Normalising flows with applications

ML Masterclass

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Summary

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Introduction

Task: model probability distribution from data

Existing methods:

- Direct analytical approaches
- Variational approaches
- Expectation maximization
- VAEs and GANs

VAEs and GANs do not allow for likelihood evaluation and may present some training issues (e.g. mode collapse, posterior collapse, vanishing gradients and training instability).

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Normalising flows basics

Let $\mathbf{Z} \in \mathbb{R}^D$ be a random variable with a known probability density function $p_{\mathbf{Z}} : \mathbb{R} \to \mathbb{R}$ and let $\mathbf{g}$ be an invertible function and $\mathbf{Y} = \mathbf{g}(\mathbf{Z})$.
Using the change of variables formula, one can compute:

$$p_{\mathbf{Y}}(\mathbf{y}) = p_{\mathbf{Z}}(f(\mathbf{y}))|\det \mathrm{D}\mathbf{g}(\mathbf{f}(\mathbf{y}))|^{-1},$$

where $\mathbf{f}$ is the inverse of $\mathbf{g}$ and $\det \mathrm{D}\mathbf{g}(\mathbf{z}) = \frac{\partial \mathbf{g}}{\partial \mathbf{z}}$ is the Jacobian of g.

The function $\mathbf{g}$ transforms the the base density $p_{\mathbf{Z}}$ into a more complex density, defining also it's generative direction.

The inverse of $\mathbf{g}$ instead moves in the opposite direction, from a complicated density to a know one.

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Application - Density estimation

- Data $y_1, \ldots, y_n \sim p_Y$
- Base noise $z \sim p_Z(.;\phi)$
- Flow model $y = \mathbf{g}_\theta(z)$ with inverse $\mathbf{f}_\theta$

$$
\begin{aligned}
\log p(y_1, \ldots, y_n \mid \theta, \phi) &= \sum_{i=1}^{n} \log p_Y\left(y_i \mid \theta, \phi\right) \\
&= \sum_{i=1}^{n} \underbrace{\log p_Z\left(\mathbf{f}\left(y_i \mid \theta\right) \mid \phi\right)}_{\text{ll under base measure}} + \underbrace{\log \left|\det D\mathbf{f}\left(y_i \mid \theta\right)\right|}_{\text{volume correction}}
\end{aligned}
$$

During training, estimate θ, ϕ to maximise the above ll.
Computational cost depends on computing $\mathbf{f}$ and $\det D\mathbf{f}$ - the *normalising direction*.

Application - sampling

To sample from p_Y, it is enough to generate noise $z \sim p_Z$ and apply the flow $\mathbf{g}$.
Performance determined by the cost of applying $\mathbf{g}$ - the *generative direction*.

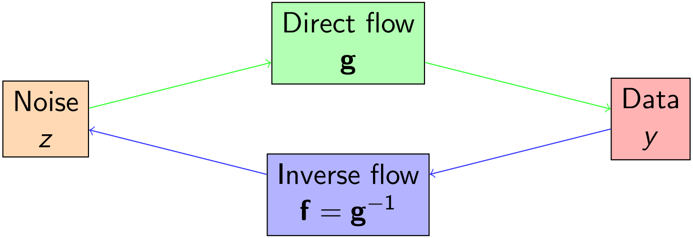

Figure: Generative direction (sampling) and Normalising direction (likelihood).

In general, want **invertible** and **expressive** $\mathbf{g}$ with **efficient evaluation** of $\mathbf{g}, \mathbf{f}$ and $\det D\mathbf{f}$. Different flows have different strengths.

Summary

Elementwise Flows

Normalizing flows should satisfy several conditions to be practical:

- be invertible,
- be sufficiently expressive to model the distribution of interest,
- be computationally efficient.

An example could be to use any bijective scalar function.
Let $h : \mathbb{R} \to \mathbb{R}$ be a scalar valued bijection. If $\mathbf{x} = (x_1, x_2, \ldots, x_D)^T$, then

$$\mathbf{g}(\mathbf{x}) = (h(x_1), h(x_2), \ldots, h(x_D))^T$$

is also a bijection whose inverse simply requires computing h^{-1} and whose Jacobian is the product of the absolute values of the derivatives of h.

Very simple approach, but limiting.

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Linear Flows

Linear mappings can express correlation between dimensions.

$$\mathbf{g}(\mathbf{x}) = \mathbf{A}\mathbf{x} + \mathbf{b}$$

where A and b are parameters. If A is invertible, then the function is invertible too. Determinant of the Jacobian can be computed in $\mathcal{O}(D^3)$.

A can be:

- diagonal: close to elementwise flows,
- upper triangular: captures correlation between dimensions and can be computed in $\mathcal{O}(D^2)$,
- permutation and orthogonal matrices can be used for faster computations,
- factorization: can be computed in $\mathcal{O}(D)$

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Coupling Flows (1)

Introduced by [Dinh et al., 2014], the idea is to only transform subsets of data at a time.

- Split input $\mathbf{x} \in R^D$ into $\mathbf{x}^A \in \mathbb{R}^d$ and $\mathbf{x}^B \in \mathbb{R}^{D-d}$.
- *Coupling function* is a bijection $\mathbf{h}(., \theta) : R^d \to R^d$.
- *Conditioner* $\Theta(.)$ used to define θ given inputs.

Define the *coupling flow* $\mathbf{g} : \mathbb{R}^D \to R^D$ as:

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The Jacobian of $\mathbf{g}$ is a block triangular matrix where diagonal blocks are $D\mathbf{h}$ and the identity. So the determinant of the Jacobian is $\det D\mathbf{h}$.

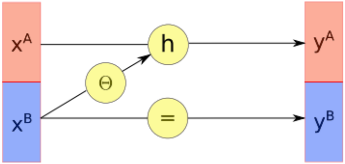

Figure: A single coupling flow illustration from [Kobyzev et al., 2020].

The power of coupling flows is in the ability to have very complex models for $\Theta(\mathbf{x}^B)$ (which do not need to be invertible), such as neural networks.

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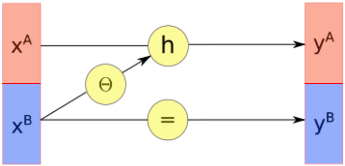

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Autoregressive Flows (1)

Similar to coupling flows, but with each entry of outputs $\mathbf{y} = \mathbf{g}(\mathbf{x})$ conditioned on the previous entries of the input.

- *Coupling function* is a bijection $h(., \theta) : \mathbb{R} \to \mathbb{R}$.
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Then the AR flow is given by:

$$y_t = h\left(x_t; \Theta_t\left(\mathbf{x}_{1:t-1}\right)\right), \quad t \in \{1, \ldots, D\}.$$

The Jacobian of $\mathbf{g}$ is triangular with inputs y_t depending only on $x_{1:t}$, so the determinant is a product of its diagonal entries.
Furthermore, $\mathbf{g}$ can be parrallelised easily due to a dependence on available subsets of $\mathbf{x}$ only.

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However, the inverse flow $\mathbf{f}$ is more complicated and is found recursively, making it hard to implement efficiently.

An alternative is proposed by [Kingma et al., 2016] under the name of *inverse autoregressive flows* (IAF), which outputs terms from $\mathbf{y}$ conditioned on previous entries of $\mathbf{y}$:

$$y_t = h(x_t; \Theta_t(\mathbf{y}_{1:t-1}))$$

While most flows are modeled in the normalising direction to ensure efficient evaluations of $\mathbf{f}$, the IAF does the opposite and models the generative direction.

- Classical AR flows have efficient density estimation.
- IAFs have efficient sampling.

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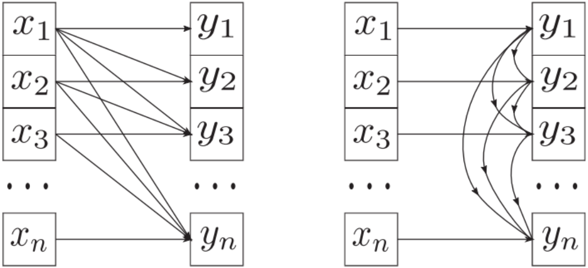
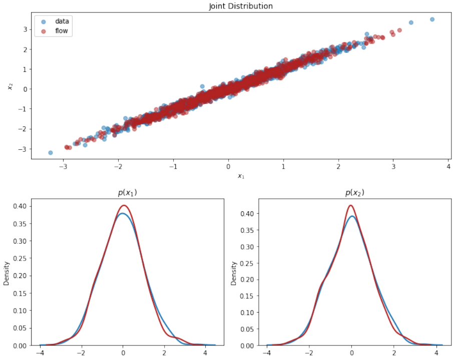


Figure: Left: classical Autoregressive Flows. Right: Inverse Autoregressive FLows.

Summary

Learning a multivariate Gaussian

- Base noise is $\mathcal{N}_2(\mathbf{0}, \mathbb{I}_2)$.
- Target density if $\mathcal{N}_2(\mathbf{0}, \begin{bmatrix} 1 & 0.99 \\ 0.99 & 1 \end{bmatrix})$.
- Use a coupling flow with affine h as $\begin{cases} y_1 = & h(x_1;\theta) = \theta_1 x_1 + \theta_2 \\ y_2 = & x_2 \end{cases}$



Learning a multivariate Gaussian

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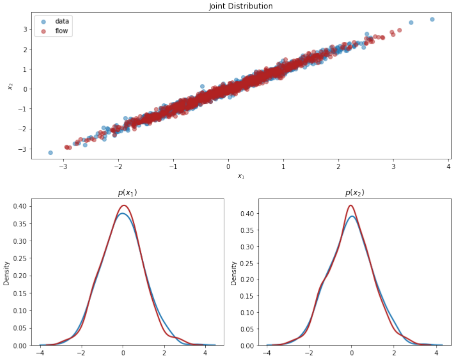

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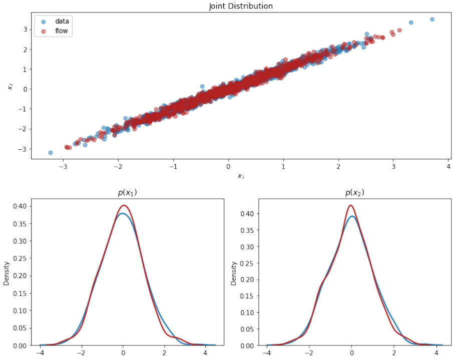

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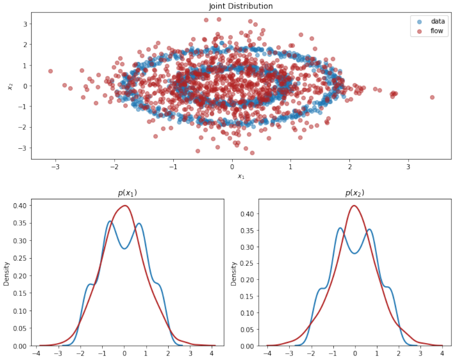

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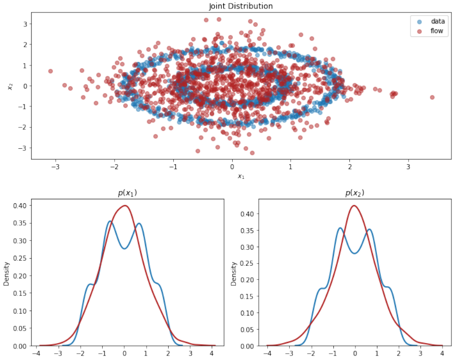

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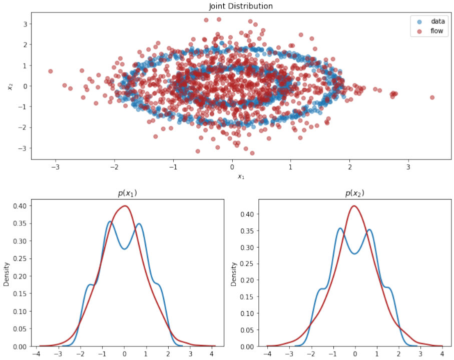

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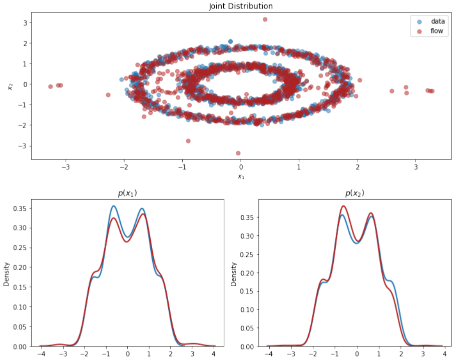

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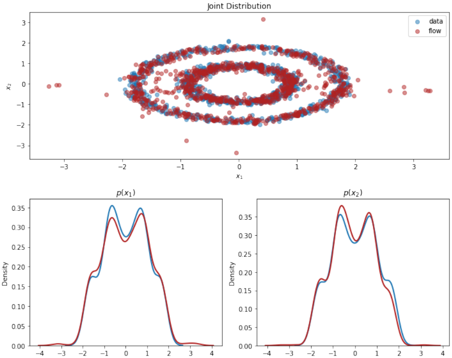

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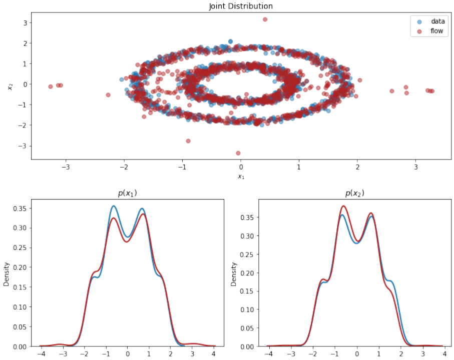

Summary

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Thank you!

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