Normalising Flows

Philip Schulz and Wilker Aziz

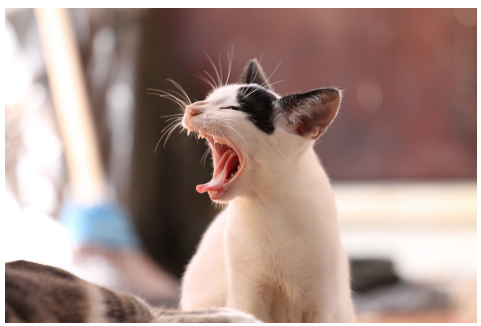
https://github.com/philschulz/VITutorial

The problem with Standard Distributions

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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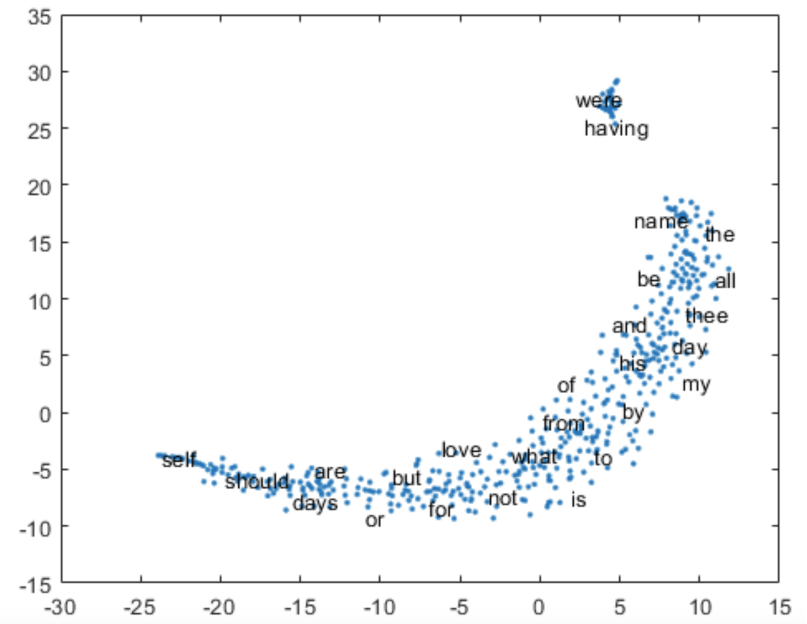

Figure: https://it.mathworks.com/help/textanalytics/ref/trainwordembedding.html

Posterior Approximations

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Counter example

Gaussian mixture model

Recap: Reparametrisation

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 $p(y)$, 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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$$h^{-1} = h_K^{-1} \circ h_{K-1}^{-1} \circ \ldots \circ h_1^{-1}$$

$$p(x) = p(y) \left| \det J_{h_1} \left(y^{(1)} \right) \right| \left| \det J_{h_2} \left(y^{(2)} \right) \right| \ldots \left| \det J_{h_K} (x) \right|$$

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Our data x is has unknown continuous density $p(x)$.
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2-step Flow

$$p(x) = p(\epsilon)\left|\det J_{h_1^{-1}}\left(\epsilon^{(1)}\right)\right|\left|\det J_{h_2^{-1}}(x)\right|$$

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The transformations h_1^{-1} and h_2^{-1} are learned by backprop. The determinants need to be computed analytically.

Designing a Transformation

Assume: $x_i = (x_{i1}, x_{i2}, \ldots x_{iM})$. Then factorise the density according to the chain rule.

$$\log p(x_i|\theta) = \sum_{j=1}^{M} \log p(x_{ij}|x_{i,<j}\theta)$$

Next assume an invertible mapping $h(x_{ij}) = \epsilon_{ij}$.

Simple Mapping

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

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Flow Mapping

$$h_1 \circ h_2 \circ \ldots \circ h_K(x) = \epsilon$$
$$h_K^{-1} \circ h_{K-1}^{-1} \circ \ldots \circ h_1^{-1}(\epsilon) = x$$

Designing a Transformation

MADE (Germain et al., 2015)

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

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

Designing a Transformation

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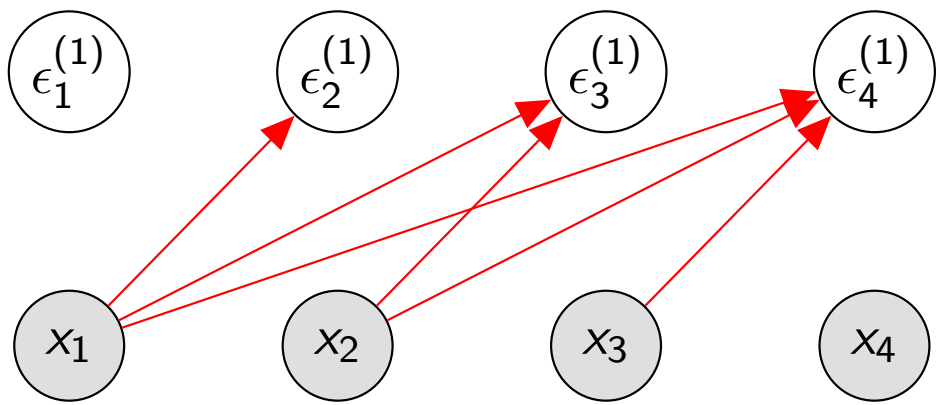

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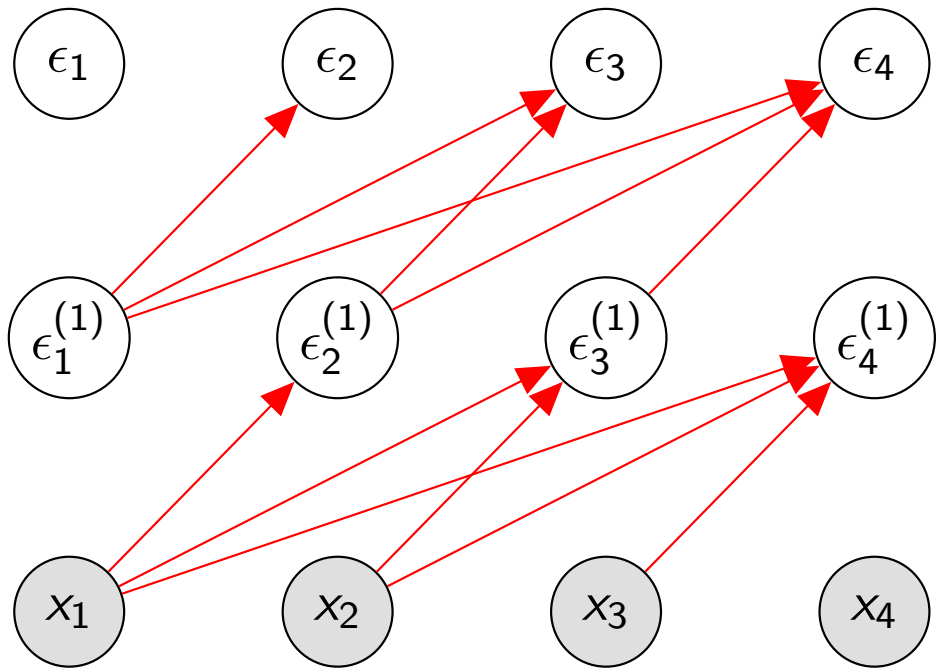

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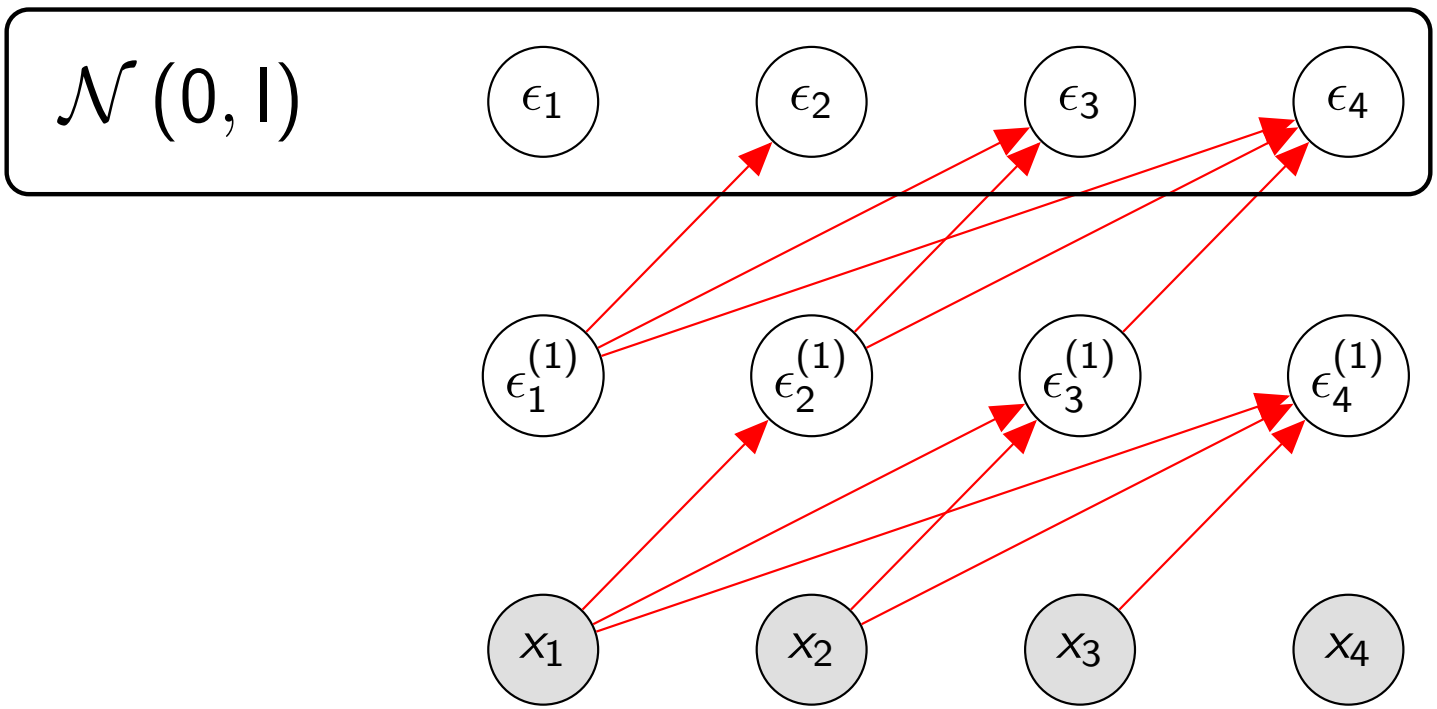

Designing a Transformation

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.

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

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The Jacobian is

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

Designing a Transformation

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

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Designing a Transformation

Simple Jacobian Determinant

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

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In practice we work with the log-likelihood.

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

2-step Flow

$$
\begin{aligned}
p(x) &= p(\epsilon)\left|\det J_{h_1^{-1}}\left(\epsilon^{(1)}\right)\right|\left|\det J_{h_2^{-1}}\left(x\right)\right| \\
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\log p(x) &= \log p(h_1^{-1}(h_2^{-1}(x))) - \sum_{j=1}^{M} \log \sigma_j^{(2)} - \sum_{j=1}^{M} \log \sigma_j^{(1)}
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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

Setting

We have a generative model $p(x|z)$. We want to approximate the posterior $p(z|x)$ using an amortized variational distribution $q(z|x)$ computed by a neural net.

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Goal

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

Normalising Flows: Inference

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

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\begin{aligned}
h(z) &= \epsilon \text{ s.t. } \epsilon \perp \lambda \\
h^{-1}(\epsilon) &= z
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&- \mathrm{KL}\left(q(z|x) \,||\, p(z|x)\right) \propto \mathrm{ELBO} = \\
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Flow Mapping

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2-step Flow

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

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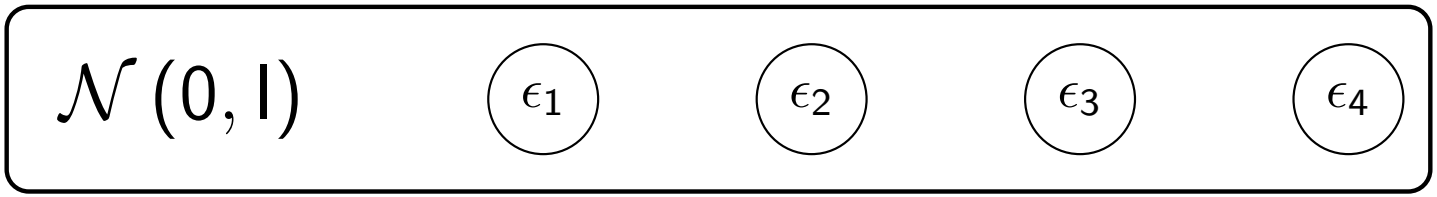
The transformations h_1^{-1} and h_2^{-1} are learned by backprop. The determinants need to be computed analytically.

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



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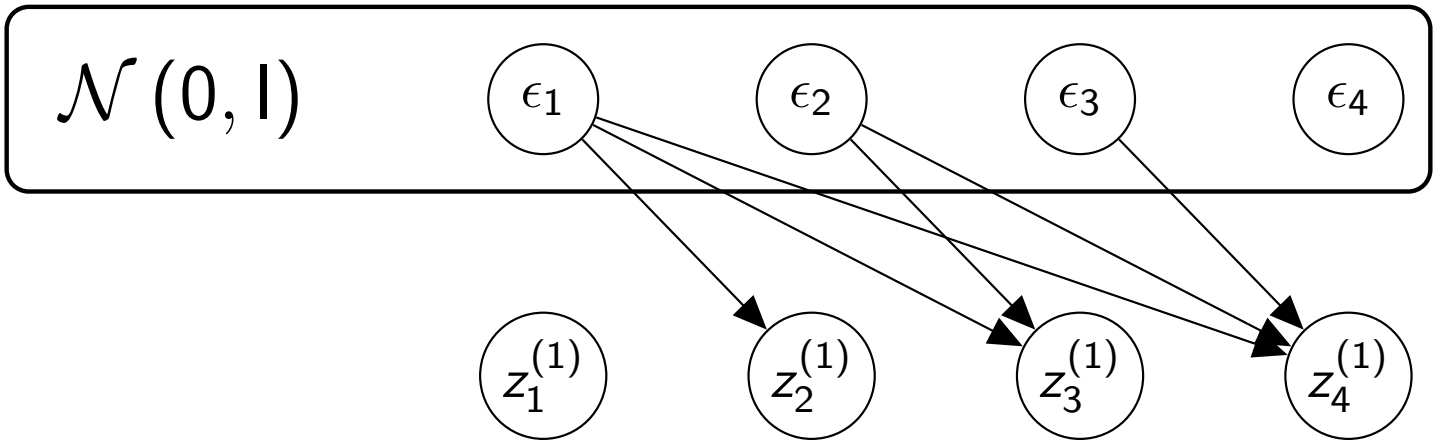

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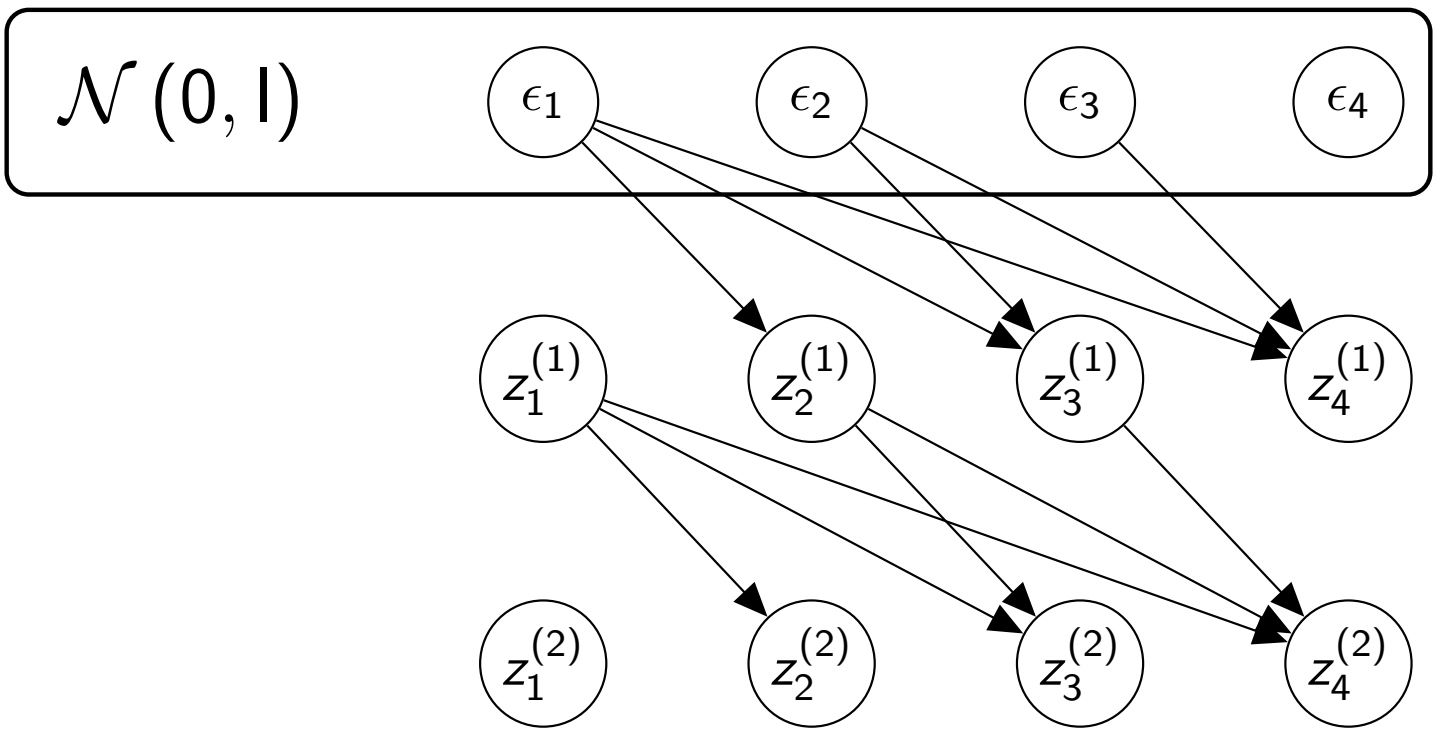

Designing a Transformation

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.

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

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$$J_{h_1}(\epsilon) = \mathrm{I}\,\sigma + J_\mu(\epsilon) + J_{\sigma\epsilon}(\epsilon)$$

Designing a Transformation

Simple Jacobian Determinant

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

In practice we work with the log-likelihood.

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

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

2-step Flow

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

$$
\log q(z^{(2)}) = \log q(h_1(h_2(z^{(2)}))) + \sum_{j=1}^{M} \log \sigma_j^{(1)} + \sum_{j=1}^{M} \log \sigma_j^{(2)}
$$

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

2-step Flow

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

$$
\log q(z^{(2)}) = \log q(h_1(h_2(z^{(2)}))) + \sum_{j=1}^{M} \log \sigma_j^{(1)} + \sum_{j=1}^{M} \log \sigma_j^{(2)}
$$

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

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

ELBO

$$\text{ELBO} = \mathbb{E}_{q(z|\lambda)}\left[\log p(x|z)\right] - \text{KL}\left(q(z^{(2)}|\lambda)) \,||\, p(z^{(2)})\right) =$$

ELBO

$$\text{ELBO} = \mathbb{E}_{q(z|\lambda)}\left[\log p(x|z)\right] - \text{KL}\left(q(z^{(2)}|\lambda)) \,||\, p(z^{(2)})\right) =$$
$$\mathbb{E}_{q(z|\lambda)}\left[\log p(x|z)\right] - \text{KL}\left(q(\epsilon)\left|\det J_h\left(z^{(2)}\right)\right| \,||\, p(z)\right)$$

ELBO

KL-term

$$\mathrm{KL}\left(q(\epsilon)\left|\det J_h\left(z^{(2)}\right)\right| \,||\, p(z)\right) =$$

ELBO

KL-term

$$\mathrm{KL}\left(q(\epsilon)\left|\det J_h\left(z^{(2)}\right)\right| \,||\, p(z)\right) =$$

$$\mathbb{E}_{q(z^{(2)}|\lambda))}\left[\frac{q(\epsilon)\left|\det J_h\left(z^{(2)}\right)\right|}{p(z^{(2)})}\right]$$

ELBO

KL-term

$$\mathrm{KL}\left(q(\epsilon)\left|\det J_h\left(z^{(2)}\right)\right| \,||\, p(z)\right) =$$

$$\mathbb{E}_{q(z^{(2)}|\lambda))}\left[\frac{q(\epsilon)\left|\det J_h\left(z^{(2)}\right)\right|}{p(z^{(2)})}\right] \overset{\text{MC}}{\approx} \frac{1}{S}\sum_{s=1}^{S}\frac{q(\epsilon)\left|\det J_h\left(z^{(2,s)}\right)\right|}{p(z^{(2,s)})}$$

ELBO

KL-term

$$\mathrm{KL}\left(q(\epsilon)\left|\det J_h\left(z^{(2)}\right)\right| \,||\, p(z)\right) =$$

$$\mathbb{E}_{q(z^{(2)}|\lambda))}\left[\frac{q(\epsilon)\left|\det J_h\left(z^{(2)}\right)\right|}{p(z^{(2)})}\right] \overset{\text{MC}}{\approx} \frac{1}{S}\sum_{s=1}^{S}\frac{q(\epsilon)\left|\det J_h\left(z^{(2,s)}\right)\right|}{p(z^{(2,s)})}$$

Jacobian

ELBO

KL-term

$$\mathrm{KL}\left(q(\epsilon)\left|\det J_h\left(z^{(2)}\right)\right| \,||\, p(z)\right) =$$

$$\mathbb{E}_{q(z^{(2)}|\lambda))}\left[\frac{q(\epsilon)\left|\det J_h\left(z^{(2)}\right)\right|}{p(z^{(2)})}\right] \overset{\text{MC}}{\approx} \frac{1}{S}\sum_{s=1}^{S}\frac{q(\epsilon)\left|\det J_h\left(z^{(2,s)}\right)\right|}{p(z^{(2,s)})}$$

Jacobian

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

Other Appliations of Normalizing Flows

- As a prior

Other Appliations of Normalizing Flows

- As a prior
- Modeling of dynamic systems

Summary

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

References I

Mathieu Germain, Karol Gregor, Iain Murray, and Hugo Larochelle. Made: Masked autoencoder for distribution estimation. In Francis Bach and David Blei, editors, *Proceedings of the 32nd International Conference on Machine Learning*, pages 881–889, 2015.

Chin-Wei Huang, David Krueger, Alexandre Lacoste, and Aaron C. Courville. Neural autoregressive flows. *CoRR*, 2018. URL http://arxiv.org/abs/1804.00779.

References II

Diederik P. Kingma, Tim Salimans, and Max Welling. Improving variational inference with inverse autoregressive flow. 2016. URL http://arxiv.org/abs/1606.04934.

Danilo Rezende and Shakir Mohamed. Variational inference with normalizing flows. In *ICML*, pages 1530–1538, 2015. URL http://proceedings.mlr.press/v37/rezende15.pdf.