Normalising Flows

Philip Schulz and Wilker Aziz
https://github.com/philschulz/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

Posterior Approximations

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

Counter example

Gaussian mixture model

The problem with Standard Distributions

Normalising Flows

Use Case 1: Density Estimation

Use Case 2: Inference (sampling)

Summary

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.

$$h(x) = y$$

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.

$$h(x) = y$$

$$p(y) = p(h^{-1}(y))|\det J_{h^{-1}}(y)| = p(x)|\det J_{h^{-1}}(y)|$$

$$p(x) = p(h(x))|\det J_h(x)| = p(y)|\det J_h(x)|$$

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.

$$
\begin{aligned}
h(x) &= y \\
p(y) &= p(h^{-1}(y))|\det J_{h^{-1}}(y)| = p(x)|\det J_{h^{-1}}(y)| \\
p(x) &= p(h(x))|\det J_h(x)| = p(y)|\det J_h(x)|
\end{aligned}
$$

The Challenge

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

Normalising Flows

Approach

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

Normalising Flows

Approach

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

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

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

Normalising Flows

Core Idea

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

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

Now we can learn K mappings with simple Jacobians.

Normalising Flows

Core Idea

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

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

Now we can learn K mappings with simple Jacobians.

$$h^{-1} = h_K^{-1} \circ h_{K-1}^{-1} \circ \ldots \circ h_1^{-1}$$

Normalising Flows

Core Idea

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

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

Now we can learn K mappings with simple Jacobians.

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

Normalising Flows

Core Idea

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

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

Now we can learn K mappings with simple Jacobians.

$$\begin{aligned}
h^{-1} &= h_K^{-1} \circ h_{K-1}^{-1} \circ \ldots \circ h_1^{-1} \\
p(x) &= p(y) \left| \det J_{h_1}\left(y^{(1)}\right) \right| \left| \det J_{h_2}\left(y^{(2)}\right) \right| \ldots \left| \det J_{h_K}(x) \right| \\
p(y) &= p(x) \left| \det J_{h_1^{-1}}\left(y^{(K-1)}\right) \right| \left| \det J_{h_2^{-1}}\left(y^{(K-2)}\right) \right| \ldots \left| \det J_{h_1^{-1}}(y) \right|
\end{aligned}$$

Normalising Flows: Density Estimation

Setting

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

Normalising Flows: Density Estimation

Setting

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

Goal

Transform known variable x into $\epsilon = h(x)$ and express the likelihood as

Normalising Flows: Density Estimation

Setting

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

Goal

Transform known variable x into $\epsilon = h(x)$ and express the likelihood as

$$p(x) = p(\epsilon)|\det J_h\,(x)|$$

Normalising Flows: Density Estimation

Setting

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

Goal

Transform known variable x into $\epsilon = h(x)$ and express the likelihood as

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

Normalising Flows: Density Estimation

Setting

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

Goal

Transform known variable x into $\epsilon = h(x)$ and express the likelihood as

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

2-step Flow

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

2-step Flow

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

2-step Flow

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

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

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

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 a mapping $h(x_{ij}) = \epsilon_{ij}$.

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

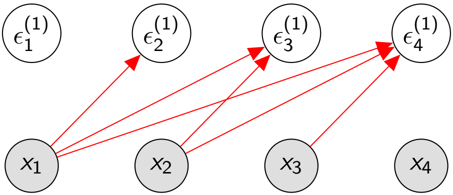
MADE (Germain et al., 2015)

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

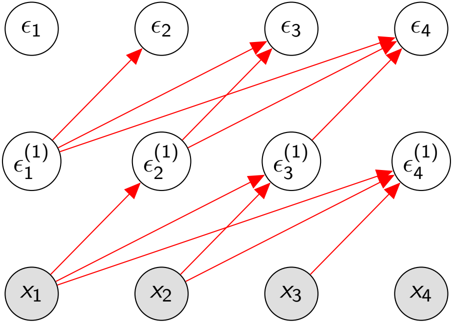
$$\begin{bmatrix} 0 & 0 & \cdots & 0 & 0 \\ 1 & 0 & \cdots & 0 & 0 \\ 1 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \cdots & \vdots & \vdots \\ 1 & 1 & \cdots & 1 & 0 \end{bmatrix}$$

Designing a Transformation

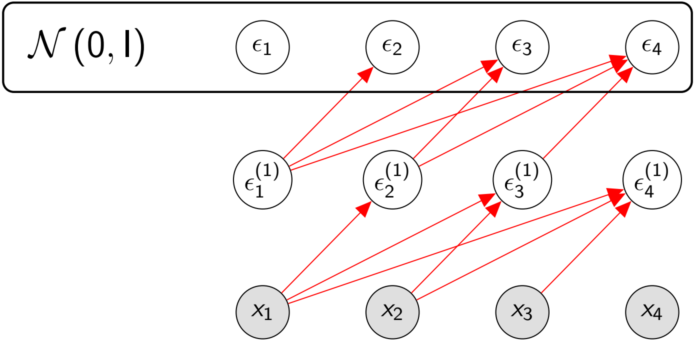
Designing a Transformation



Designing a Transformation



Designing a Transformation



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.

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

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.

$$\begin{aligned} \epsilon_j^{(1)} = h_2^{-1}(x)_j &= \frac{x - \mu(x_{<j})}{\sigma(x_{<j})} \\ \epsilon^{(1)} = h_2^{-1}(x) &= \frac{x - \mu}{\sigma} \end{aligned}$$

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.

$$\begin{aligned}
\epsilon_j^{(1)} = h_2^{-1}(x)_j &= \frac{x - \mu(x_{<j})}{\sigma(x_{<j})} \\
\epsilon^{(1)} = h_2^{-1}(x) &= \frac{x - \mu}{\sigma}
\end{aligned}$$

The Jacobian is

$$J_{h_2^{-1}}(x) =$$

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.

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

$$\epsilon^{(1)} = h_2^{-1}(x) = \frac{x - \mu}{\sigma}$$

The Jacobian is

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

Designing a Transformation

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

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

Designing a Transformation

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

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

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

Designing a Transformation

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

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

$$\begin{bmatrix} \sigma_{11}^{-1} & 0 & \cdots & 0 & 0 \\ 0 & \sigma_{22}^{-1} & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ldots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & \sigma_{mm}^{-1} \end{bmatrix} + \begin{bmatrix} 0 & 0 & \cdots & 0 & 0 \\ \alpha_{21} & 0 & \cdots & 0 & 0 \\ \alpha_{31} & \alpha_{32} & \cdots & 0 & 0 \\ \vdots & \vdots & \ldots & \vdots & \vdots \\ \alpha_{m1} & \alpha_{m2} & \cdots & \alpha_{m,m-1} & 0 \end{bmatrix}$$

Designing a Transformation

Simple Jacobian Determinant

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

Designing a Transformation

Simple Jacobian Determinant

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

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

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

2-step Flow

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

$$
\log p(x) = \log p(h_1^{-1}(h_2^{-1}(x)))
$$

2-step Flow

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

$$
\log p(x) = \log p(h_1^{-1}(h_2^{-1}(x))) - \sum_{j=1}^{M} \log \sigma_j^{(2)} - \sum_{j=1}^{M} \log \sigma_j^{(1)}
$$

2-step Flow

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

$$
\log p(x) = \log p(h_1^{-1}(h_2^{-1}(x))) - \sum_{j=1}^{M} \log \sigma_j^{(2)} - \sum_{j=1}^{M} \log \sigma_j^{(1)}
$$

$$
\epsilon^{(1)} = h_2^{-1} = \frac{x - \mu^{(2)}}{\sigma^{(2)}} \text{ where } \left[\mu^{(2)}, \sigma^{(2)}\right] = g^{(2)}(x)
$$

2-step Flow

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

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

$$\log p(x) = \log p(h_1^{-1}(h_2^{-1}(x))) - \sum_{j=1}^{M} \log \sigma_j^{(2)} - \sum_{j=1}^{M} \log \sigma_j^{(1)}$$

$$\epsilon^{(1)} = h_2^{-1} = \frac{x - \mu^{(2)}}{\sigma^{(2)}} \text{ where } \left[\mu^{(2)}, \sigma^{(2)}\right] = g^{(2)}(x)$$

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

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

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.

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.

Goal

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

Normalising Flows: Inference

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

Simple Mapping

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

Normalising Flows: Inference

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

Flow Mapping

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

2-step Flow

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

2-step Flow

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

2-step Flow

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

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

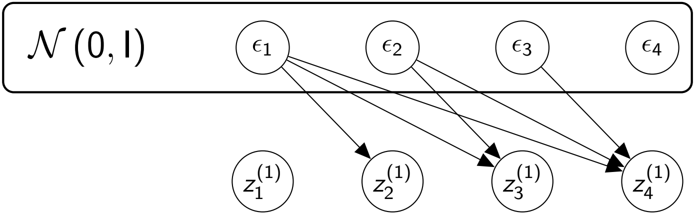
Designing a Transformation

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

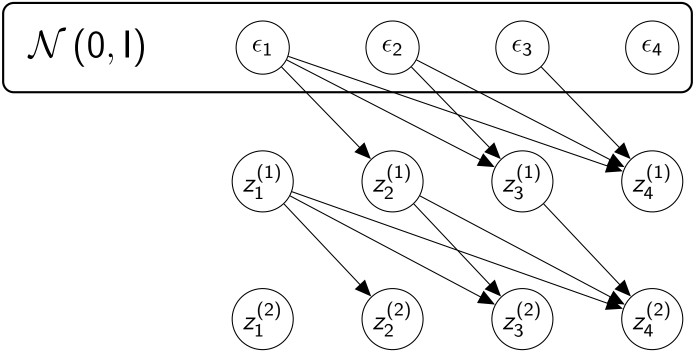
Designing a Transformation

$\mathcal{N}(0, I)$ ϵ_1 ϵ_2 ϵ_3 ϵ_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.

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

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.

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

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.

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

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

Designing a Transformation

Simple Jacobian Determinant

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

In practice we work with the log-likelihood.

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

2-step Flow

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

2-step Flow

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

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

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

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

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

ELBO

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

ELBO

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

ELBO

KL-term

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

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

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

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

Jacobian

ELBO

KL-term

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

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

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
- 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.