

Normalising Flows

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<https://vitutorial.github.io/tour/ua2020>



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- 1 The problem with Known Distributions
- 2 Normalising Flows
- 3 Use Case 1: Density Estimation
- 4 Use Case 2: Inference (sampling)
- 5 Summary

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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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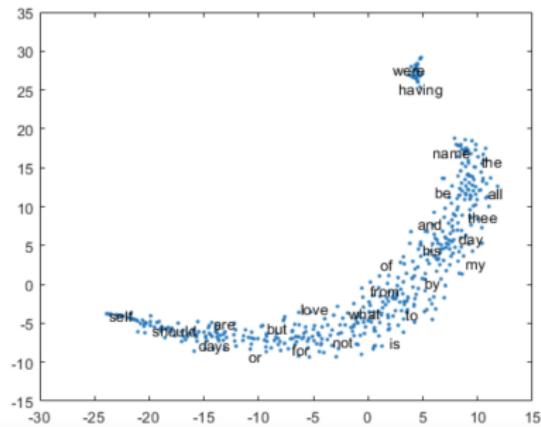


Figure: <https://it.mathworks.com/help/textanalytics/ref/trainwordembedding.html>

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

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Recap: Reparametrisation

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

$$h(x) = y$$

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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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If we want $p_Y(y)$, 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 $h : \mathcal{X} \rightarrow \mathcal{Y}$ into

$$h = h_1 \circ h_2 \circ \dots \circ h_K$$

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

Normalising Flows

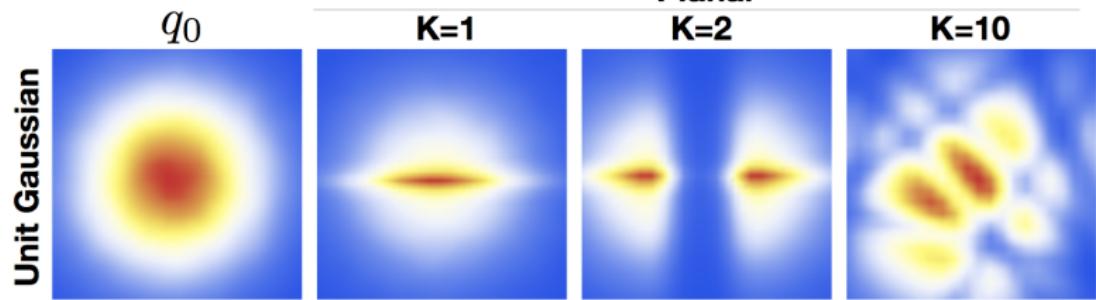


Figure: Taken from [Rezende and Mohamed \(2015\)](#)

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

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2-step Flow

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

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

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

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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

$$h_1 \circ h_2 \circ \dots \circ h_K(x) = \epsilon$$

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Designing a Transformation

MADE (Germain et al., 2015)

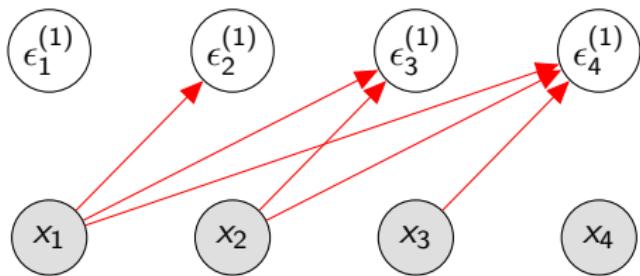
An autoregressive network that takes constant time. Its connectivity matrix is lower-triangular.

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

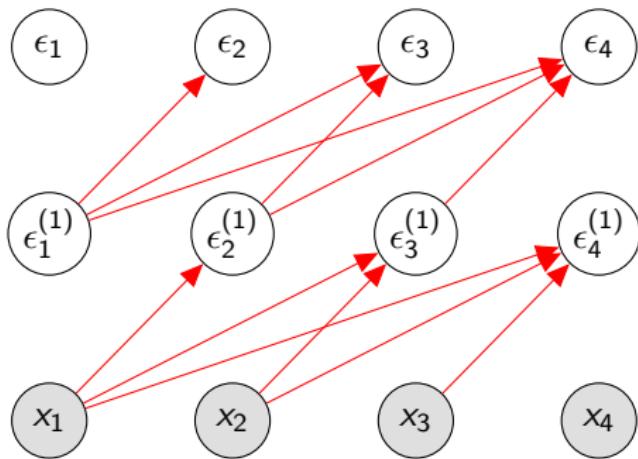
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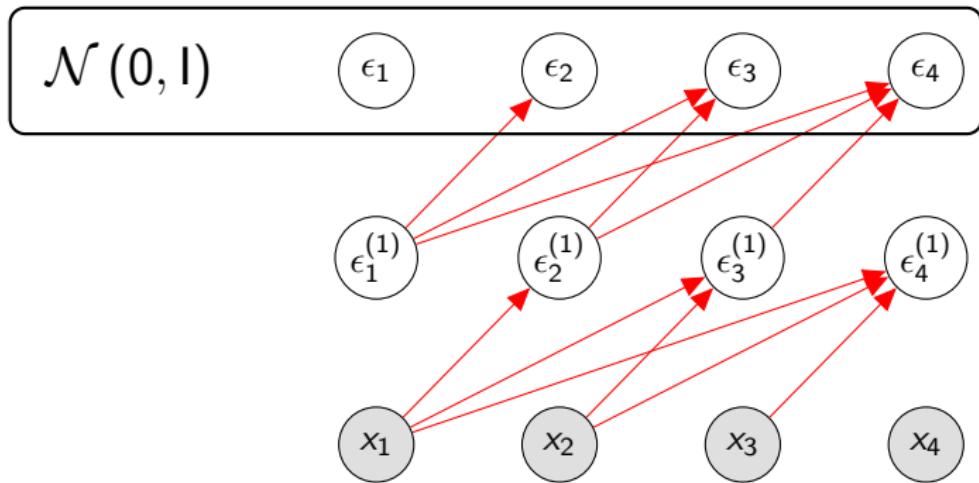
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We use a MADE $g_\theta^{(2)}$ to predict the parameters of the first transformation: $[\mu_j \ \sigma_j] = g_\theta^{(2)}(x_{<j})$. Then we apply the first transformation.

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

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

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

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In practice we work with the log-likelihood.

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

2-step Flow

$$\begin{aligned} p_X(x) &= p_\epsilon(\epsilon) |\det J_{h_1}(\epsilon^{(1)})| |\det J_{h_2}(x)| \\ &= p_\epsilon(h_1(h_2(x))) |\det J_{h_1}(h_2(x))| |\det J_{h_2}(x)| \end{aligned}$$

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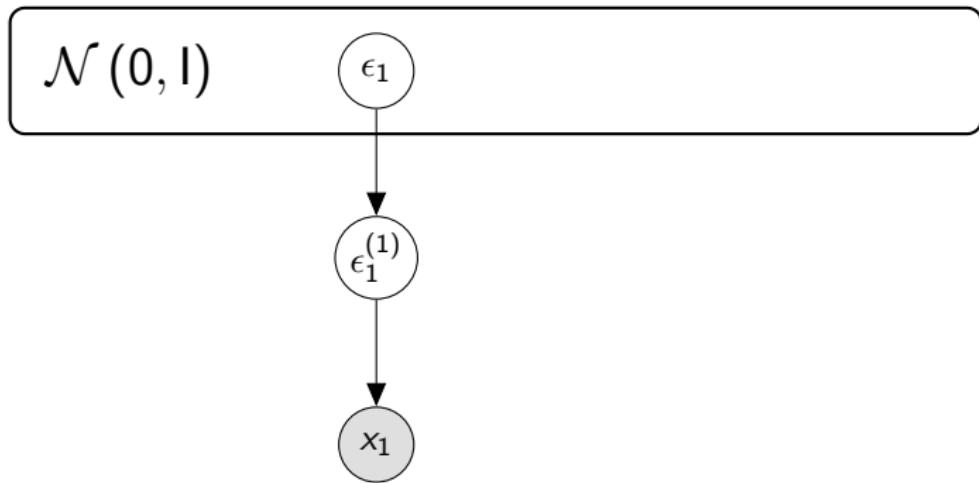
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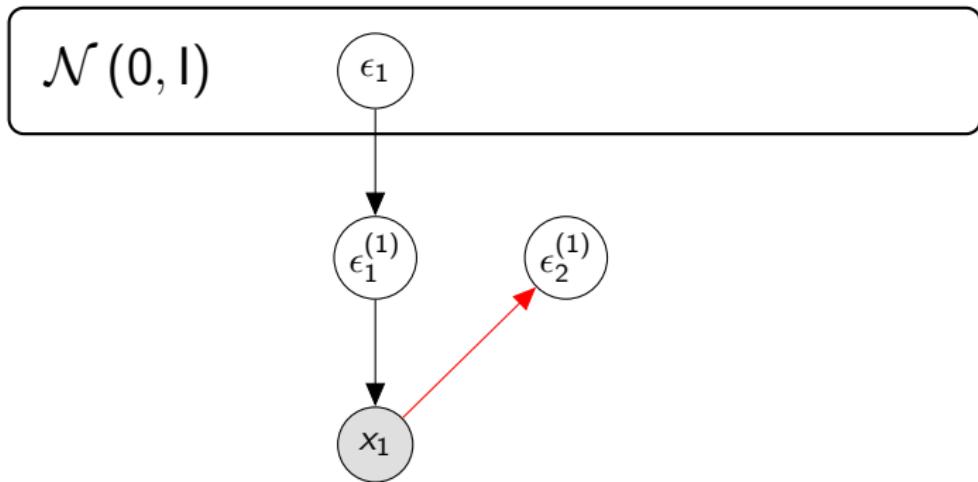
Intermediate Summary

- 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

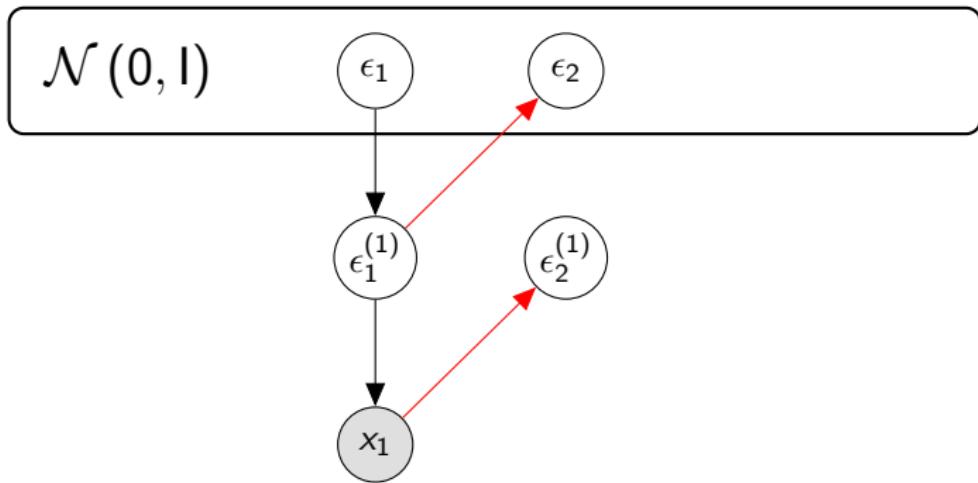
Sampling From the Flow



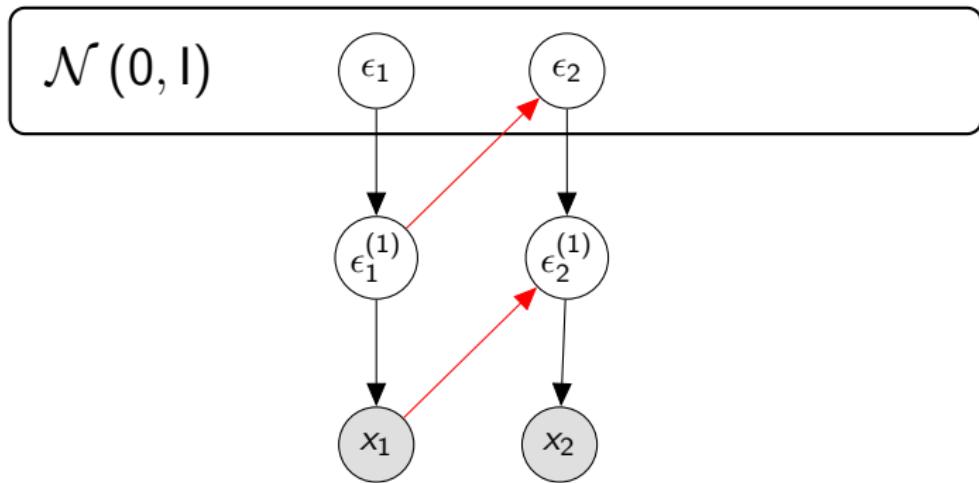
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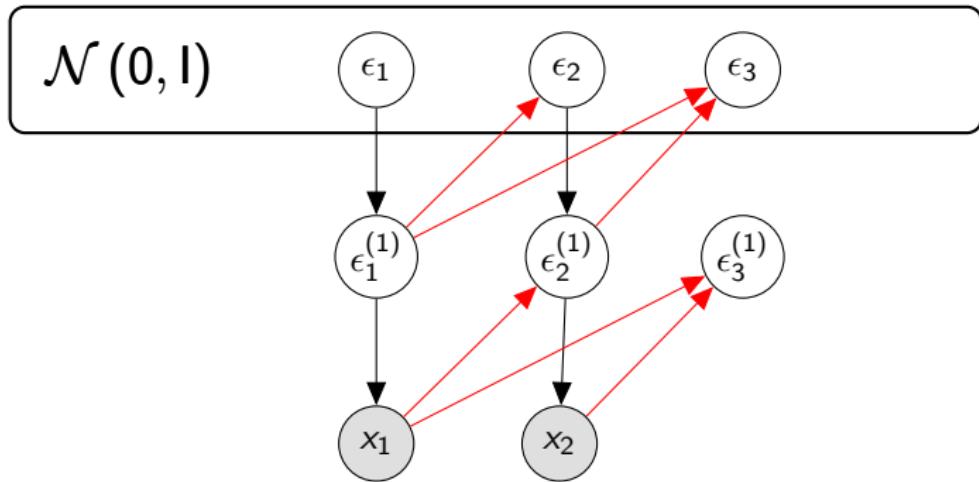
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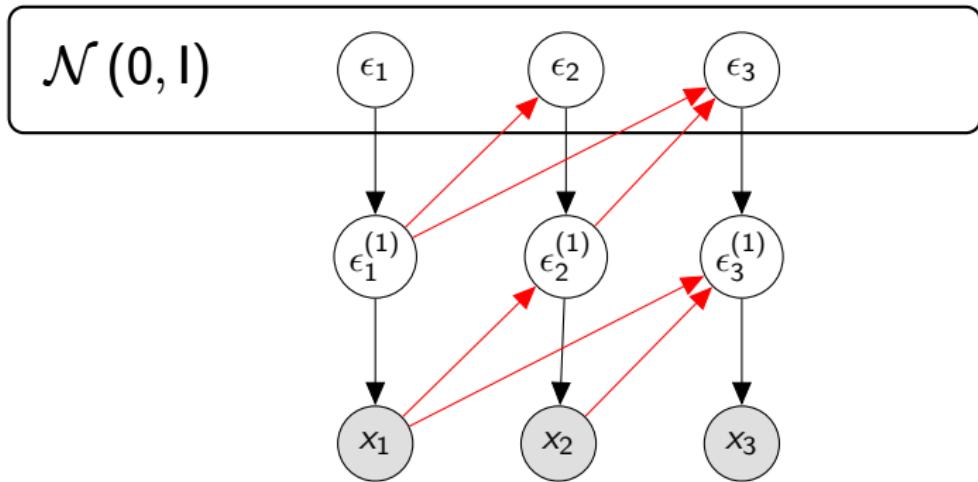
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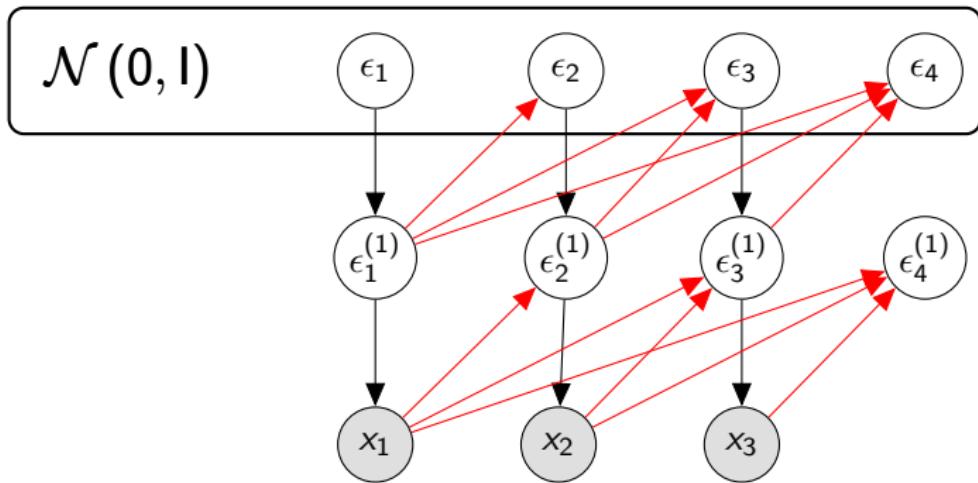
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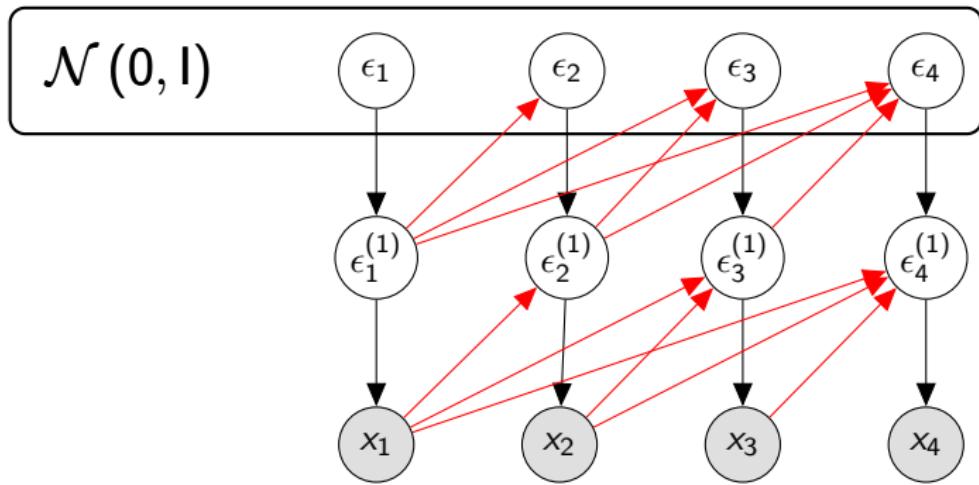
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Goal

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

Normalising Flows: Inference

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

Simple Mapping

$$\begin{aligned}
 h(z) &= \epsilon \text{ s.t. } \epsilon \perp \lambda \\
 h^{-1}(\epsilon) &= z
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$$\begin{aligned}
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2-step Flow

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

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

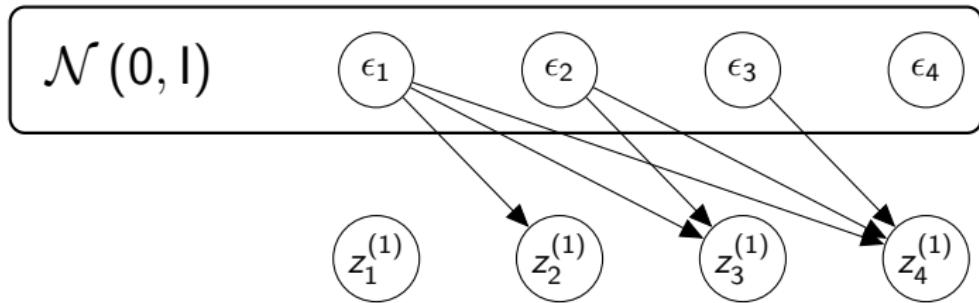
Designing a Transformation

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

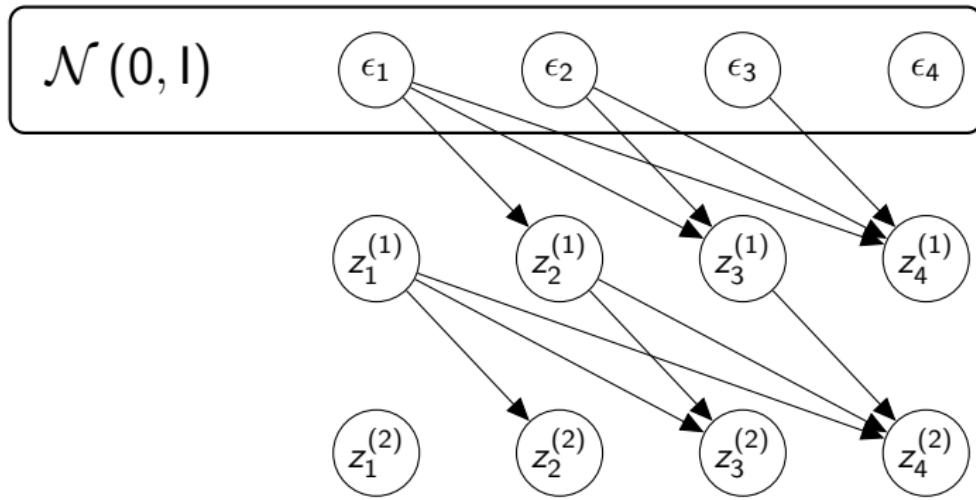
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 $\mathcal{N}(0, I)$ ϵ_1 ϵ_2 ϵ_3 ϵ_4

Designing a Transformation



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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.

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

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

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

$$\begin{aligned} q_Z(z^{(2)}) &= q_\epsilon(\epsilon) \left| \det J_{h_1^{-1}}(\textcolor{red}{z}^{(1)}) \right| \left| \det J_{h_2^{-1}}(\textcolor{blue}{z}^{(2)}) \right| \\ &= q_\epsilon(\epsilon) \left| \det J_{h_1^{-1}}(\textcolor{red}{h}_1^{-1}(\epsilon)) \right| \left| \det J_{h_2^{-1}}(\textcolor{blue}{h}_2^{-1}(h_1^{-1}(\epsilon))) \right| \end{aligned}$$

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

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

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

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

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

ELBO

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

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

ELBO

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

ELBO

KL-term

$$\text{KL}(q(\epsilon) | \det J_h(z) | \parallel p(z)) =$$

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Jacobian

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Jacobian

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

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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- but we can construct other flows using other bijections, e.g. a permutation (volume preserving)
- or any strictly monotone function
 - e.g. a neural network with positive weights and strictly monotone activations
- also note that, we require invertibility (strict monotonicity), not **analytical** invertibility

Closing

- Check our website for reading lists
- Write to us if you have questions
- Make DGMs part of research agenda ;D

Thank you all!

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