Variational Mixture of Normalizing Flows

Guilherme Grijó Pen Freitas Pires

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Thesis to obtain the Master of Science degree in
Electrical and Computer Engineering

Supervisor: Prof. Mário A. T. Figueiredo

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- Goal of this work: **mixture of flexible distributions**.

Introduction and Motivation

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  - What should the **mixture components** be?

Introduction and Motivation

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  - What should the **mixture components** be?
  - How should their **parameters** be **estimated**?

Introduction and Motivation

- Deep generative models: an active area of research

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  - **Implicit distributions**: Generative adversarial networks [Goodfellow et al., 2014], Variational Autoencoder [Kingma and Welling, 2014]
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  - **Explicit distributions**: Normalizing flows [Rezende and Mohamed, 2015]
    - Explicit access to the density function
    - No approach to introduce discrete structure (multi-modality)

Outline

- Mixture Models

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- Experiments and results
- Conclusions and future work

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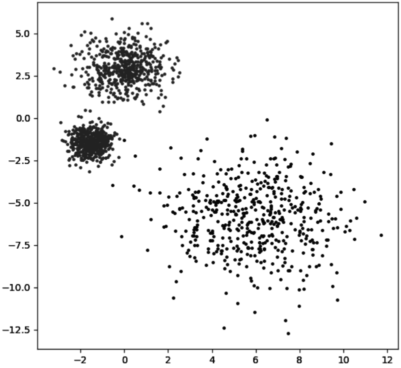
Mixture Models: Mixture of Gaussians



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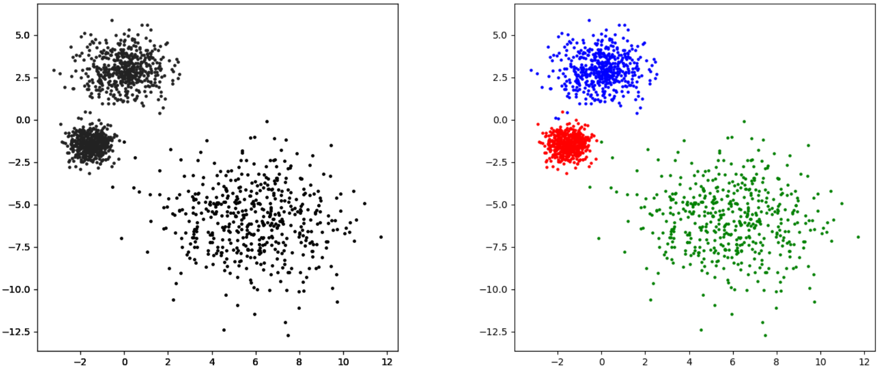

Mixture Models: Definition

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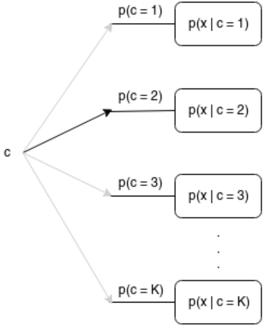
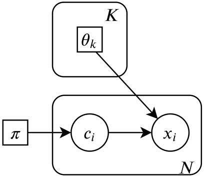


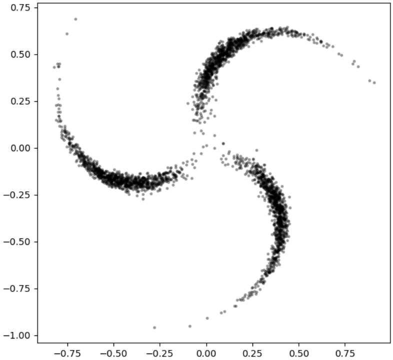
Mixture Models: Joint

For N data points, $X = \{\boldsymbol{x_i} : i = 1, 2, ..., N\}$, and hidden variables $C = \{c_i : i = 1, 2, ..., N\}$



$$
\begin{aligned}
p(\boldsymbol{x}, \boldsymbol{c}) &= \\
&= \prod_{i=1}^{N} \sum_{k=1}^{K} p_c(c_i = k) p_{\boldsymbol{x}|c}(\boldsymbol{x_i} | c_i = k, \theta_k) \\
&= \prod_{i=1}^{N} \sum_{k=1}^{K} \pi_k p_{\boldsymbol{x}|c}(\boldsymbol{x_i} | c_i = k, \theta_k)
\end{aligned}
$$

Mixture Models: Difficult case



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Normalizing Flows: Change of Variables

Given

$$\begin{cases} \boldsymbol{z} \sim p(\boldsymbol{z}) \\ \boldsymbol{x} = g(\boldsymbol{z}; \boldsymbol{\theta}) \end{cases}$$

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then:

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This can be **optimized w.r.t. θ**, to approximate an **arbitrary distribution**

Requirements for feasibility

Normalizing Flows: Change of Variables

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b. **Determinant** of the **Jacobian** of g - computationally cheap

c. **Gradient** of $\det\left(\frac{d}{d\boldsymbol{z}} g(\boldsymbol{z};\boldsymbol{\theta})\right)$ w.r.t $\boldsymbol{\theta}$ - computationally cheap

Normalizing Flows: Change of Variables

- Normalizing Flows: **composition** of several "good" transformations

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Normalizing Flows: Change of Variables

- Normalizing Flows: **composition** of several "good" transformations
- I.e., $g = h_{L-1} \circ h_{L-2} \circ \ldots \circ h_1 \circ h_0$
- Applying the formula to g, and taking the logarithm:

$$\log f_X(\boldsymbol{x}) = \log f_Z(g^{-1}(\boldsymbol{x})) - \sum_{\ell=0}^{L-1} \log \left| \det \left(\frac{d}{d\boldsymbol{x}_\ell} h_\ell(\boldsymbol{x}_\ell) \right) \right|.$$

Normalizing Flows: Affine Coupling Layer

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$$\begin{cases} \boldsymbol{x_1} &= \boldsymbol{z_1} \odot \exp\left(s(\boldsymbol{z_2})\right) + t(\boldsymbol{z_2}) \\ \boldsymbol{x_2} &= \boldsymbol{z_2}. \end{cases}$$

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- The respective Jacobian matrix:

$$J_{f(z)} = \begin{bmatrix} \frac{\partial \boldsymbol{x}_1}{\partial \boldsymbol{z}_1} & \frac{\partial \boldsymbol{x}_1}{\partial \boldsymbol{z}_2} \\ \frac{\partial \boldsymbol{x}_2}{\partial \boldsymbol{z}_1} & \frac{\partial \boldsymbol{x}_2}{\partial \boldsymbol{z}_2} \end{bmatrix} = \begin{bmatrix} \mathrm{diag}\Big(\exp\left(s(\boldsymbol{z}_2)\right)\Big) & \frac{\partial \boldsymbol{x}_1}{\partial \boldsymbol{z}_2} \\ \boldsymbol{0} & \boldsymbol{I} \end{bmatrix}$$

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Variational Inference: Preamble

- Joint probability distribution $p(\boldsymbol{x}, \boldsymbol{c})$.

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- Inference about $\boldsymbol{c}$, given $\boldsymbol{x}$, by **Bayes' Law**:

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p(\boldsymbol{c}|\boldsymbol{x}) &= \frac{p(\boldsymbol{x}|\boldsymbol{c})p(\boldsymbol{c})}{p(\boldsymbol{x})} \\
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- Problem: The integral is normally **intractable**
  - **Variational inference**: an **approximate inference** framework to overcome this intractability.

Variational Inference: Goal

Given a family $q(\boldsymbol{c}; \boldsymbol{\lambda})$, find the parameters $\boldsymbol{\lambda}^*$ such that:

$$\boldsymbol{\lambda}^* = \underset{\boldsymbol{\lambda}}{\operatorname{argmin}}\, KL(q(\boldsymbol{c}; \boldsymbol{\lambda}) || p(\boldsymbol{c}|\boldsymbol{x}))$$

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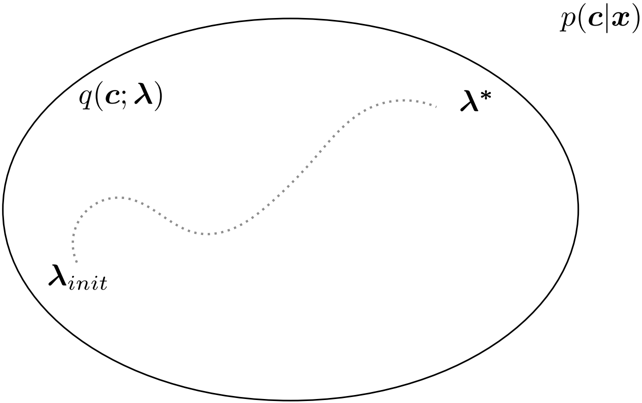
Variational Inference: Goal



Variational Inference: ELBO

$$KL(q(\boldsymbol{c})||p(\boldsymbol{c}|\boldsymbol{x})) = \int q(\boldsymbol{c}) \log \frac{q(\boldsymbol{c})}{p(\boldsymbol{c}|\boldsymbol{x})} d\boldsymbol{c}$$

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&= \int q(\boldsymbol{c})(\log q(\boldsymbol{c}) - (\log p(\boldsymbol{x}, \boldsymbol{c}) - \log p(\boldsymbol{x}))) d\boldsymbol{c}
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&= \int q(\boldsymbol{c})(\log q(\boldsymbol{c}) - (\log p(\boldsymbol{x}, \boldsymbol{c}) - \log p(\boldsymbol{x}))) d\boldsymbol{c} \\
&= \mathbb{E}_q[\log q(\boldsymbol{c})] - \mathbb{E}_q[\log p(\boldsymbol{x}, \boldsymbol{c})] + \log p(\boldsymbol{x})
\end{aligned}
$$

Variational Inference: ELBO

$$KL(q(\boldsymbol{c})||p(\boldsymbol{c}|\boldsymbol{x})) + \mathbb{E}_q[\log p(\boldsymbol{x}, \boldsymbol{c})] - \mathbb{E}_q[\log q(\boldsymbol{c})] = \log p(\boldsymbol{x})$$

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$$\overbrace{KL(q(\boldsymbol{c})||p(\boldsymbol{c}|\boldsymbol{x}))}^{\geqslant 0} + \mathbb{E}_q[\log p(\boldsymbol{x}, \boldsymbol{c})] - \mathbb{E}_q[\log q(\boldsymbol{c})] = \log p(\boldsymbol{x})$$

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$$\begin{aligned} \mathrm{ELBO}(q) &= \mathbb{E}_q[\log p(\boldsymbol{x}, \boldsymbol{c})] - \mathbb{E}_q[\log q(\boldsymbol{c})] \\ &= \mathbb{E}_q[\log p(\boldsymbol{x}|\boldsymbol{c})] + \mathbb{E}_q[\log p(\boldsymbol{c})] - \mathbb{E}_q[\log q(\boldsymbol{c})] \end{aligned}$$

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VMoNF: Introduction

Is it possible to **combine** the ideas from the previous sections, to obtain a mixture of flexible models?

VMoNF: Definition

- Mixture of K normalizing flows

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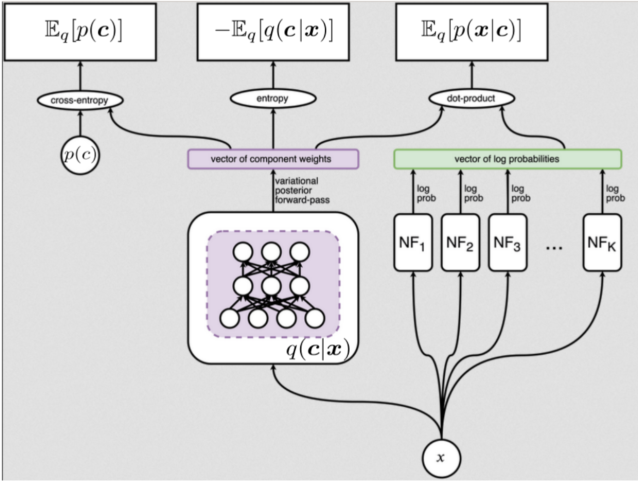
- Recall $ELBO(q) = \mathbb{E}_q[\log p(\boldsymbol{x}|c)] + \mathbb{E}_q[\log p(c)] - \mathbb{E}_q[\log q(c)]$
- The components $p(\boldsymbol{x}|c)$ are **normalizing flows**
- Optimize the ELBO, by **jointly** learning the variational posterior and the generative components.

VMoNF: Overview



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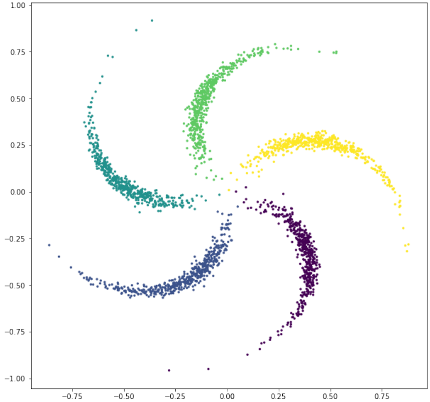
VMoNF: Experiments - Pinwheel (5 wings)



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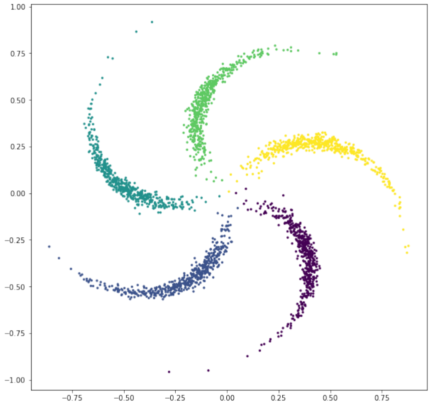
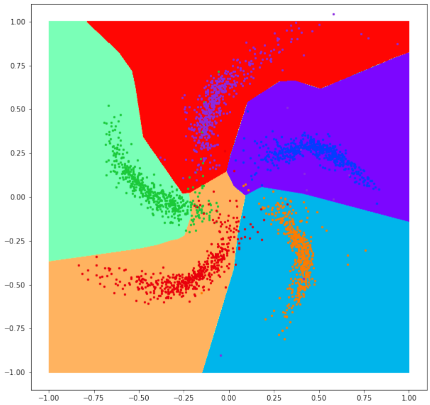
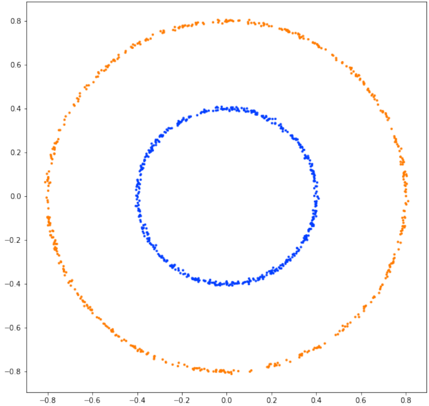




Trainining Animation

VMoNF: Experiments - 2 Circles



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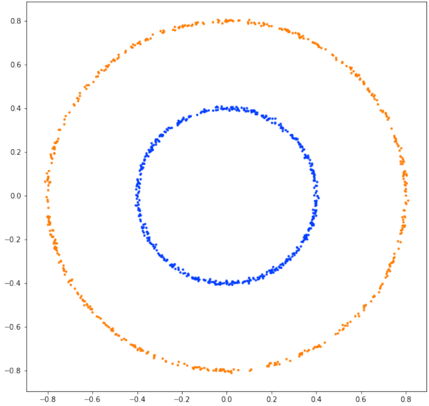

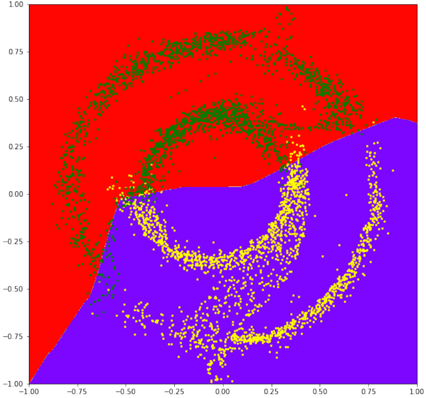

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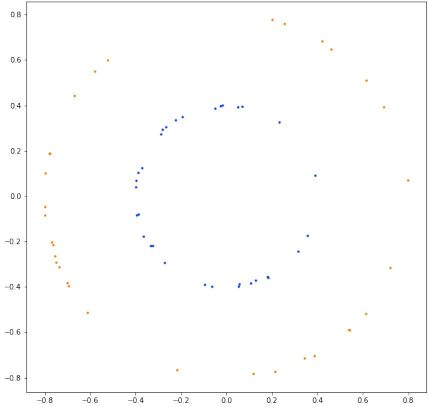
VMoNF: Experiments - 2 Circles (semi supervised)



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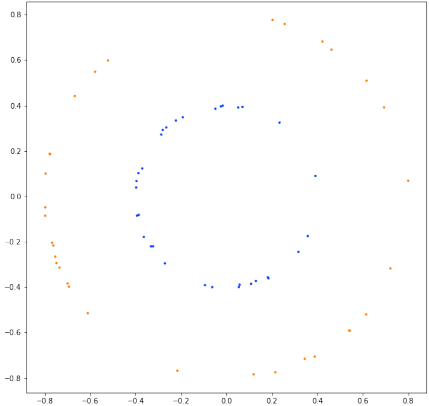
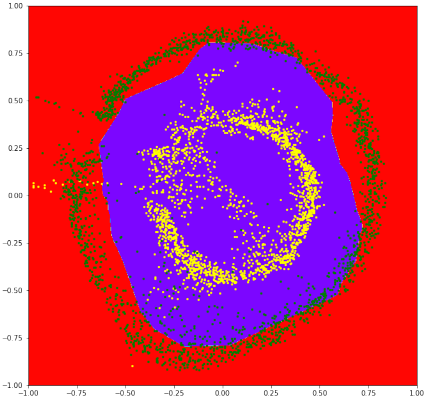
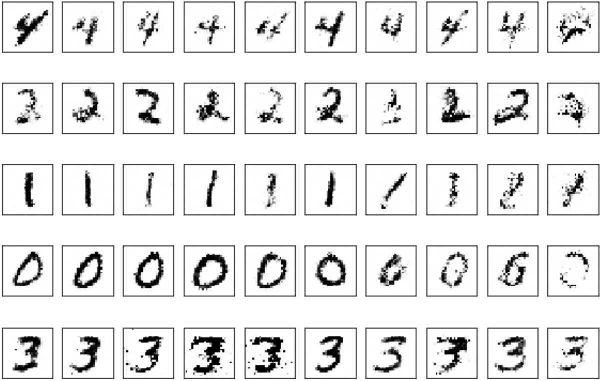




Note: 32 labeled points, 1024 unlabeled points

VMoNF: Experiments - MNIST



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Conclusions and Future Work

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- Weight-sharing between components

- Balance between complexities

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- Investigate the effect of a consistency loss regularization term
- Weight-sharing between components
- Balance between complexities
- (Controlled) component anihilation

Thank you!