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 have been an active area of research, with promising results.

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- Deep generative models have been an active area of research, with promising results.
  - **Implicit distributions**: Generative adversarial networks [Goodfellow et al., 2014], Variational Autoencoder [Kingma and Welling, 2014]
    - Don't allow explicit access to the density function
  - **Explicit distributions**: Normalizing flows [Rezende and Mohamed, 2015]
    - Allow explicit access to the density function
    - Lack an approach to introduce discrete structure (multi-modality) in the modelled distribution.

Introduction and Motivation: Goal

– The goal of this work was the development of a mixture of flexible distributions.

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- This requires answering two questions:
  - What should be the “family” of the mixture components?
  - How should the mixture components’ parameters be estimated?

Outline

- Mixture Models

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- Experiments and results
- Conclusions and future work

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Mixture Models: Definition

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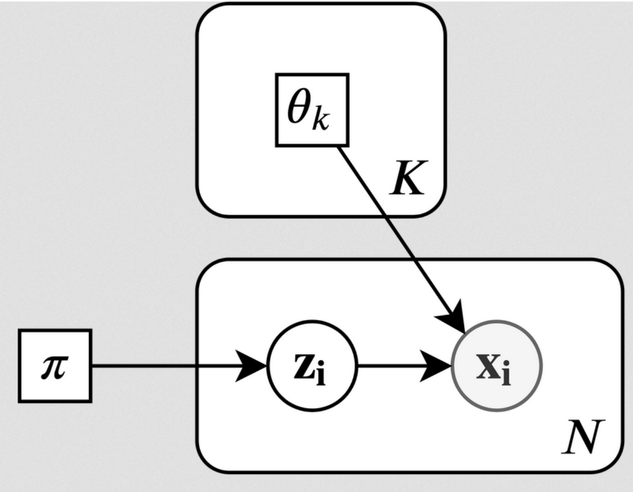
- Typically, it is assumed that the "subgroup-conditional" distributions belong to the same family, but have different parameters.
- Formally, a mixture model's joint distribution (for a single instance $\boldsymbol{x}$) is given by:

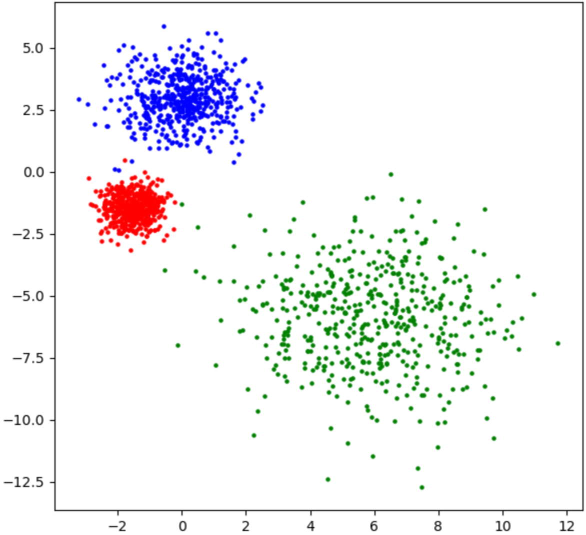
  $$p(\boldsymbol{x}, c) = p(\boldsymbol{x}|c)p(c),$$

  where c is the latent variable that indexes the subgroup to which $\boldsymbol{x}$ belongs

Mixture Models: Plate diagram



Mixture Models: Mixture of Gaussians



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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. $\boldsymbol{\theta}$, so as to approximate an arbitrary distribution

Normalizing Flows: Change of Variables

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- The gradient of the determinant of the Jacobian of g w.r.t $\boldsymbol{\theta}$ is computationally cheap

Normalizing Flows: Change of Variables

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I.e., the function g is a composition of L functions h_ℓ, $\ell = 0, 1, ..., L-1$. Applying the formula to g, and taking the logarithm, yields:

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

Normalizing Flows: Affine Coupling Layer

An example of such a transformation is the Affine Coupling Layer {[Dinh, Sohl-Dickstein, and Bengio, 2017]}.

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

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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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This transformation has the following Jacobian matrix:

$$J_{f(z)} = \begin{bmatrix} \frac{\partial x_1}{\partial z_1} & \frac{\partial x_1}{\partial z_2} \\ \frac{\partial x_2}{\partial z_1} & \frac{\partial x_2}{\partial z_2} \end{bmatrix} = \begin{bmatrix} \text{diag}\Big(\exp\big(s(z_2)\big)\Big) & \frac{\partial x_1}{\partial z_2} \\ \mathbf{0} & I \end{bmatrix}$$

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Variational Inference: Preamble

Consider a joint probability distribution $p(\boldsymbol{x}, \boldsymbol{z})$.

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$$\begin{aligned} p(\boldsymbol{z}|\boldsymbol{x}) &= \frac{p(\boldsymbol{x}|\boldsymbol{z})p(\boldsymbol{z})}{p(\boldsymbol{x})} \\ &= \frac{p(\boldsymbol{x}|\boldsymbol{z})p(\boldsymbol{z})}{\int p(\boldsymbol{x}|\boldsymbol{z}')p(\boldsymbol{z}')d\boldsymbol{z}'} \end{aligned}$$

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Problem: The integral in the denominator is intractable for most interesting models.

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Problem: The integral in the denominator is intractable for most interesting models.

- Variational inference is an approximate inference framework, that can be used to overcome this intractability.

Variational Inference: Goal

Given a parametric family of distributions $q(\boldsymbol{z};\boldsymbol{\lambda})$, find the parameters $\boldsymbol{\lambda}$ that minimize the Kullback-Leibler divergence between $q(\boldsymbol{z};\boldsymbol{\lambda})$ and $p(\boldsymbol{z}|\boldsymbol{x})$

Variational Inference: ELBO

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

Variational Inference: ELBO

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

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

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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:

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

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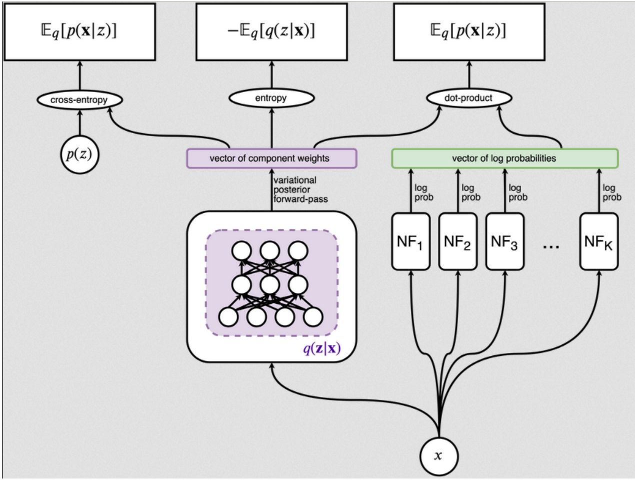
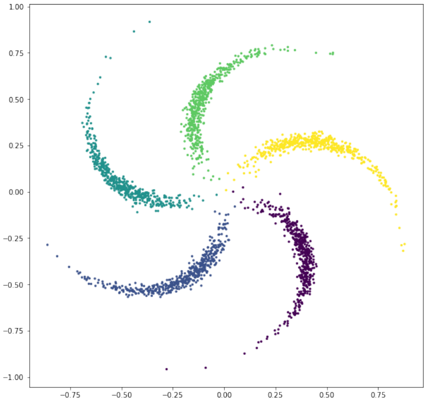
Let the variational posterior $q(z|x)$ be parameterized by a neural network.

We optimize this objective, by **jointly** learning the variational posterior and the generative components.

VMoNF: Overview



VMoNF: Experiments - Pinwheel (5 wings)



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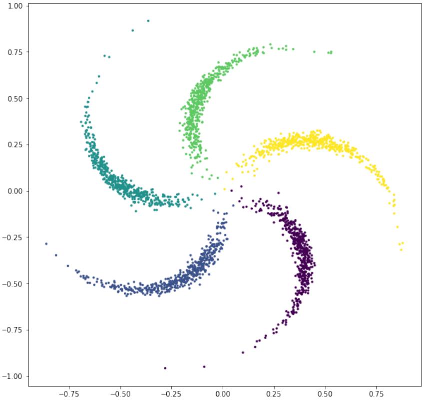

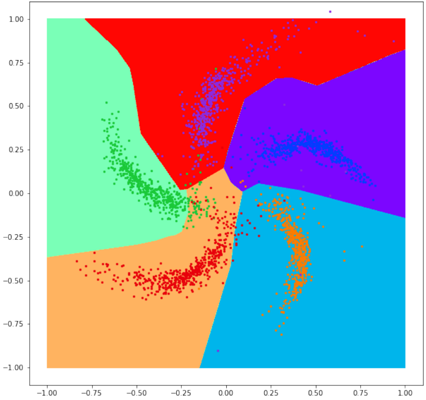

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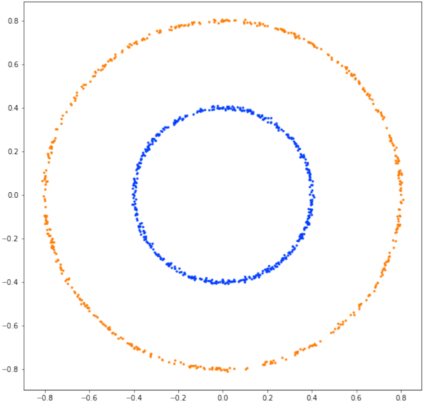
VMoNF: Experiments - Pinwheel (3 wings)

Trainining Animation

VMoNF: Experiments - 2 Circles



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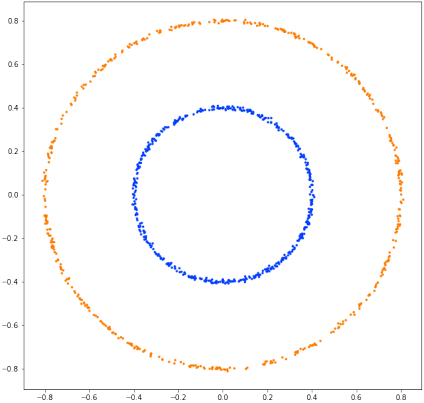
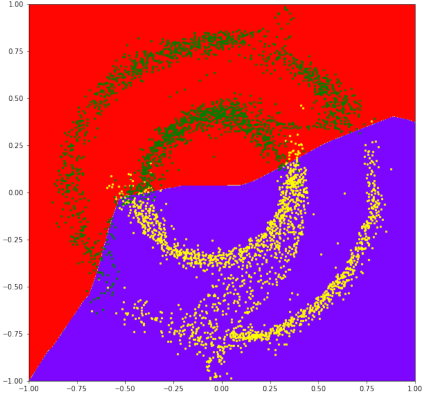
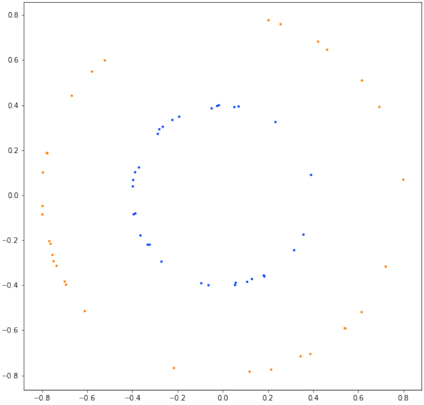




VMoNF: Experiments - 2 Circles (semi supervised)



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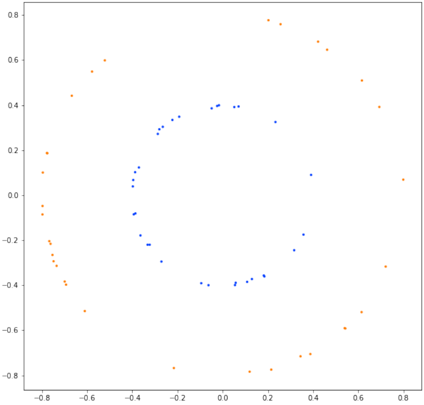
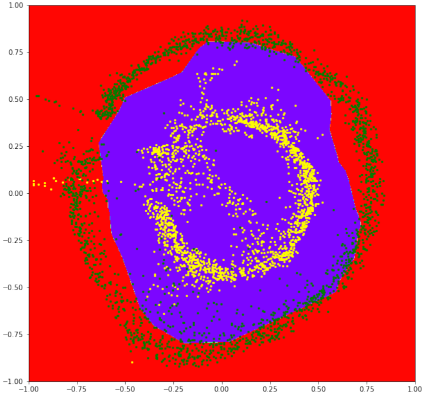
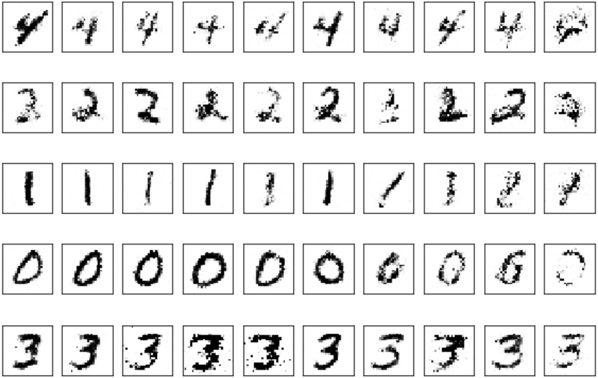




Note: 32 labeled points, 1024 unlabeled points

VMoNF: Experiments - MNIST



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Conclusions and Future Work

- Similar work is being pursued and published in prominent venues: [Dinh, Sohl-Dickstein, et al., 2019; Izmailov et al., 2019]

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

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Thank you!