Variational Mixture of Normalizing Flows

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November 20, 2019

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

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Introduction and Motivation

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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)

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Introduction and Motivation: Goal

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

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

Outline

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- Experiments and results
- Conclusions and future work

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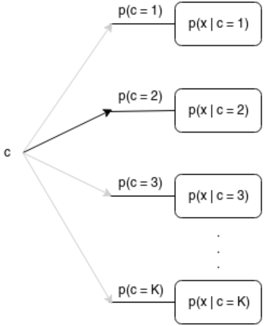

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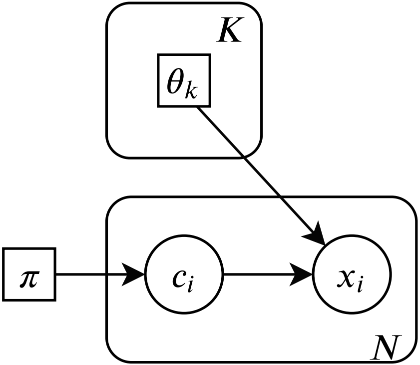
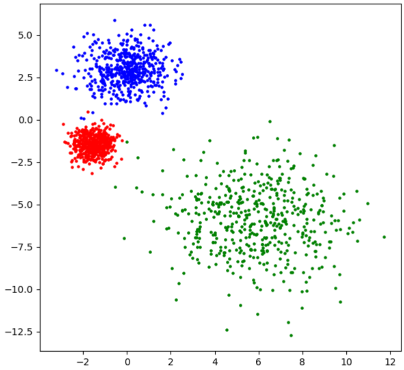
Mixture Models: Plate diagram



Mixture Models: Mixture of Gaussians



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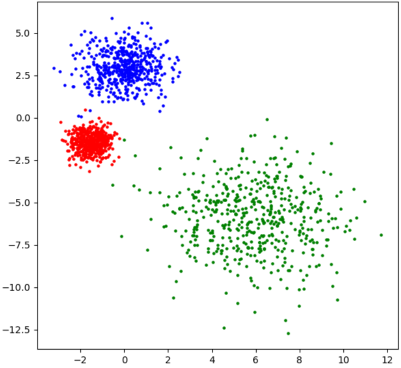

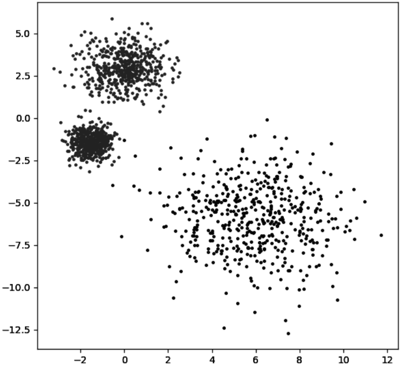

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Given

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then:

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

Requirements for feasibility

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2. **Determinant** of the **Jacobian** of g: computationally cheap
3. **Gradient** of b w.r.t $\boldsymbol{\theta}$: computationally cheap

Normalizing Flows: composition of several “good” transformations

Normalizing Flows: Change of Variables

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Normalizing Flows: Change of Variables

Normalizing Flows: composition of several "good" transformations I.e., $g = h_{L-1} \odot h_{L-2} \odot \ldots \odot h_1 \odot h_0$ 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]$\}$.

Splitting $\boldsymbol{z}$ into $(\boldsymbol{z_1}, \boldsymbol{z_2})$,

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Splitting $\boldsymbol{z}$ into $(\boldsymbol{z}_1, \boldsymbol{z}_2)$,

$$\begin{cases} \boldsymbol{x}_1 & = \boldsymbol{z}_1 \odot \exp\left(s(\boldsymbol{z}_2)\right) + t(\boldsymbol{z}_2) \\ \boldsymbol{x}_2 & = \boldsymbol{z}_2. \end{cases}$$

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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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Variational Inference: Preamble

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

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Inference about $\boldsymbol{z}$, given $\boldsymbol{x}$, by Bayes' Law:

$$
\begin{aligned}
p(\boldsymbol{z}|\boldsymbol{x}) &= \frac{p(\boldsymbol{x}|\boldsymbol{z})p(\boldsymbol{z})}{p(\boldsymbol{x})} \\
&= \frac{p(\boldsymbol{x}|\boldsymbol{z})p(\boldsymbol{z})}{\int p(\boldsymbol{x}|\boldsymbol{z}')p(\boldsymbol{z'})d\boldsymbol{z'}}
\end{aligned}
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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 $q(\boldsymbol{z}; \boldsymbol{\lambda})$, find the parameters $\boldsymbol{\lambda}$ that minimize the Kullback-Leibler divergence between $q(\boldsymbol{z}; \boldsymbol{\lambda})$ and $p(\boldsymbol{z}|\boldsymbol{x})$

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

Variational Inference: ELBO

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

Variational Inference: ELBO

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

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

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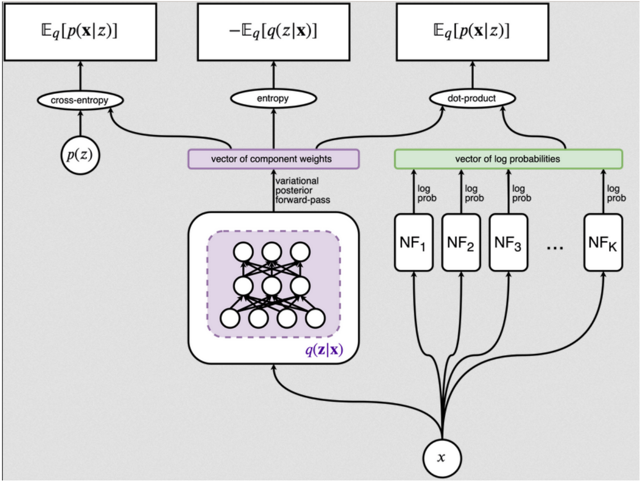
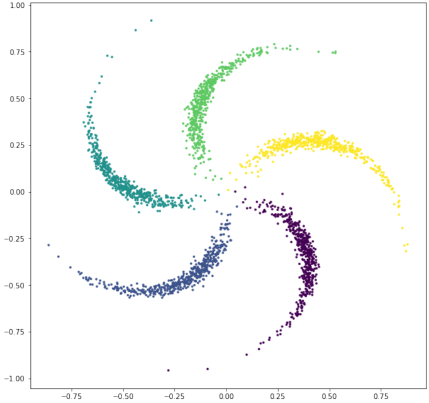
Optimize the ELBO, by **jointly** learning the variational posterior and the generative components.

VMoNF: Overview



VMoNF: Experiments - Pinwheel (5 wings)



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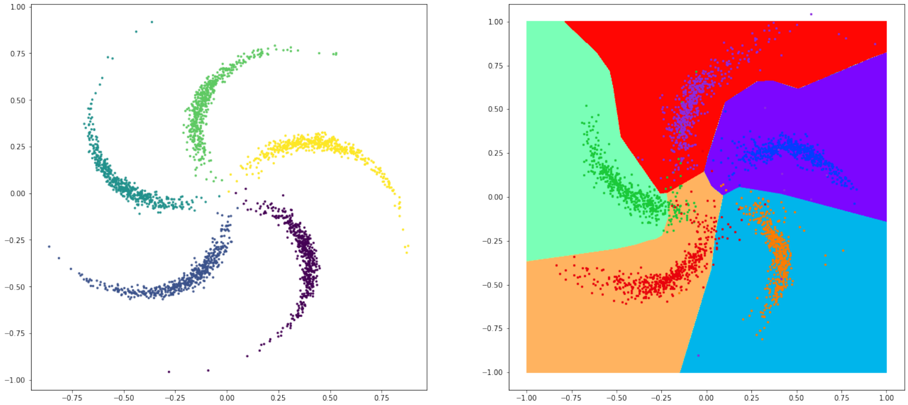
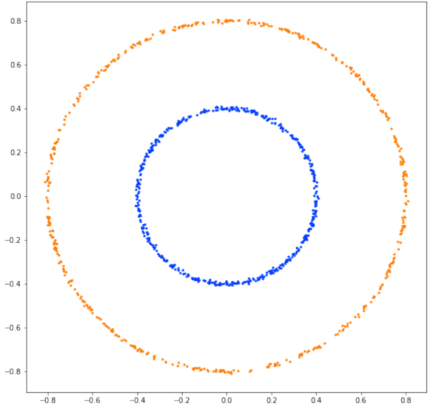


VMoNF: Experiments - Pinwheel (3 wings)

Trainining Animation

VMoNF: Experiments - 2 Circles



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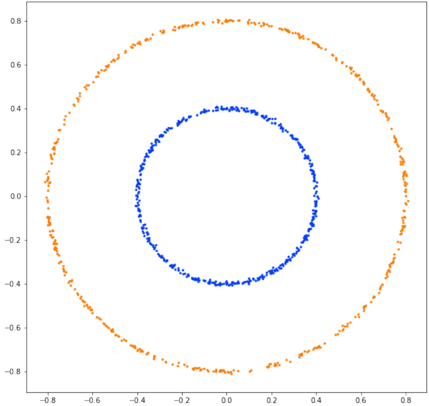
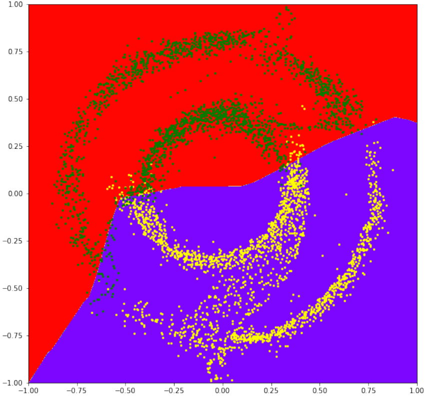
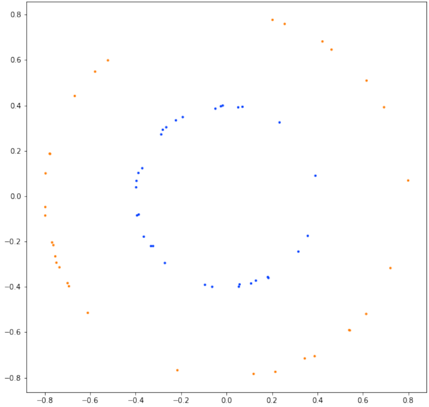




VMoNF: Experiments - 2 Circles (semi supervised)



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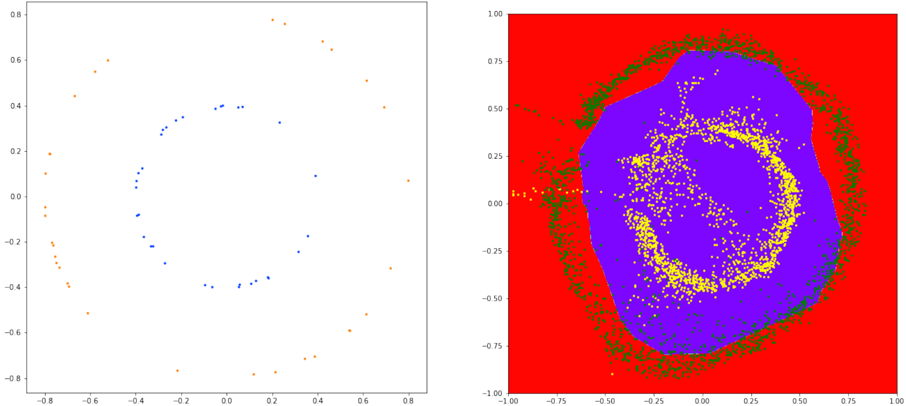
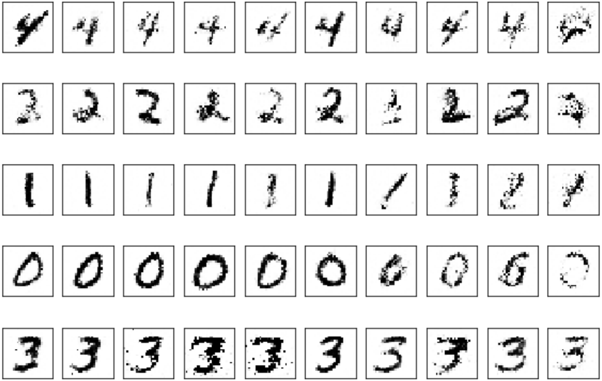


Note: 32 labeled points, 1024 unlabeled points

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!