Normalising flows and continuously indexed flows for machine learning

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Outline

1. Normalising flows overview
2. Variational inference
3. Density estimation
4. Practical implementations
5. Limitations
6. Continuously-indexed flows

Overview

Motivation

It is often important to parameterise an expressive families of densities

Key tasks:

- Variational inference: find $\operatorname{argmin}_\phi \mathrm{KL}(q_\phi \parallel p(\cdot \mid \overline{X}))$
- Density estimation: determine p_{data} from $X_1, \ldots, X_n \overset{\text{i.i.d.}}{\sim} p_{\mathrm{data}}$

Normalising flows use neural networks to parameterise families of diffeomorphisms, which induce densities via the change-of-variables formula

Key idea

Parameterise a family of diffeomorphisms f_ψ and choose a fixed noise distribution p_Z

Define model p_ψ to be the W marginal of the following generative process:

$$Z \sim p_Z \qquad W := f_\psi(Z)$$

This gives a procedure for sampling from p_ψ

Can also compute densities via change-of-variables:

$$p_\psi(w) = p_Z(f_\psi^{-1}(w)) \left| \det \mathrm{D} f_\psi^{-1}(w) \right|$$

where $\mathrm{D} f_\psi^{-1}(w)$ denotes the Jacobian of f_ψ^{-1} evaluated at w.

Variational inference

Overview

Assume a Bayesian model $p_{\overline{X},Y}$ with prior p_Y and likelihood $p_{\overline{X}|Y}$, e.g.

$$p_{\overline{X},Y}(\overline{x}, y) = p_Y(y) \prod_{i=1}^{n} p_{X|Y}(x_i \mid y)$$

Observe data $\overline{X} = (X_1, \ldots, X_n)$, and seek posterior $p_{Y|\overline{X}}(\cdot \mid \overline{X})$

Variational inference: (non-amortised)

1. Posit a family of approximate posteriors q_ϕ on Y-space
2. Approximate the true posterior via

$$\operatorname{argmin}_\phi \mathrm{KL}(q_\phi \,\|\, p_{Y|\overline{X}}(\cdot \mid \overline{X}))$$

Mean-field approximation

For high-quality inference, expressiveness of q_ϕ is key; otherwise $\min_\phi \mathrm{KL}(q_\phi \parallel p_{Y|\overline{X}}(\cdot \mid \overline{X}))$ will be large (for complex posteriors)

One approach is mean-field:

$$q_\phi(y) = \prod_{i=1}^{\dim(Y)} q_i(y_i; \phi),$$

where e.g. $\phi = (\overline{\mu}, \overline{\sigma})$ and $q_i(y_i; \phi) = \mathrm{Normal}(y_i; \mu_i, \sigma_i)$

Can rewrite as

$$q_\phi(y) = \mathrm{Normal}(y; \overline{\mu}, \overline{\sigma}\, I),$$

so unimodal and axis-aligned, i.e. fairly limited expressiveness

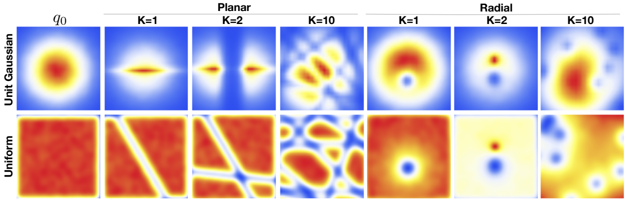
Normalising flows for variational inference

Key idea of Rezende and Mohamed [2015]: use normalising flows to parameterise a more expressive approximate posterior q_ϕ

In particular, take q_ϕ to be distribution of Y, where

$$Z \sim p_Z \qquad Y := f_\phi(Z)$$

with f_ϕ a diffeomorphism



The evidence lower bound (ELBO)

Can compute

$$\begin{aligned}
\mathrm{KL}(q_\phi \parallel p_{Y|\overline{X}}(\cdot \mid \overline{X})) &= -\int q_\phi(y) \log \frac{p_{Y|\overline{X}}(y \mid \overline{X})}{q_\phi(y)}\, dy \\
&= -\int q_\phi(y) \left(\log \frac{p_{\overline{X},Y}(\overline{X}, y)}{q_\phi(y)} - \log p_{\overline{X}}(\overline{X}) \right) dy \\
&= -\int q_\phi(y) \log \frac{p_{\overline{X},Y}(\overline{X}, y)}{q_\phi(y)}\, dy + \log p_{\overline{X}}(\overline{X}),
\end{aligned}$$

so that

$$\mathrm{argmin}_\phi\, \mathrm{KL}(q_\phi \parallel p_{Y|\overline{X}}(\cdot \mid \overline{X})) = \mathrm{argmax}_\phi \underbrace{\int q_\phi(y) \log \frac{p_{\overline{X},Y}(\overline{X}, y)}{q_\phi(y)}\, dy}_{=:\mathrm{ELBO}(\phi)}$$

Optimising the ELBO

A general strategy for optimising the ELBO is stochastic gradient ascent

For normalising flows, since q_ϕ is the pushforward of p_Z by f_ϕ,

$$\begin{aligned} \mathrm{ELBO}(\phi) &:= \int q_\phi(y) \log \frac{p_{\overline{X},Y}(\overline{X}, y)}{q_\phi(y)} \, dy \\ &= \int p_Z(z) \log \frac{p_{\overline{X},Y}(\overline{X}, f_\phi(z))}{q_\phi(f_\phi(z))} \, dz \end{aligned}$$

By differentiating under the integral sign,

$$\nabla_\phi \, \mathrm{ELBO}(\phi) = \int p_Z(z) \, \nabla_\phi \log \frac{p_{\overline{X},Y}(\overline{X}, f_\phi(z))}{q_\phi(f_\phi(z))} \, dz,$$

so that if $Z \sim p_Z$, then $\nabla_\phi \log \frac{p_{\overline{X},Y}(\overline{X}, f_\phi(Z))}{q_\phi(f_\phi(Z))}$ is an unbiased estimate of $\nabla_\phi \, \mathrm{ELBO}(\phi)$ suitable for optimisation

Summary

When using normalising flows for variational inference:

1. Choose p_Z and parameterise f_ϕ
2. Sample $Z \sim p_Z$ and compute $\nabla_\phi \log \frac{p_{\overline{X},Y}(\overline{X}, f_\phi(Z))}{q_\phi(f_\phi(Z))}$
3. Update ϕ via stochastic gradient ascent

In practice:

- Use neural network for f_ϕ (can for p_Z also if reparameterisable)
- Obtain ϕ gradient via autodiff
- Must be able to sample efficiently from q_ϕ (i.e. compute $f_\phi(z)$)
- Only need to be able to compute efficiently

$$q_\phi(f_\phi(Z)) = p_Z(f_\phi^{-1}(f_\phi(Z))) \left|\det \mathrm{D} f_\phi^{-1}(f_\phi(Z))\right| = p_Z(Z) \left|\det \mathrm{D} f_\phi(Z)\right|^{-1}$$

  (or an unbiased estimate of its log), i.e. not $f_\phi^{-1}(y)$ given only y
- Can amortise this procedure

Density estimation

Overview

Aim: determine p_{data} from samples $X_1, \ldots, X_n \overset{\text{i.i.d.}}{\sim} p_{\mathrm{data}}$

Applications:

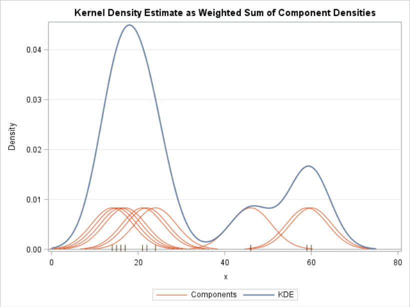
- Out-of-distribution detection
- Synthetic data generation

Illustrative approach

Kernel density estimation: approximate density of p_{data} by

$$p(x) := \frac{1}{n}\sum_{i=1}^{n} k(x - X_i),$$

where k is e.g. a scaled Gaussian



Source: `blogs.sas.com`

Motivation

Curse of dimensionality $\Rightarrow$ different strategies needed in high dimensions

Neural networks have had great success with high-dimensional data e.g. in classification problems

How can we leverage this expressiveness for density estimation?

High-level strategy

Alternatively, consider projecting p_{data} onto a model family, i.e. estimate is

$$\operatorname{argmin}_{\theta \in \Theta} \mathrm{KL}(p_{\mathrm{data}} \parallel p_\theta)$$

where p_θ is a parametrised density

As with variational inference, expressiveness of p_θ is clearly important

Normalising flows for density estimation

A popular idea is to use normalising flows to define p_θ, i.e. p_θ is the X marginal of the following generative process:

$$Z \sim p_Z \qquad X := f_\theta(Z),$$

where f_θ is a parameterised diffeomorphism

This gives a procedure for sampling from p_θ

Can also compute densities via change-of-variables:

$$p_\theta(x) = p_Z(f_\theta^{-1}(x)) \left| \det \mathrm{D} f_\theta^{-1}(x) \right|$$

where $\mathrm{D} f_\theta^{-1}(x)$ denotes the Jacobian of f_θ^{-1} evaluated at x

A nice feature is that this is often exactly tractable by construction

Gradient estimation

By differentiating under the integral sign

$$\nabla_\theta \, \mathrm{KL}(p_{\mathrm{data}} \parallel p_\theta) = -\nabla_\theta \int p_{\mathrm{data}}(x) \log \frac{p_\theta(x)}{p_{\mathrm{data}}(x)} \, dx$$
$$= -\int p_{\mathrm{data}}(x) \, \nabla_\theta \log p_\theta(x) \, dx,$$

so if $X \sim p_{\mathrm{data}}$, then $-\nabla_\theta \log p_\theta(X)$ is an unbiased gradient estimate

This allows finding $\mathrm{argmin}_\theta \, \mathrm{KL}(p_{\mathrm{data}} \parallel p_\theta)$ by stochastic gradient descent

Summary

When using normalising flows for density estimation:

1. Choose p_Z and parameterise f_θ
2. Obtain $X \sim p_{\mathrm{data}}$ and compute $-\nabla_\theta \log p_\theta(X)$
3. Update θ via stochastic gradient descent

In practice:

- Use neural network for f_θ
- Obtain θ gradient via autodiff
- Must be able to compute efficiently

$$p_\theta(x) = p_Z(f_\theta^{-1}(x)) \left|\det \mathrm{D} f_\theta^{-1}(x)\right|$$

(or an unbiased estimate of $\nabla_\theta \log p_\theta(x)$)

- Don't need to be able to sample from p_θ

Some flow architectures

Key considerations

Want to parameterise a family of diffeomorphisms f_ψ

Key requirements:

- f_ψ must be invertible (in practice this may be implicit)
- Tractable log Jacobian (or tractable unbiased estimate)

Can compose flows to obtain greater complexity

RealNVP

For $w \in \mathbb{R}^D$ and $1 \leq d < D$, Dinh et al. [2017] defines

$$f_\psi(w) = \begin{bmatrix} w_{1:d} \\ \exp(s(w_{1:d};\psi)) \odot w_{d+1:D} + t(w_{1:d};\psi) \end{bmatrix}$$

where $s, t : \mathbb{R}^d \to \mathbb{R}^{D-d}$ are unconstrained neural networks

Clear that this is invertible

Jacobian matrix is lower-triangular, so determinant is tractable

Inverse Autoregressive Flow / Masked Autoregressive Flow

For $w \in \mathbb{R}^D$, define

$$f_i(w; \psi) = \exp(s_i(w_{1:i-1}; \psi)) \odot w_i + t_i(w_{1:i-1}; \psi),$$

where $s_i, t_i : \mathbb{R}^{i-1} \to \mathbb{R}$ are unconstrained neural networks, and set

$$f_\psi(w) := \begin{bmatrix} f_1(w; \psi) \\ \vdots \\ f_D(w; \psi) \end{bmatrix}$$

Again invertible and triangular Jacobian matrix

For efficiency (in one direction), MADE [Germain et al., 2015] provides a way to parameterise an autoregressive neural network

Used by Kingma et al. [2016] (for VI) and Papamakarios et al. [2017] (for density estimation)

Residual Flows

Triangular Jacobians seem to reduce expressiveness

Alternative strategy [Behrmann et al., 2019, Chen et al., 2020]: if $g_\psi : \mathbb{R}^D \to \mathbb{R}^D$ has $\operatorname{Lip} g_\psi < 1$, then we get a diffeomorphism

$$f_\psi(w) := w + g_\psi(w)$$

Can ensure a neural network g_ψ is Lipschitz via spectral normalisation

Can estimate Jacobians unbiasedly by expanding as a matrix power series, and using debiasing techniques plus the Skilling-Hutchinson trace estimator

Can be inverted numerically by Banach Fixed Point theorem

Limitations of normalising flows

Intuition

Diffeomorphisms preserve topological properties of their input space, e.g.

- Number of connected components
- Number of "holes"
- How the space is "knotted"

Intuitively suggests that if $X = f(Z)$ then the supports of X and Z will share the same topological properties

Precise result

Theorem (Cornish et al. [2020])

If $\operatorname{supp} p_Z$ *is not homeomorphic to* $\operatorname{supp} p_{\mathrm{data}}$*, then a sequence of diffeomorphisms* f_n *can yield* $f_n(Z) \to p_{\mathrm{data}}$ *in distribution only if*

$$\max\{\mathrm{Lip}\, f_n, \mathrm{Lip}\, f_n^{-1}\} \to \infty$$

Convergence in distribution straightforwardly implies a version in terms of being "approximately not homeomorphic"

General consequence: numerical noninvertibility (observed by Behrmann et al. [2020])

Consequences for Residual Flows

The following densities were learned using a Gaussian prior with a 10-layer Residual Flow [Behrmann et al., 2019, Chen et al., 2020]

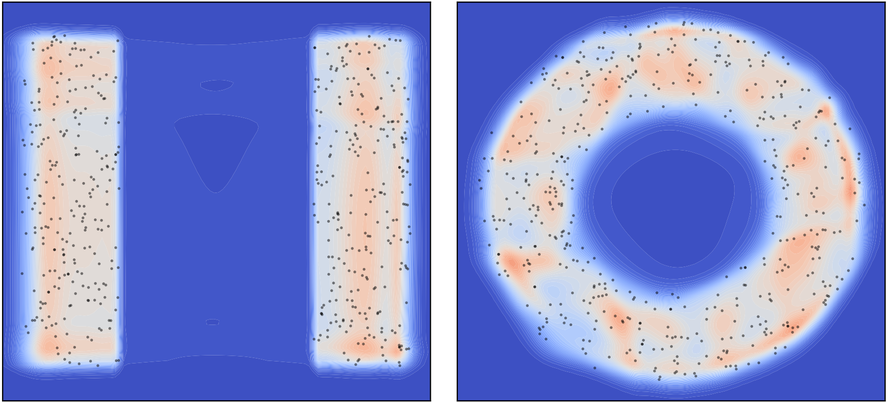


Figure: Darker regions indicate lower density. Data shown in black.

Continuously-Indexed Normalizing Flows (for density estimation)

Continuously-Indexed Flow Layer

To gain expressiveness over baseline flows, continuously-indexed flows (CIFs) now model the data as the X-marginal of

$$Z \sim p_Z, \qquad U \mid Z \sim p_{U|Z}(\cdot \mid Z), \qquad X := F(Z; U)$$

where

- U is a continuous index variable
- $p_{U|Z}$ is a (parametrized) conditional distribution
- $F(\cdot; u)$ is a diffeomorphism for every u

Any existing normalizing flow f can be used to construct F, e.g. via

$$F(z; u) := f\left(e^{s(u)} \odot z + t(u)\right)$$

for neural networks s, t outputting values in Z-space

Multi-Layer CIFs

An L-layer CIF is obtained by stacking the single-layer model:

$$
\begin{aligned}
& && Z_0 \sim p_{Z_0}, \\
U_1 &\sim p_{U_1|Z_0}(\cdot \mid Z_0), && Z_1 := F_1(Z_0; U_1), \\
& && \cdots \\
U_L &\sim P_{U_L|Z_{L-1}}(\cdot \mid Z_{L-1}), && X := F_L(Z_{L-1}; U_L)
\end{aligned}
$$

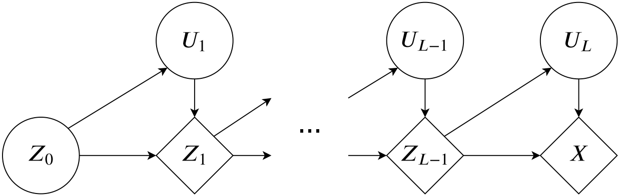


Figure: Graphical multi-layer CIF generative model

Training and inference

The marginal p_X is intractable, but the *joint* $p_{X,U_{1:L}}$ has a closed-form, e.g. for a single layer

$$p_{X,U}(x,u) = p_Z(F^{-1}(x;u))p_{U|Z}(u \mid F^{-1}(x;u))|\det \mathrm{D}F^{-1}(x;u)|$$

Given an inference model $q_{U_{1:L}|X}$, we can use the *ELBO* for training:

$$\mathcal{L}(x) := \mathbb{E}_{u_{1:L} \sim q_{U_{1:L}|X}(\cdot|x)}\left[\log \frac{p_{X,U_{1:L}}(x,u_{1:L})}{q_{U_{1:L}|X}(u_{1:L} \mid x)}\right] \leq \log p_X(x)$$

At test time, we can estimate $\log p_X(x)$ to arbitrary precision using an m-sample *IWAE* estimate with $m \gg 1$

Inference model

To obtain an efficient inference model $q_{U_{1:L}|X}$, we exploit the *conditional independence structure* of $p_{U_{1:L}|X}$ from the forward model:

$$
\begin{aligned}
& Z_L := X, \\
U_L \sim q_{U_L|Z_L}(\cdot \mid Z_L), \qquad & Z_{L-1} := F_L^{-1}(Z_L; U_L), \\
& \cdots \\
U_1 \sim q_{U_1|Z_1}(\cdot \mid Z_1), \qquad & Z_0 := F_1^{-1}(Z_1; U_1)
\end{aligned}
$$

In other words,

$$q_{U_{1:L}|X}(u_{1:L} \mid x) := \prod_{\ell=1}^{L} q_{U_\ell|Z_\ell}(u_\ell \mid z_\ell)$$

This induces a natural weight-sharing scheme between the forward and inverse models, since the same F_ℓ are used in both cases

Benefits over Standard Flows

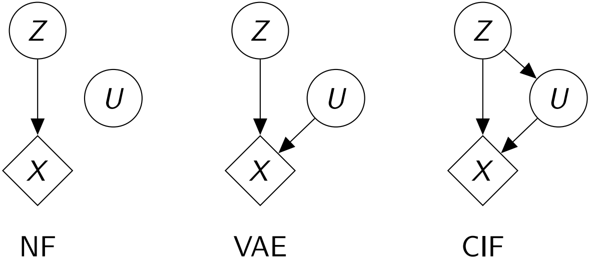
Intuitively, the additional flexibility afforded by $p_{U|Z}$ allows a CIF to "clean up" mass that would be misplaced by a single bijection

Proposition: Under mild conditions on the target and F, there exists $p_{U|Z}$ such that the model p_X has the same support as the target $p_X^\star$

Proposition: If $F(z; \cdot)$ is surjective for each z, there exists $p_{U|Z}$ such that p_X matches $p_X^\star$ exactly

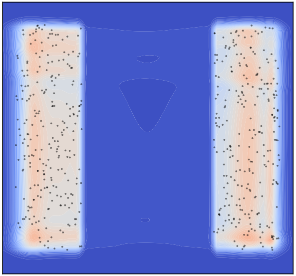
Comparison with Related Models

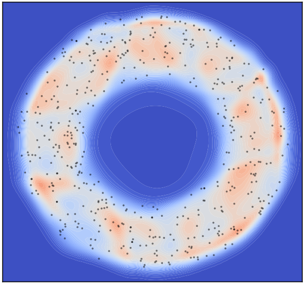
CIFs may be understood as a hybrid between standard normalizing flow and VAE density models:

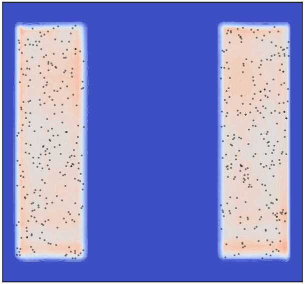


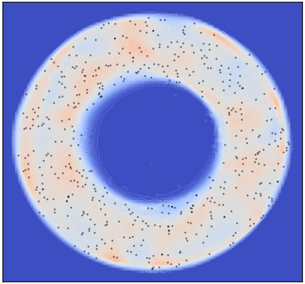
In all cases, $X = F(Z; U)$ for some family of bijections F

2D ResFlow Experiments









2D Masked Autoregressive Flow (MAF) Experiments

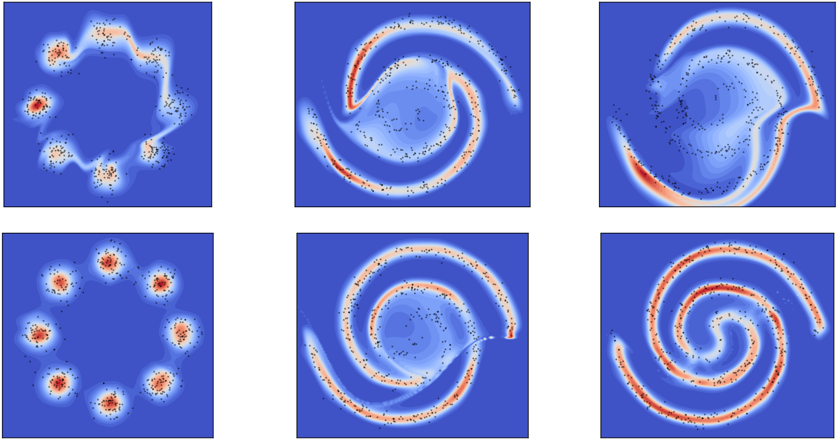


Figure: Density models learned by a 20-layer MAF (above) and a 5-layer CIF-MAF (below) for 2-D target distributions. The far right column uses a higher-capacity model for each method.

High-Dimensional ResFlow Experiments

Table: Test set bits per dimension. Lower is better.

	MNIST	CIFAR-10
ResFlow (small)	1.074	3.474
ResFlow (big)	1.018	3.422
CIF-ResFlow	**0.922**	**3.334**

NB: These ResFlows were smaller than those from Chen et al. [2019]

We obtained similar improvements on several other problems and flow models

Thank you!

Figure: Joint work with Anthony Caterini, George Deligiannidis, Arnaud Doucet, and Dino Sejdinovic

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