Variational Mixture of Normalizing Flows

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November 15, 2019

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

TÉCNICO LISBOA

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5. Variational Mixture of Normalizing Flows
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Introduction and Motivation

- Deep generative models have been an active area of research, with promising results.

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  - **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

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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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- Conclusions and future work

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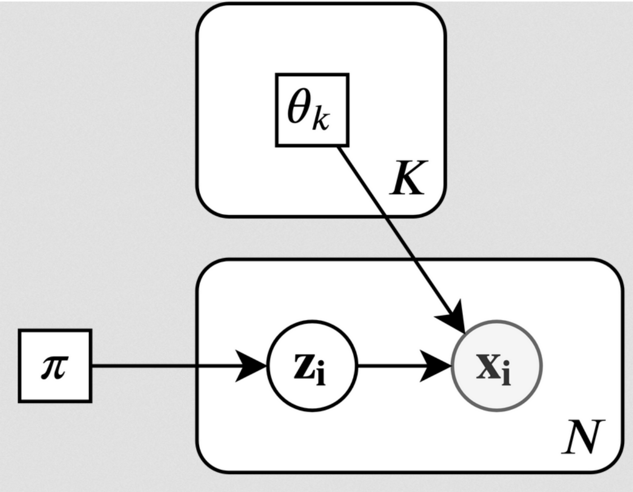
- Typically, it is assumed that the “subgroup-conditional” distributions belong to the same family, but have different parameters.
- Formally, a mixture model’s joint distribution (for a single instance $\boldsymbol{x}$) is given by:

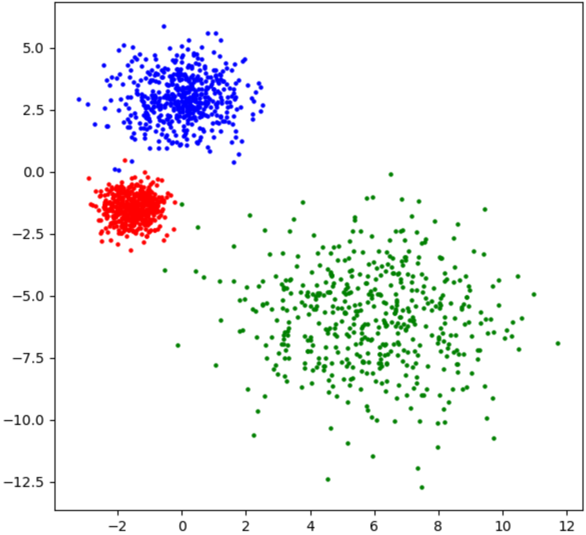
$$p(\boldsymbol{x}, c) = p(\boldsymbol{x}|c)p(c),$$

  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

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

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

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- The base density has a closed form expression and is easy to sample from
- The determinant of the Jacobian of g is computationally cheap - not the case, in general
- The gradient of the determinant of the Jacobian of g w.r.t $\boldsymbol{\theta}$ is computationally cheap

Normalizing Flows: Change of Variables

The framework of Normalizing Flows consists of composing several transformations that fulfill the three listed conditions.

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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This transformation has the following Jacobian matrix:

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

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

Variational Inference: Goal

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

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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$$

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: Motivation

How can we leverage the flexibility of normalizing flows, and endow it with multimodal, discrete structure, like in a mixture model?

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Mixture of normalizing flows. $\rightarrow$ Approximate inference is required.

VMoNF: Definition

Recall the ELBO:

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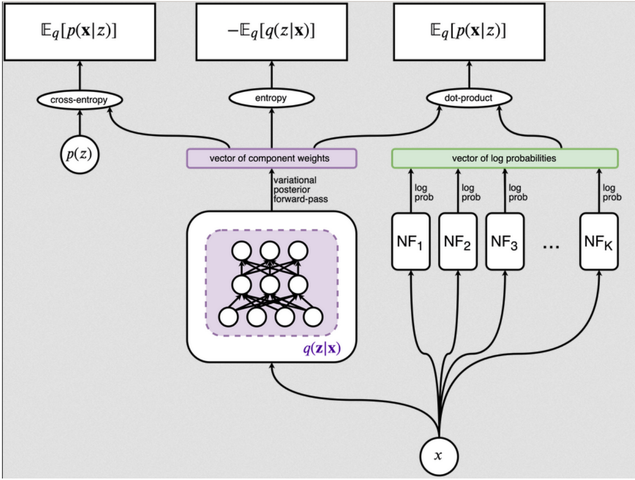
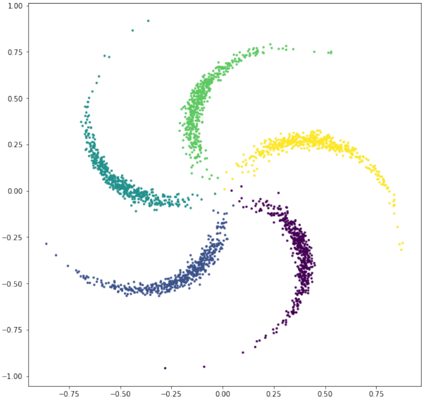
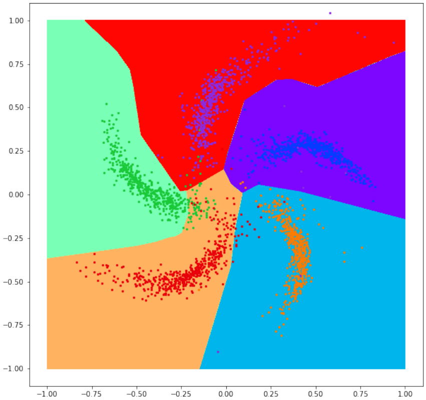
Let the variational posterior $q(z|x)$ be parameterized by a neural network. We jointly optimize this objective, hence we learn the variational posterior and the generative components simultaneously.

VMoNF: Overview



VMoNF: Experiments - Pinwheel (5 wings)

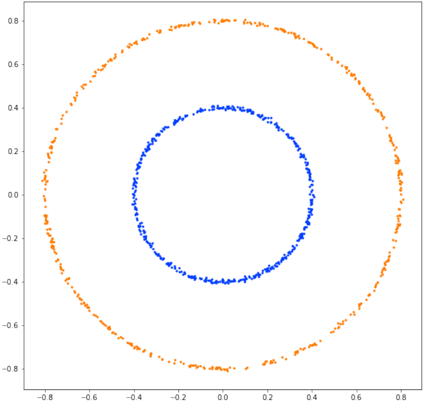


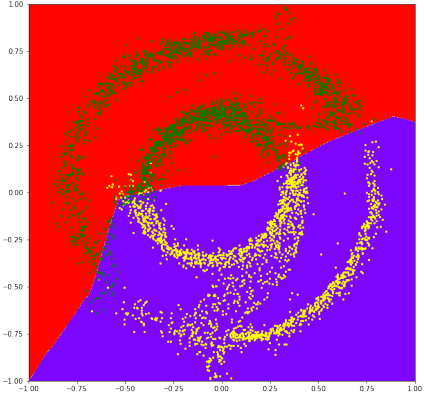


VMoNF: Experiments - Pinwheel (3 wings)

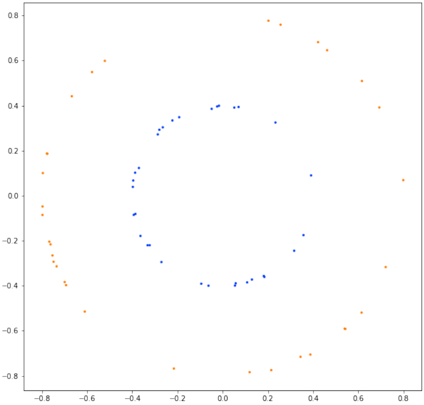
Trainining Animation

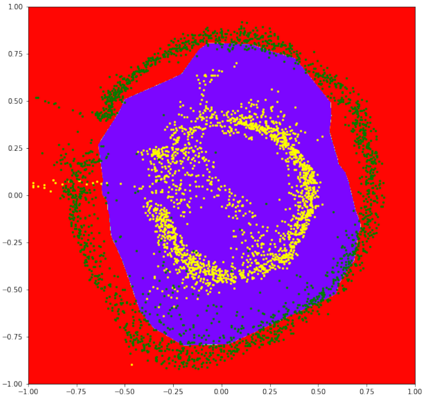
VMoNF: Experiments - 2 Circles





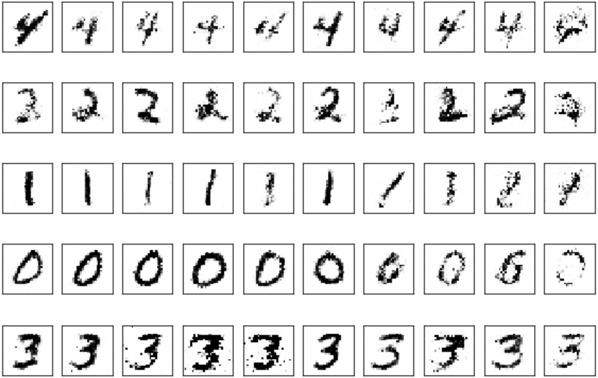
VMoNF: Experiments - 2 Circles (semi supervised)





Note: 32 labeled points, 1024 unlabeled points

VMoNF: Experiments - MNIST



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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!