# Variational Inference with Continuously-Indexed Normalizing Flows ICML 2020 INNF+ Workshop

Anthony Caterini, Rob Cornish, Dino Sejdinovic, Arnaud Doucet

University of Oxford

July 18, 2020

#### Variational Inference

Given a joint target  $p_{X,Z}(x,z)$  over data  $x \in \mathcal{X}$  and latent variables  $z \in \mathcal{Z}$ , variational inference (VI) seeks to approximate the intractable posterior  $p_{Z|X}$ 

University of Oxford VI with CIFs July 18, 2020

#### Variational Inference

Given a joint target  $p_{X,Z}(x,z)$  over data  $x \in \mathcal{X}$  and latent variables  $z \in \mathcal{Z}$ , variational inference (VI) seeks to approximate the intractable posterior  $p_{Z|X}$ 

VI methods introduce an approximate posterior  $q_Z$ , and are trained to maximize the evidence lower bound (ELBO) objective

#### Variational Inference

Given a joint target  $p_{X,Z}(x,z)$  over data  $x \in \mathcal{X}$  and latent variables  $z \in \mathcal{Z}$ , variational inference (VI) seeks to approximate the intractable posterior  $p_{Z|X}$ 

VI methods introduce an approximate posterior  $q_Z$ , and are trained to maximize the evidence lower bound (ELBO) objective

Can also amortize inference across observations

• e.g. Encoder in a VAE [Kingma and Welling, 2014]

## Explicit VI with Normalizing Flows

Explicit VI involves specifying  $q_Z$  with tractable sampling and density evaluation

## Explicit VI with Normalizing Flows

Explicit VI involves specifying  $q_Z$  with tractable sampling and density evaluation

Normalizing flows (NFs) [Rezende and Mohamed, 2015] define  $q_Z$  explicitly according to the generative process

$$W \sim q_W$$
,  $Z := g(W)$ 

 $\bullet$  g is a diffeomorphism,  $q_W$  is a simple base density

## Explicit VI with Normalizing Flows

Explicit VI involves specifying  $q_Z$  with tractable sampling and density evaluation

Normalizing flows (NFs) [Rezende and Mohamed, 2015] define  $q_Z$  explicitly according to the generative process

$$W \sim q_W, \qquad Z := g(W)$$

 $\bullet$  g is a diffeomorphism,  $q_W$  is a simple base density

Although powerful, NFs can suffer from expressiveness issues, even becoming pathological when the topologies of  $q_W$  and  $p_{Z|X}$  don't match [Cornish et al., 2020]

## Implicit VI with Continuously-Indexed Normalizing Flows

Main contribution: We can gain expressiveness in VI by instead using continuously indexed flows (CIFs) [Cornish et al., 2020], with generative process

$$W \sim q_W$$
,  $U \mid W \sim q_{U \mid W}(\cdot \mid W)$ ,  $Z := G(W; U)$ ,

where  $q_{U|W}$  is trainable, and each  $G(\cdot; u)$  is a normalizing flow

## Implicit VI with Continuously-Indexed Normalizing Flows

Main contribution: We can gain expressiveness in VI by instead using continuously indexed flows (CIFs) [Cornish et al., 2020], with generative process

$$W \sim q_W$$
,  $U \mid W \sim q_{U \mid W}(\cdot \mid W)$ ,  $Z := G(W; U)$ ,

where  $q_{U|W}$  is trainable, and each  $G(\cdot; u)$  is a normalizing flow

Any existing normalizing flow g can be used to construct G, e.g.

$$G(w; u) := e^{s(u)} \odot g(w) + t(u)$$

## Implicit VI with Continuously-Indexed Normalizing Flows

Main contribution: We can gain expressiveness in VI by instead using continuously indexed flows (CIFs) [Cornish et al., 2020], with generative process

$$W \sim q_W$$
,  $U \mid W \sim q_{U \mid W}(\cdot \mid W)$ ,  $Z := G(W; U)$ ,

where  $q_{U|W}$  is trainable, and each  $G(\cdot; u)$  is a normalizing flow

Any existing normalizing flow g can be used to construct G, e.g.

$$G(w; u) := e^{s(u)} \odot g(w) + t(u)$$

Now,  $q_Z(z) := \int q_{Z,U}(z,u) \, \mathrm{d}u$  is defined implicitly over auxiliary variables  $u \in \mathcal{U}$ , rendering the original ELBO intractable

4□ > 4□ > 4 ≥ > 4 ≥ > ≥ 900

#### Auxiliary Variational Inference

Since  $q_{Z,U}$  is tractable for CIFs, we can train using the framework of auxiliary variational inference [Agakov and Barber, 2004]

## Auxiliary Variational Inference

Since  $q_{Z,U}$  is tractable for CIFs, we can train using the framework of auxiliary variational inference [Agakov and Barber, 2004]

New objective is the auxiliary ELBO, having auxiliary inference distribution  $r_{U|Z}$ 

## Auxiliary Variational Inference

Since  $q_{Z,U}$  is tractable for CIFs, we can train using the framework of auxiliary variational inference [Agakov and Barber, 2004]

New objective is the auxiliary ELBO, having auxiliary inference distribution  $r_{U|Z}$ 

CIFs already provide an auxiliary inference distribution

For multi-layer CIFs, this has the correct factorization structure

#### Results - Mixture of Gaussians

We compare explicit VI with a neural spline flow (NSF) [Durkan et al., 2019] to a CIF-NSF on a mixture of Gaussians inference problem with varied initial noise  $\sigma_0$ 

#### Results - Mixture of Gaussians

We compare explicit VI with a neural spline flow (NSF) [Durkan et al., 2019] to a CIF-NSF on a mixture of Gaussians inference problem with varied initial noise  $\sigma_0$ 

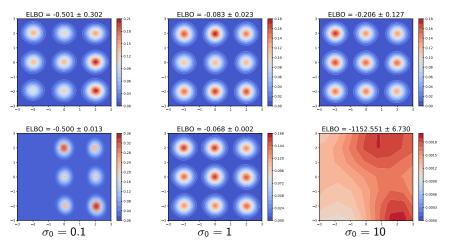


Figure 1: CIFs on top, NSFs on bottom.

#### Results - Image Datasets

We further compare the performance of generative models which use either NSFs, CIF-NSFs, or baseline VAEs as an amortized inference method

#### Results - Image Datasets

We further compare the performance of generative models which use either NSFs, CIF-NSFs, or baseline VAEs as an amortized inference method

Table 1: Test-set marginal log-likelihood averaged over three runs.

	VAE	NSF	CIF-NSF
MNIST FASHION-MNIST	$-87.37_{\pm 0.15} \\ -217.82_{\pm 0.07}$	$-82.95_{\pm 0.11} \\ -215.45_{\pm 0.08}$	$-82.22_{\pm 0.13} \\ -214.50_{\pm 0.11}$

## Thank you!







Figure 2: Joint work with Rob Cornish, Dino Sejdinovic, and Arnaud Doucet

July 18, 2020

#### References

- Anthony Caterini, Rob Cornish, Dino Sejdinovic, and Arnaud Doucet. Variational inference with continuously-indexed normalizing flows. In *ICML Workshop on Invertible Neural Networks and Normalizing Flows*, 2020.
- Rob Cornish, Anthony L Caterini, George Deligiannidis, and Arnaud Doucet. Relaxing bijectivity constraints with continuously-indexed normalising flows. In *International Conference on Machine Learning*, 2020.
- Diederik P. Kingma and Max Welling. Auto-encoding variational bayes. In 2nd International Conference on Learning Representations, ICLR, 2014.
- Danilo Rezende and Shakir Mohamed. Variational inference with normalizing flows. In *International Conference on Machine Learning*, pages 1530–1538, 2015.
- Felix V Agakov and David Barber. An auxiliary variational method. In *International Conference on Neural Information Processing*, pages 561–566. Springer, 2004.
- Conor Durkan, Artur Bekasov, Iain Murray, and George Papamakarios. Neural spline flows. In *Advances in Neural Information Processing Systems*, pages 7509–7520, 2019.