right)\right|\left|\det J_{h_2^{-1}}\left(h_2^{-1}(h_1^{-1}(\epsilon))\right)\right|
\end{aligned}
$$

2-step Flow

$$q_Z(z^{(2)}) = q_\epsilon(\epsilon)\left|\det J_{h_1^{-1}}\left(z^{(1)}\right)\right|\left|\det J_{h_2^{-1}}\left(z^{(2)}\right)\right|$$
$$= q_\epsilon(\epsilon)\left|\det J_{h_1^{-1}}\left(h_1^{-1}(\epsilon)\right)\right|\left|\det J_{h_2^{-1}}\left(h_2^{-1}(h_1^{-1}(\epsilon))\right)\right|$$

The transformations h_1^{-1} and h_2^{-1} are learned by backprop (while still being invertible). The determinants need to be computed analytically.

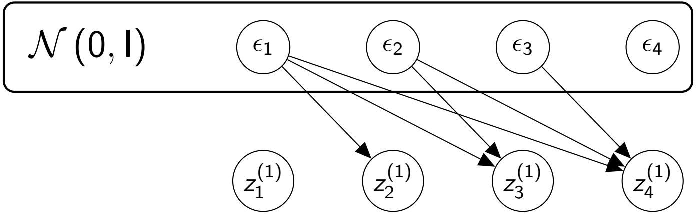
Designing a Transformation

We are again going to use a MADE to predict parameters.
However, this time we will use it in the other direction.

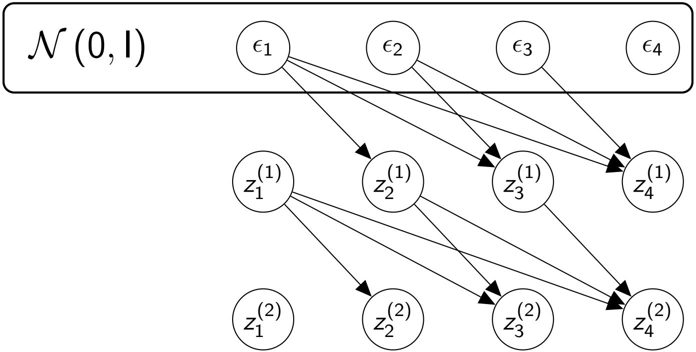
Designing a Transformation

$\mathcal{N}(0, I)$ $\quad \epsilon_1 \quad \epsilon_2 \quad \epsilon_3 \quad \epsilon_4$

Designing a Transformation



Designing a Transformation



Designing a Transformation

We use a MADE f_λ to predict the parameters of the first transformation: $\begin{bmatrix}\mu_j & \sigma_j\end{bmatrix} = f_\lambda(\epsilon_{<j})$. Then we apply the first transformation.

$$z_j^{(1)} = h_1^{-1}(\epsilon)_j \; = \mu(\epsilon_{<j}) + \sigma(\epsilon_{<j})\epsilon_j$$

Designing a Transformation

We use a MADE f_λ to predict the parameters of the first transformation: $\begin{bmatrix}\mu_j & \sigma_j\end{bmatrix} = f_\lambda(\epsilon_{<j})$. Then we apply the first transformation.

$$\begin{aligned} z_j^{(1)} &= h_1^{-1}(\epsilon)_j &= \mu(\epsilon_{<j}) + \sigma(\epsilon_{<j})\epsilon_j \\ z^{(1)} &= h_1^{-1}(\epsilon) &= \mu + \sigma\epsilon \end{aligned}$$

Designing a Transformation

We use a MADE f_λ to predict the parameters of the first transformation: $\begin{bmatrix}\mu_j & \sigma_j\end{bmatrix} = f_\lambda(\epsilon_{<j})$. Then we apply the first transformation.

$$
\begin{aligned}
z_j^{(1)} &= h_1^{-1}(\epsilon)_j &&= \mu(\epsilon_{<j}) + \sigma(\epsilon_{<j})\epsilon_j \\
z^{(1)} &= h_1^{-1}(\epsilon) &&= \mu + \sigma\epsilon
\end{aligned}
$$

$$
J_{h_1^{-1}}(\epsilon) = \mathrm{I}\sigma + J_\mu(\epsilon) + J_{\sigma\epsilon}(\epsilon)
$$

Designing a Transformation

Simple Jacobian Determinant

$$\left|\det J_{h_1^{-1}}(\epsilon)\right| = \prod_{j=1}^{M} \sigma_j$$

In practice we work with the log-likelihood.

$$\log \left|\det J_{h_1^{-1}}(\epsilon)\right| = \sum_{j=1}^{M} \log \sigma_j$$

2-step Flow

$$
\begin{aligned}
q_Z(z^{(2)}) &= q_\epsilon(\epsilon) \left| \det J_{h_1^{-1}} \left(z^{(1)} \right) \right| \left| \det J_{h_2^{-1}} \left(z^{(2)} \right) \right| \\
&= q_\epsilon(\epsilon) \left| \det J_{h_1^{-1}} \left(h_1^{-1}(\epsilon) \right) \right| \left| \det J_{h_2^{-1}} \left(h_2^{-1}(h_1^{-1}(\epsilon)) \right) \right|
\end{aligned}
$$

2-step Flow

$$
\begin{aligned}
q_Z(z^{(2)}) &= q_\epsilon(\epsilon) \left| \det J_{h_1^{-1}} \left(z^{(1)} \right) \right| \left| \det J_{h_2^{-1}} \left(z^{(2)} \right) \right| \\
&= q_\epsilon(\epsilon) \left| \det J_{h_1^{-1}} \left(h_1^{-1}(\epsilon) \right) \right| \left| \det J_{h_2^{-1}} \left(h_2^{-1}(h_1^{-1}(\epsilon)) \right) \right|
\end{aligned}
$$

$$
\log q_Z(z^{(2)}) = \log q_\epsilon(\epsilon)
$$

2-step Flow

$$
\begin{aligned}
q_Z(z^{(2)}) &= q_\epsilon(\epsilon) \left| \det J_{h_1^{-1}} \left(z^{(1)} \right) \right| \left| \det J_{h_2^{-1}} \left(z^{(2)} \right) \right| \\
&= q_\epsilon(\epsilon) \left| \det J_{h_1^{-1}} \left(h_1^{-1}(\epsilon) \right) \right| \left| \det J_{h_2^{-1}} \left(h_2^{-1}(h_1^{-1}(\epsilon)) \right) \right| \\
\log q_Z(z^{(2)}) &= \log q_\epsilon(\epsilon) + \sum_{j=1}^{M} \log \sigma_j^{(1)} + \sum_{j=1}^{M} \log \sigma_j^{(2)}
\end{aligned}
$$

2-step Flow

$$
\begin{aligned}
q_Z(z^{(2)}) &= q_\epsilon(\epsilon)\left|\det J_{h_1^{-1}}\left(z^{(1)}\right)\right|\left|\det J_{h_2^{-1}}\left(z^{(2)}\right)\right| \\
&= q_\epsilon(\epsilon)\left|\det J_{h_1^{-1}}\left(h_1^{-1}(\epsilon)\right)\right|\left|\det J_{h_2^{-1}}\left(h_2^{-1}(h_1^{-1}(\epsilon))\right)\right|
\end{aligned}
$$

$$
\log q_Z(z^{(2)}) = \log q_\epsilon(\epsilon) + \sum_{j=1}^{M} \log \sigma_j^{(1)} + \sum_{j=1}^{M} \log \sigma_j^{(2)}
$$

$$
z^{(1)} = \mu^{(1)} + \sigma^{(1)}\epsilon \text{ where } \left[\mu^{(1)}, \sigma^{(1)}\right] = f_\lambda^{(1)}(\epsilon)
$$

2-step Flow

$$
\begin{aligned}
q_Z(z^{(2)}) &= q_\epsilon(\epsilon) \left| \det J_{h_1^{-1}} \left(z^{(1)} \right) \right| \left| \det J_{h_2^{-1}} \left(z^{(2)} \right) \right| \\
&= q_\epsilon(\epsilon) \left| \det J_{h_1^{-1}} \left(h_1^{-1}(\epsilon) \right) \right| \left| \det J_{h_2^{-1}} \left(h_2^{-1}(h_1^{-1}(\epsilon)) \right) \right|
\end{aligned}
$$

$$
\log q_Z(z^{(2)}) = \log q_\epsilon(\epsilon) + \sum_{j=1}^{M} \log \sigma_j^{(1)} + \sum_{j=1}^{M} \log \sigma_j^{(2)}
$$

$$
z^{(1)} = \mu^{(1)} + \sigma^{(1)}\epsilon \text{ where } \left[\mu^{(1)}, \sigma^{(1)}\right] = f_\lambda^{(1)}(\epsilon)
$$

$$
z^{(2)} = \mu^{(2)} + \sigma^{(2)} z^{(1)} \text{ where } \left[\mu^{(2)}, \sigma^{(2)}\right] = f_\lambda^{(2)}(z^{(1)})
$$

ELBO

Recall: $z = z^{(2)}$

$$\text{ELBO} = \mathbb{E}_{q(z|\lambda)}\left[\log p(x|z)\right] - \text{KL}\left(q(z)|\lambda)\right) \mid\mid p(z)) =$$

ELBO

Recall: $z = z^{(2)}$

$$\text{ELBO} = \mathbb{E}_{q(z|\lambda)}\left[\log p(x|z)\right] - \text{KL}\left(q(z)|\lambda)\right) \,||\, p(z)) =$$
$$\mathbb{E}_{q(z|\lambda)}\left[\log p(x|z)\right] - \text{KL}\left(q(\epsilon)|\det J_{h^{-1}}\,(z)|\,||\, p(z)\right)$$

ELBO

KL-term

$$\mathrm{KL}\left(q(\epsilon)|\det J_h\left(z\right)| \;||\; p(z)\right) =$$

ELBO

KL-term

$$\mathrm{KL}\left(q(\epsilon)|\det J_h\left(z\right)| \;||\; p(z)\right) =$$

$$\mathbb{E}_{q(z|\lambda))}\left[\log \frac{q(\epsilon)|\det J_{h^{-1}}\left(z\right)|}{p(z)}\right]$$

ELBO

KL-term

$$\mathrm{KL}\left(q(\epsilon)|\det J_h\left(z\right)| \mid\mid p(z)\right) =$$

$$\mathbb{E}_{q(z|\lambda))}\left[\log \frac{q(\epsilon)|\det J_{h^{-1}}\left(z\right)|}{p(z)}\right] \overset{\mathrm{MC}}{\approx} \frac{1}{S}\sum_{s=1}^{S} \log \frac{q(\epsilon)\left|\det J_{h^{-1}}\left(z^{(s)}\right)\right|}{p\left(z^{(s)}\right)}$$

ELBO

KL-term

$$\mathrm{KL}\left(q(\epsilon)|\det J_h(z)| \;||\; p(z)\right) =$$

$$\mathbb{E}_{q(z|\lambda))}\left[\log \frac{q(\epsilon)|\det J_{h^{-1}}(z)|}{p(z)}\right] \overset{\text{MC}}{\approx} \frac{1}{S}\sum_{s=1}^{S} \log \frac{q(\epsilon)\left|\det J_{h^{-1}}\left(z^{(s)}\right)\right|}{p(z^{(s)})}$$

Jacobian

ELBO

KL-term

$$\mathrm{KL}\left(q(\epsilon)|\det J_h(z)| \,||\, p(z)\right) =$$

$$\mathbb{E}_{q(z|\lambda))}\left[\log \frac{q(\epsilon)|\det J_{h^{-1}}(z)|}{p(z)}\right] \overset{\mathrm{MC}}{\approx} \frac{1}{S}\sum_{s=1}^{S} \log \frac{q(\epsilon)\left|\det J_{h^{-1}}\left(z^{(s)}\right)\right|}{p\left(z^{(s)}\right)}$$

Jacobian

$$\left|\det J_{h^{-1}}\left(z^{(s)}\right)\right| = \sum_{j=1}^{M} \log \sigma_j^{(1)} + \sum_{j=1}^{M} \log \sigma_j^{(2)}$$

Summary

- NFs model arbitrary continuous distributions
- They allow for density computation
- Need to have simple Jacobian determinants
- Depending on direction, they are good at either sampling or density computation (not both)

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