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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Summary

This work in one sentence:

- The development of a mixture of **normalizing flows** and a (variational) training procedure for it.

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1 Introduction and Motivation

2 Probabilistic Modelling

3 Variational Inference

4 Normalizing Flows

5 Variational Mixture of Normalizing Flows

6 Conclusions

Introduction and Motivation

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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

Introduction and Motivation

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  - How to endow normalizing flows with discrete structure?

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  - How to endow normalizing flows with discrete structure?
  - Or, how to endow mixture models with more expressiveness/flexibility?

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- Experiments and results
- Conclusions and future work

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Probabilistic Modelling: Goal

Given data, find the probability distribution (commonly referred to as the *model*) that is the closest possible approximation to the true distribution of the data.

Probabilistic Modelling: Goal

Informally, via Bayes' Law:

$$p(\text{hypothesis}|\text{data}) = \frac{p(\text{data}|\text{hypothesis})p(\text{hypothesis})}{p(\text{data})}.$$

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The goal of probabilistic modelling is to find the optimal hypothesis that maximizes (some form of) this expression.

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- All of the above, combined

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A mixture model is defined as:

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

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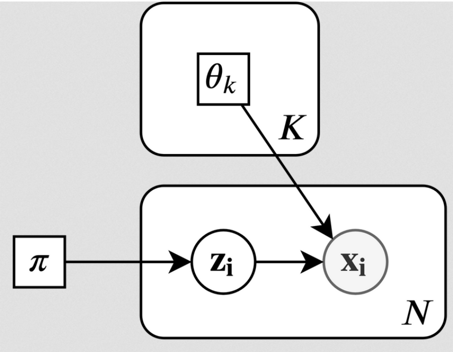

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Maximum-likelihood:

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Maximum a posteriori:

$$\begin{cases} \hat{\boldsymbol{\theta}}_{MAP} = \text{argmax}_{\boldsymbol{\theta}}\, p(\boldsymbol{\theta}|\boldsymbol{x}), \\ p(\boldsymbol{\theta}|\boldsymbol{x}) = \frac{p(\boldsymbol{x}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{p(\boldsymbol{x})}. \end{cases}$$

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$\rightarrow$ Approximate inference is required.

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

Variational Inference: ELBO

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

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This transformation has the following Jacobian matrix:

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

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VMoNF: Motivation

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

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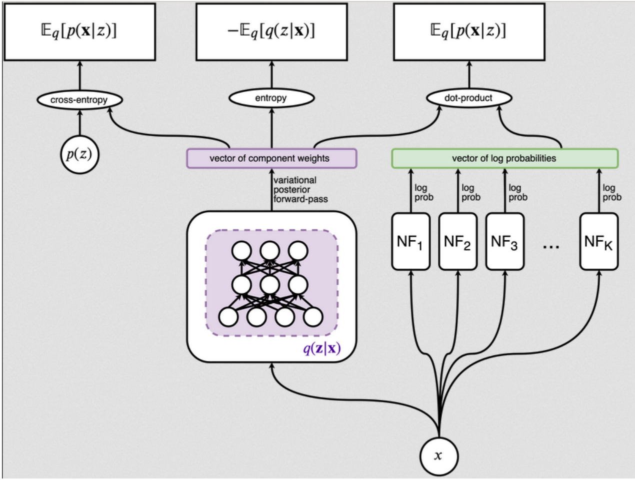
Let the variational posterior $q(z|x)$ be parameterized by a neural network. We jointly optimize this objective, hence we learn the variational posterior and the generative components simultaneously.

VMoNF: Overview



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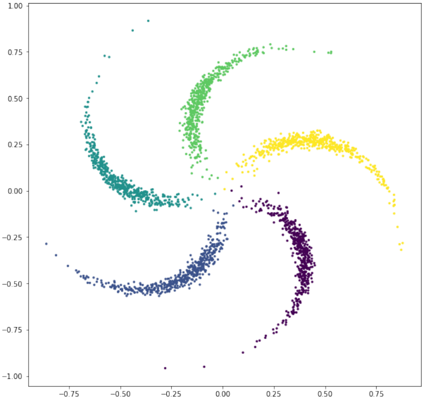
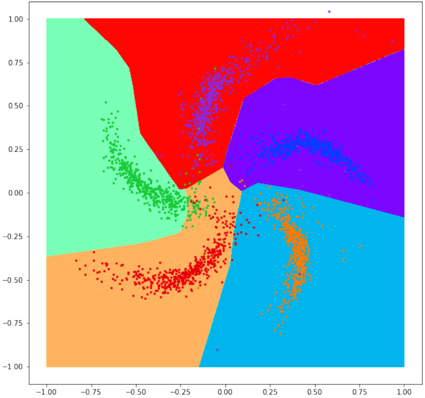
VMoNF: Experiments - Pinwheel (5 wings)





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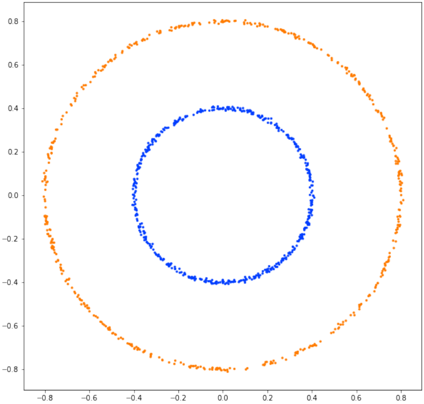
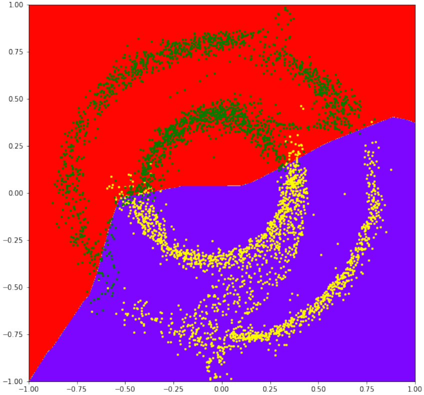
VMoNF: Experiments - Pinwheel (3 wings)

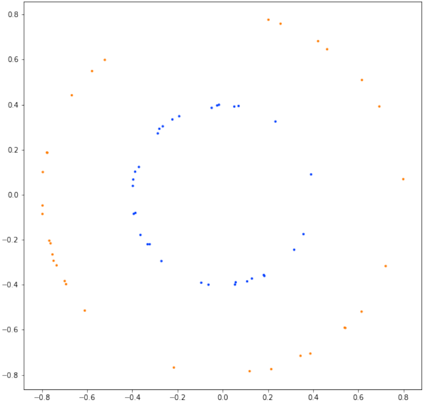
Trainining Animation

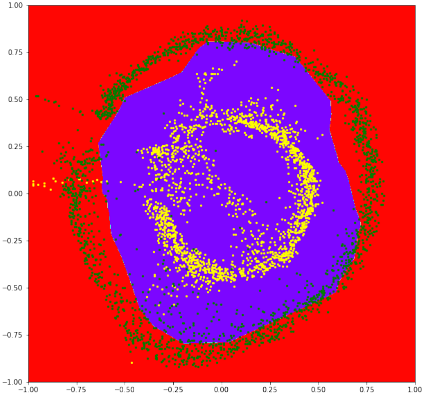
VMoNF: Experiments - 2 Circles





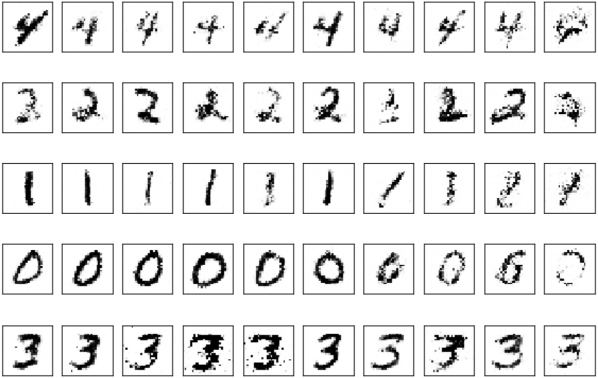
VMoNF: Experiments - 2 Circles (semi supervised)





Note: 32 labeled points, 1024 unlabeled points

VMoNF: Experiments - MNIST



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

Thank you!