Normalising Flows

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VI Tutorial @ University of Alicante
https://vitutorial.github.io/tour/ua2020

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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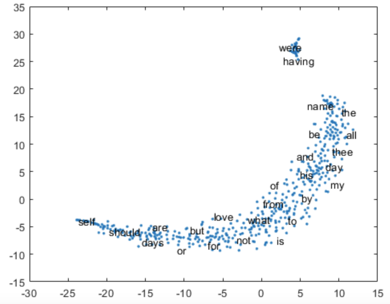

Figure: https://it.mathworks.com/help/textanalytics/ref/trainwordembedding.html

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 $h : \mathcal{X} \rightarrow \mathcal{Y}$ 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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If we want $p_Y(y)$, we need to provide $\left|\det J_{h^{-1}}(y)\right|$ **in the forward pass**. But that's hard!

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

Normalising Flows

Core Idea

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

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Normalising Flows

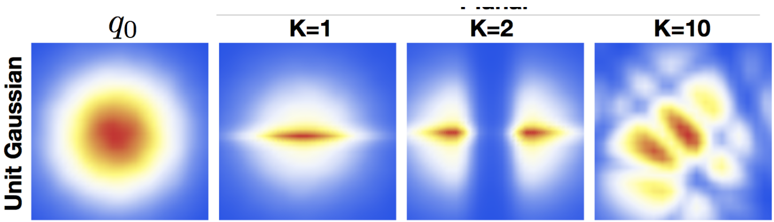

Figure: Taken from Rezende and Mohamed (2015)

Normalising Flows: Density Estimation

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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

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

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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

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

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

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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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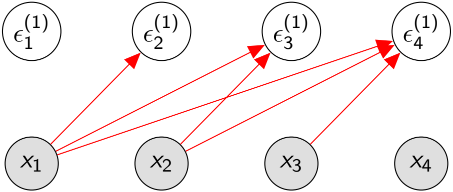

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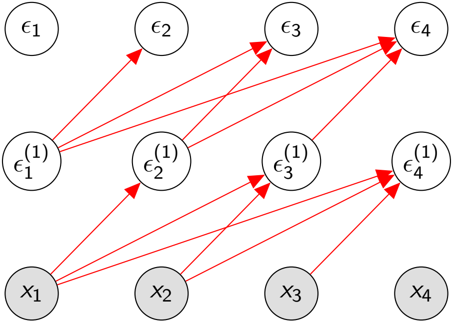

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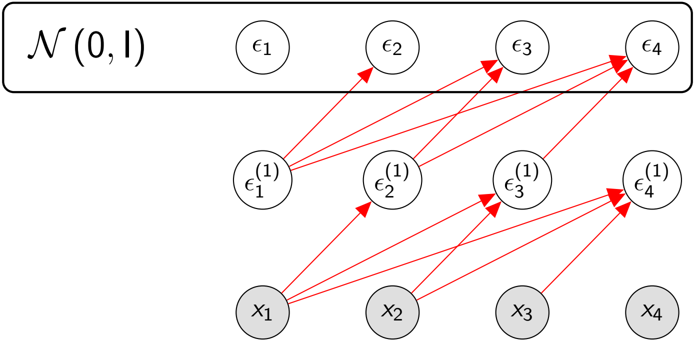

Designing a Transformation

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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The Jacobian is

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

Designing a Transformation

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

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Simple Jacobian Determinant

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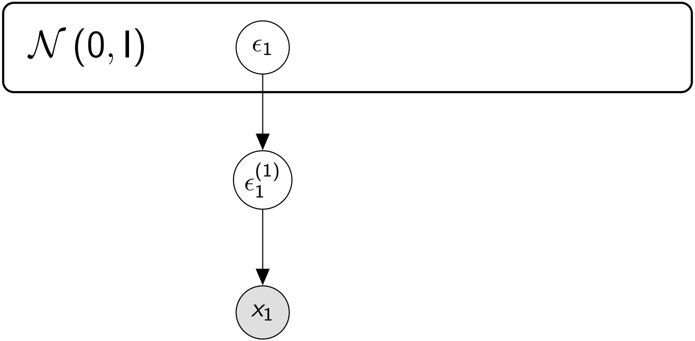
Intermediate Summary

- 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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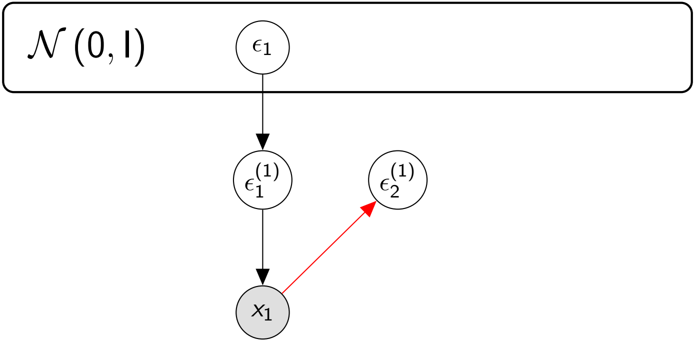

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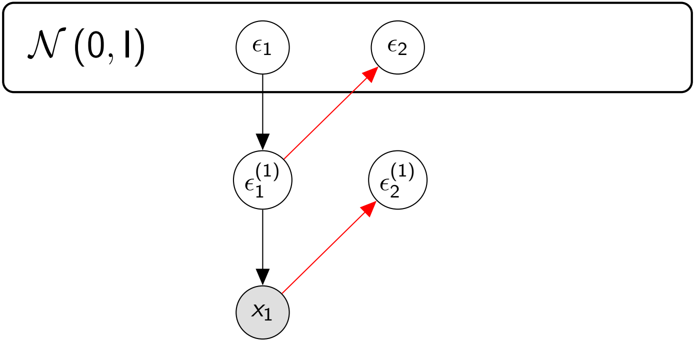

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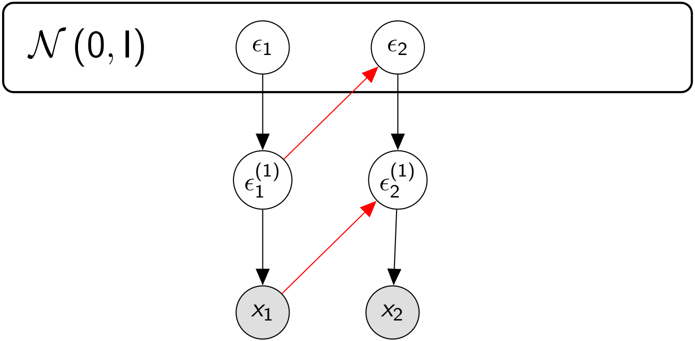

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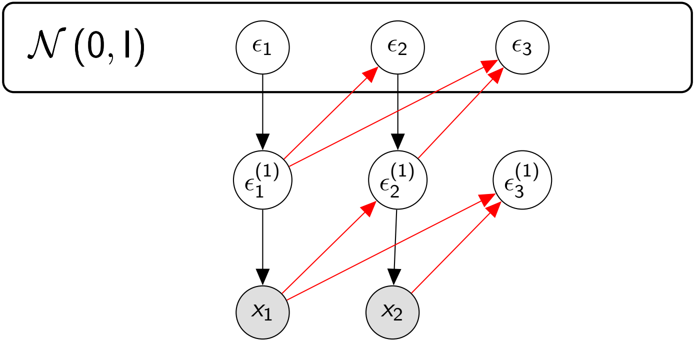

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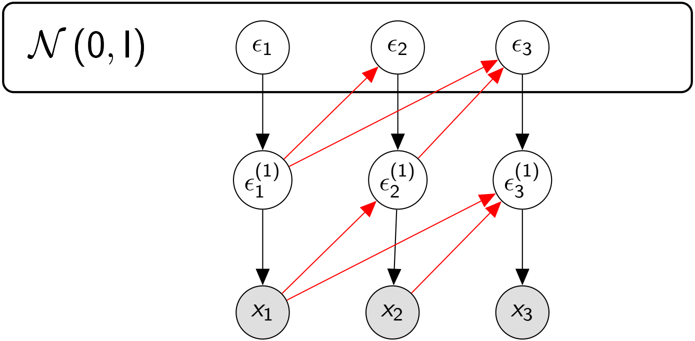

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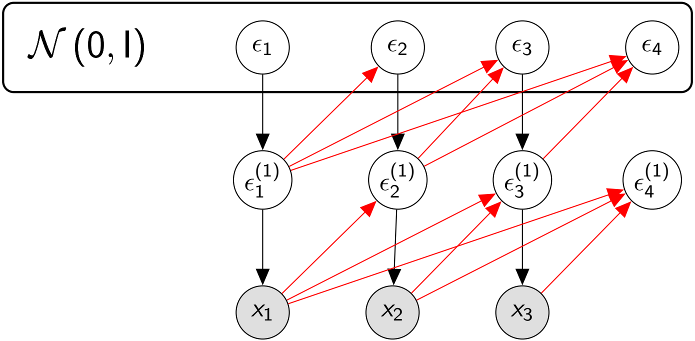

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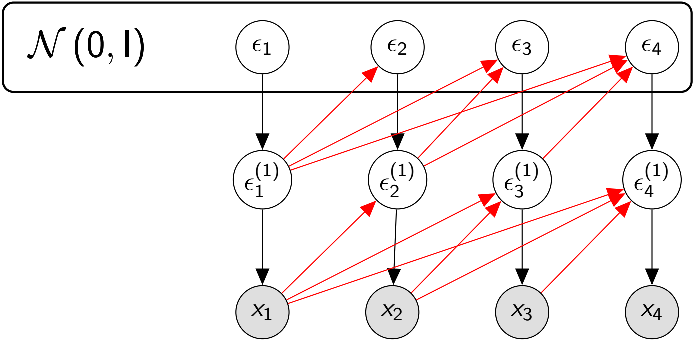

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We have a generative model $p(x, z)$. We want to approximate the posterior $p(z|x)$ using an amortized variational distribution $q(z|x)$ computed by a neural net.

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

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

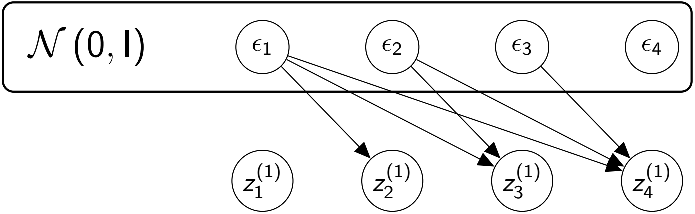
Designing a Transformation

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

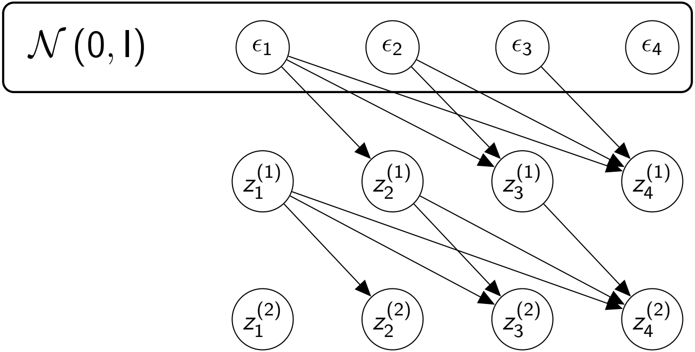
Designing a Transformation

$\mathcal{N}(0, \mathrm{I})$ 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.

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

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

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

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

2-step Flow

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

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

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$$
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$$

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

ELBO

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

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

ELBO

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

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

ELBO

KL-term

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

ELBO

KL-term

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

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

ELBO

KL-term

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

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

ELBO

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Jacobian

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Jacobian

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

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)

Beyond

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Beyond

- We built flows using an affine transformation (with non-zero scale) because its is trivially invertible,
- 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!

References I

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