Variational Mixture of Normalizing Flows

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

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Introduction and Motivation

- Deep generative models: an active area of research

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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)

Introduction and Motivation: Goal

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- Two questions:

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

  - How should their **parameters** be **estimated**?

Outline

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- Variational Inference

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    - The chosen framework for estimating the parameters of the proposed model

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- Experiments and results

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- Experiments and results
- Conclusions and future work

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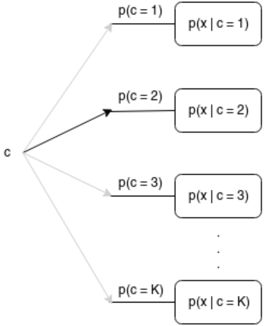
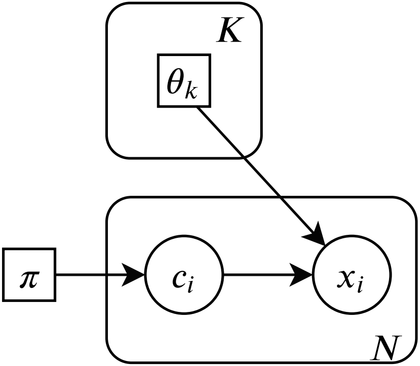


Mixture Models: Plate diagram



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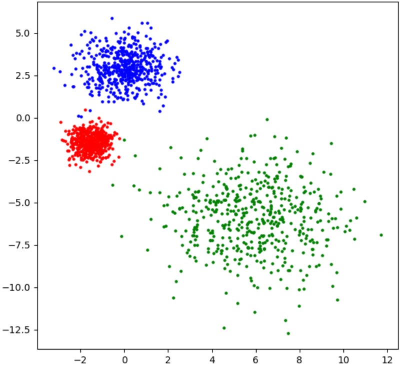
Mixture Models: Mixture of Gaussians



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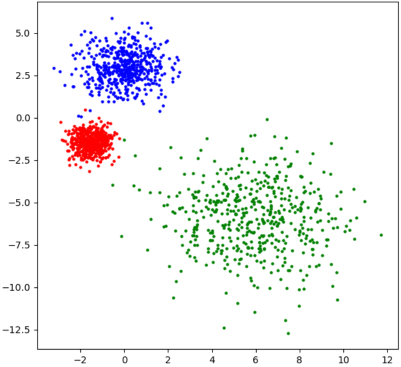

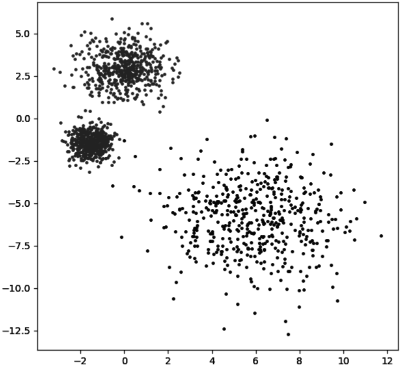

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$$\begin{cases} \boldsymbol{z} \sim p(\boldsymbol{z}) \\ \boldsymbol{x} = g(\boldsymbol{z}; \boldsymbol{\theta}) \end{cases}$$

Normalizing Flows: Change of Variables

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then:

$$\begin{aligned} f_X(\boldsymbol{x}) &= f_Z(g^{-1}(\boldsymbol{x}; \boldsymbol{\theta})) \left| \det \left(\frac{d}{d\boldsymbol{x}} g^{-1}(\boldsymbol{x}; \boldsymbol{\theta}) \right) \right| \\ &= f_Z(g^{-1}(\boldsymbol{x}; \boldsymbol{\theta})) \left| \det \left(\frac{d}{d\boldsymbol{z}} g(\boldsymbol{z}; \boldsymbol{\theta}) \Big|_{\boldsymbol{z}=g^{-1}(\boldsymbol{x};\boldsymbol{\theta})} \right) \right|^{-1} \end{aligned}$$

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This can be **optimized w.r.t. $\boldsymbol{\theta}$**, to approximate an **arbitrary distribution**

Normalizing Flows: Change of Variables

Requirements for feasibility

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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

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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

- An example: Affine Coupling Layer [Dinh, Sohl-Dickstein, and Bengio, 2017]

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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:

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

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$$p(\boldsymbol{z}|\boldsymbol{x}) = \frac{p(\boldsymbol{x}|\boldsymbol{c})p(\boldsymbol{c})}{p(\boldsymbol{x})}$$
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- Problem: The integral is normally **intractable**

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- Problem: The integral is normally **intractable**
  - **Variational inference**: an **approximate inference** framework to overcome this intractability.

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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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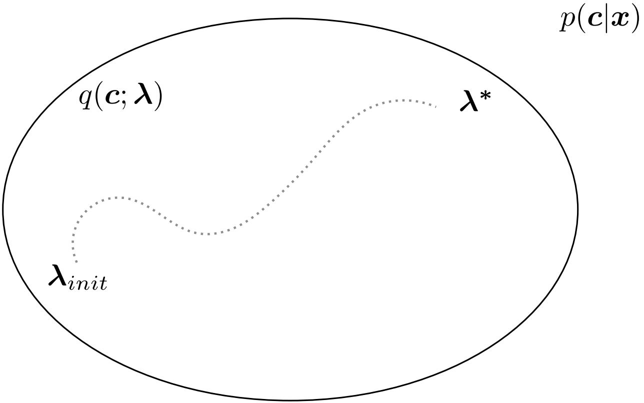
Variational Inference: Goal



Variational Inference: ELBO

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

Variational Inference: ELBO

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KL(q(\boldsymbol{c})||p(\boldsymbol{z}|\boldsymbol{x})) &= \int q(\boldsymbol{c}) \log \frac{q(\boldsymbol{c})}{p(\boldsymbol{c}|\boldsymbol{x})} d\boldsymbol{c} \\
&= \int q(\boldsymbol{c})(\log q(\boldsymbol{c}) - \log 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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Which yields the lower bound (ELBO):

$$
\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

- Recall the ELBO:

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

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- Parameterize $q(z|x)$ with a **neural network**
- Optimize the ELBO, by **jointly** learning the variational posterior and the generative components.

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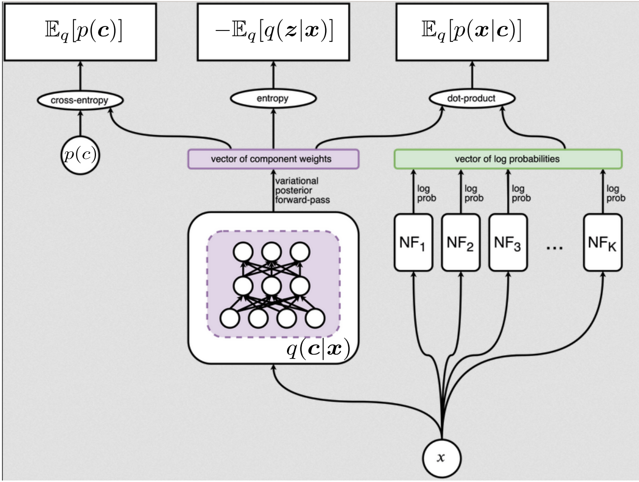
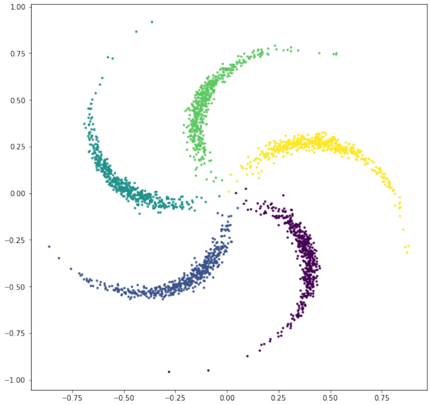
VMoNF: Overview



VMoNF: Experiments - Pinwheel (5 wings)



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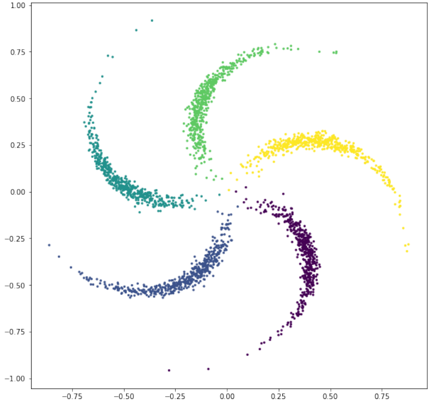
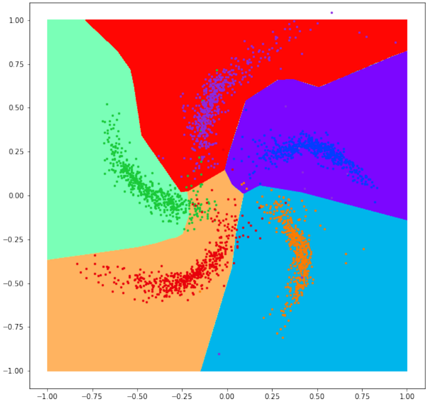
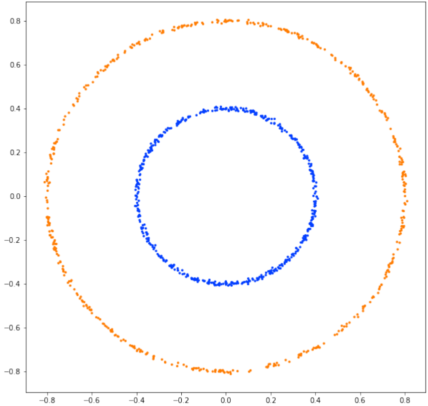




VMoNF: Experiments - Pinwheel (3 wings)

Trainining Animation

VMoNF: Experiments - 2 Circles



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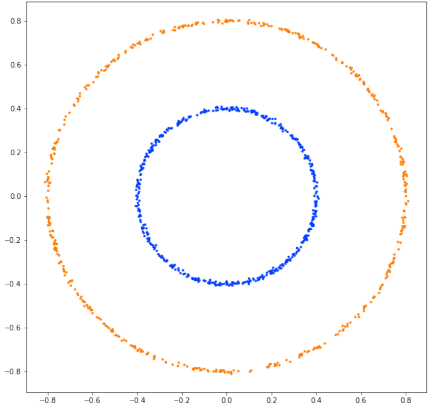
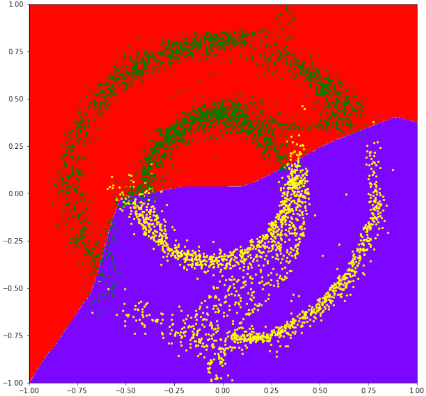
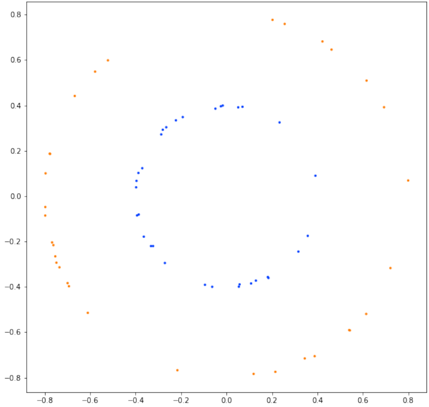




VMoNF: Experiments - 2 Circles (semi supervised)



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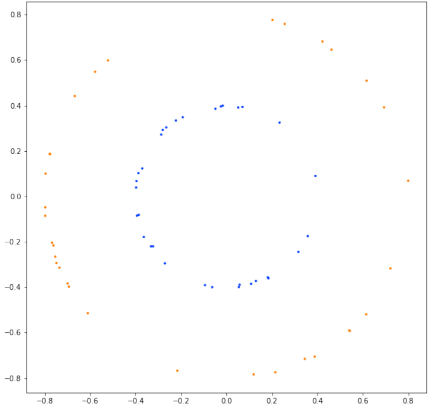

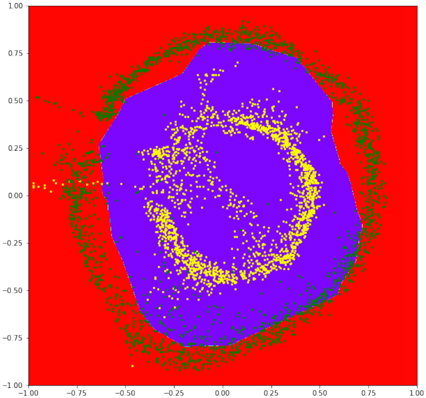

Note: 32 labeled points, 1024 unlabeled points

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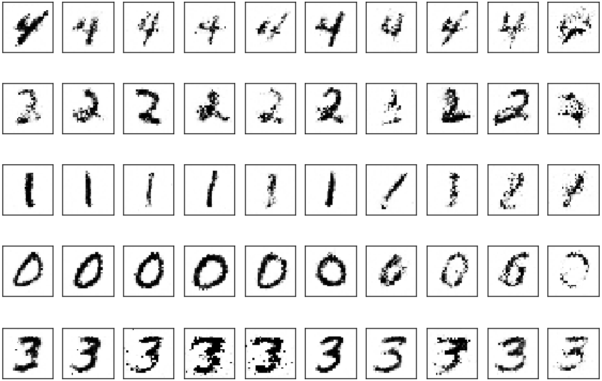
VMoNF: Experiments - MNIST



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Conclusions and Future Work

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- Weight-sharing between components
- Balance between complexities
- (Controlled) component anihilation

Thank you!