

Normalising Flows

Philip Schulz and Wilker Aziz

[https:](https://github.com/philschulz/VITutorial)

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The problem with Known Distributions

Normalising Flows

Use Case 1: Density Estimation

Use Case 2: Inference (sampling)

Summary

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Summary

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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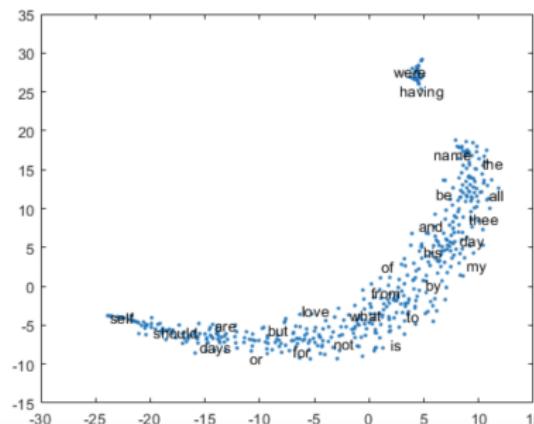


Figure: <https://it.mathworks.com/help/textanalytics/ref/trainwordembedding.html>

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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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 $h : \mathcal{X} \rightarrow \mathcal{Y}$ into

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

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$$p_X(x) = p_Y(y) |\det J_{h_1}(y^{(1)})| |\det J_{h_2}(y^{(2)})| \dots |\det J_{h_K}(x)|$$

$$p_Y(y) = p_X(x) \left| \det J_{h_1^{-1}}(y^{(K-1)}) \right| \left| \det J_{h_2^{-1}}(y^{(K-2)}) \right| \dots \left| \det J_{h_1^{-1}}(y) \right|$$

Normalising Flows

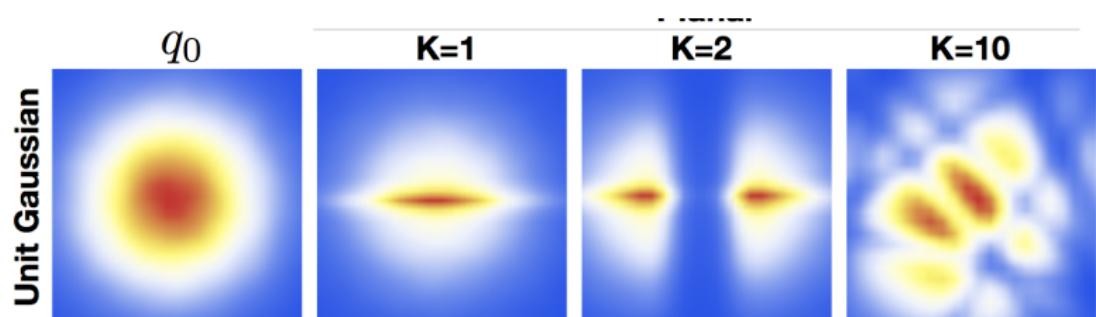


Figure: Taken from [Rezende and Mohamed \(2015\)](#)

The problem with Known Distributions

Normalising Flows

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Use Case 2: Inference (sampling)

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Normalising Flows: Density Estimation

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

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2-step Flow

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

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

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

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

Simple Mapping

$$\begin{aligned} h(x) &= \epsilon \\ h^{-1}(\epsilon) &= x \end{aligned}$$

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Flow Mapping

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

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

Designing a Transformation

MADE (Germain et al., 2015)

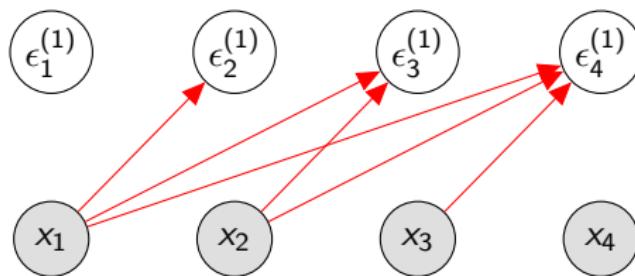
An autoregressive network that takes constant time.
Its connectivity matrix is lower-triangular.

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

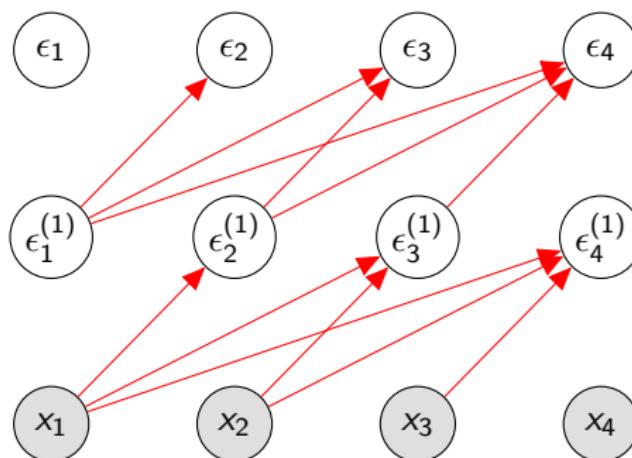
Designing a Transformation



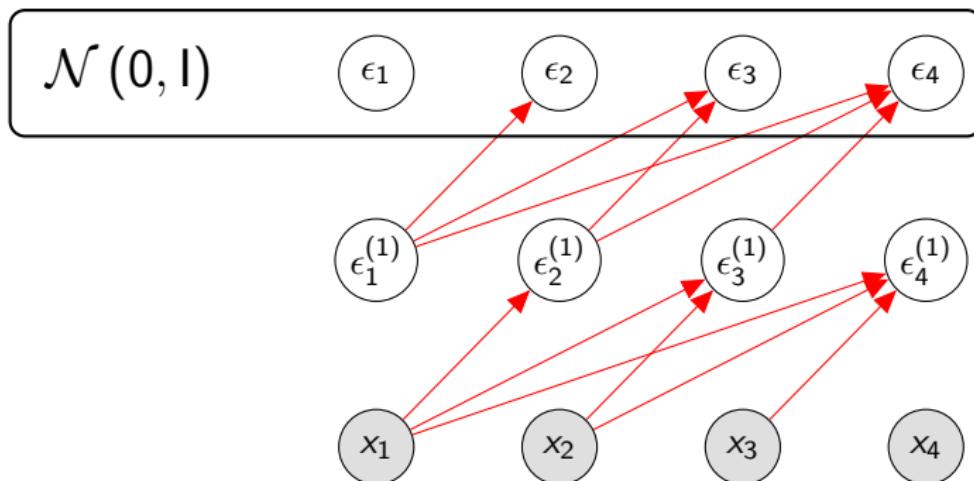
Designing a Transformation



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Designing a Transformation

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.

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

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The Jacobian is

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

Designing a Transformation

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

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

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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

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

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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

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

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$$\epsilon = h_1^{-1} = \frac{\epsilon^{(1)} - \mu^{(1)}}{\sigma^{(1)}} \text{ where } [\mu^{(1)}, \sigma^{(1)}] = g^{(1)}(\epsilon^{(1)})$$

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

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Use Case 1: Density Estimation

Use Case 2: Inference (sampling)

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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

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

Normalising Flows: Inference

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Flow Mapping

$$\begin{aligned} h_1 \circ h_2 \circ \dots \circ h_K(z) &= \epsilon \text{ s.t. } \epsilon \perp \lambda \\ h_K^{-1} \circ h_{K-1}^{-1} \circ \dots \circ h_1^{-1}(\epsilon) &= z \end{aligned}$$

2-step Flow

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

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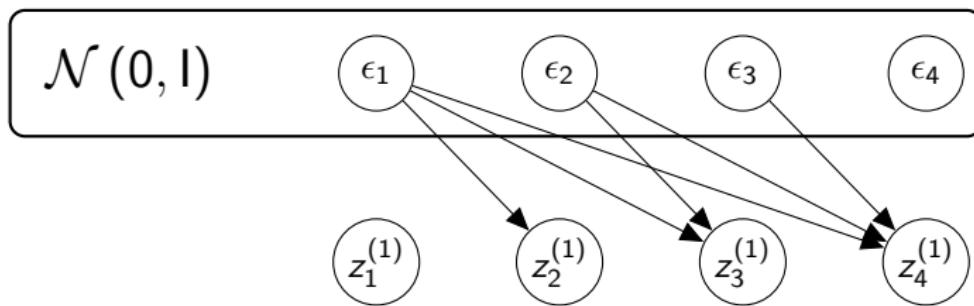
Designing a Transformation

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

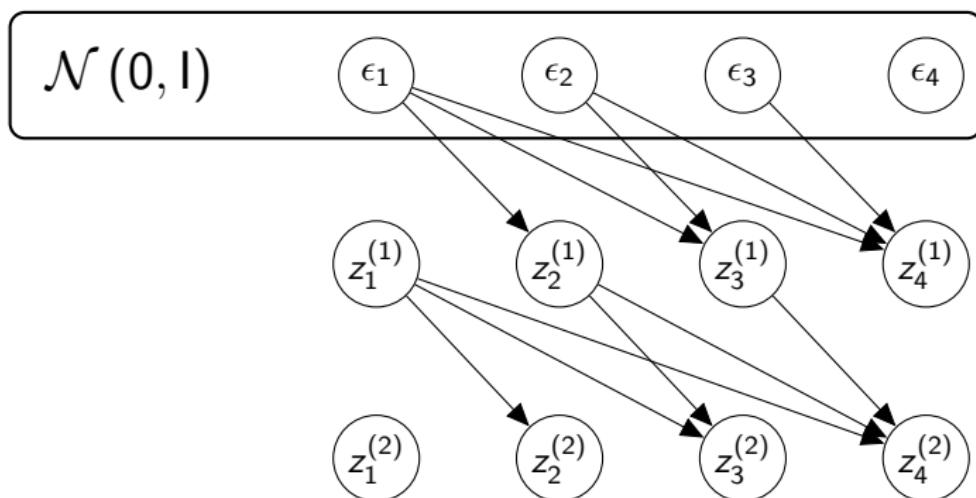
Designing a Transformation

 $\mathcal{N}(0, I)$ 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: $[\mu_j \ \sigma_j] = f_\lambda(\epsilon_{<j})$. 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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$$J_{h_1}(\epsilon) = \mathbb{I}\sigma + J_\mu(\epsilon) + J_{\sigma\epsilon}(\epsilon)$$

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.

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

2-step Flow

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

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

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

ELBO

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

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

ELBO

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

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

ELBO

KL-term

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

ELBO

KL-term

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

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

ELBO

KL-term

$$\begin{aligned} \text{KL}(q(\epsilon) | \det J_h(z) | \parallel p(z)) &= \\ \mathbb{E}_{q(z|\lambda))} \left[\log \frac{q(\epsilon) | \det J_h(z) |}{p(z)} \right] &\stackrel{\text{MC}}{\approx} \frac{1}{S} \sum_{s=1}^S \log \frac{q(\epsilon) | \det J_h(z^{(s)}) |}{p(z^{(s)})} \end{aligned}$$

ELBO

KL-term

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

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

Jacobian

ELBO

KL-term

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

Jacobian

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

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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