Normalizing Flow

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Normalizing flows (NFs) are a class of generative models that gradually transform noise into data through an *invertible* mapping, following the **change-of-variables formula** of probability densities.

Definition 1 (Change-of-Variables Formula)

For $x \sim p_x(x)$, given a smooth invertible mapping $f : \mathbb{R}^d \to \mathbb{R}^d$ such that $y = f(x)$, the probability density $p_y(y)$ is

$$p_y(y) = p_x(x) \cdot \left| \frac{\partial f^{-1}}{\partial y} \right| = p_x(x) \cdot \left| \frac{\partial f}{\partial x} \right|^{-1},$$

where f^{-1} denotes the inverse of f such that $x = f^{-1}(y)$[1].

Proof. Informally, using the change-of-variables rule in multivariate calculus, we can prove that for any $\Omega \subset \mathbb{R}^d$

$$\int_\Omega p_y(y)\,\mathrm{d}y = \int_{f^{-1}(\Omega)} p_x(x)\,\mathrm{d}x = \int_{f^{-1}(\Omega)} p_x(x) \left| \frac{\partial f^{-1}}{\partial y} \right| \mathrm{d}y.$$

Invertible Transformation

The essence of normalizing flows is to build a parametrized invertible mapping $f_\theta : \mathbb{R}^d \to \mathbb{R}^d$ by composing a sequence of K simpler learnable invertible mappings $\{f_k\}_{k=0}^{K-1}$ such that

$$f_\theta = f_{K-1} \circ \cdots f_1 \circ f_0.$$

[1]Note that $x = f^{-1}(f(x))$, and therefore $(\partial f^{-1}/\partial y) \cdot (\partial f/\partial x) = I$.

Specifically, starting from a prior noise distribution[2] $p_0(x_0)$, we gradually tranform a sampled noise $x_0 \sim p_0$ such that

$$x_{k+1} = f_k(x_k), \text{where } k \in \{0, ..., K-1\},$$

and consequently

$$x_K = f_{k-1}(x_{k-1}) = (f_{K-1} \circ \cdots f_1 \circ f_0)(x_0).$$

The probability density $p_K(x_K; \theta)$ over x_K is given by the change-of-variables formula as follows:

$$p_K(x_K; \theta) = p_0(x_0) \prod_{k=0}^{K-1} \left| \frac{\partial f_k}{\partial x_k} \right|^{-1},$$

or equivalently the log-density is

$$\log p_K(x_K; \theta) = \log p_0(x_0) - \sum_{k=0}^{K} \log \left| \frac{\partial f_k}{\partial x_k} \right|,$$

where $x_0 = (f_0^{-1} \circ f_1^{-1} \cdots \circ f_{K-1}^{-1})(x_K)$.

Learning normalizing flows essentially amouts to maximizing the log-likelihood of $p_K(\cdot; \theta)$ w.r.t. an empirical data distribution $p_{\text{data}}(x)$

$$\begin{aligned}\theta^* &= \arg\max_\theta \mathbb{E}_{x \sim p_{\text{data}}(x)}[\log p_K(x; \theta)] \\ &= \arg\min_\theta \mathbb{D}_{\text{KL}}(p_{\text{data}}(x) \parallel p_K(x; \theta))\end{aligned}$$

Examples

The major challenge of normalizing flows is to design learnable mappings f_k that is *(a)* suffciently expressive, *(b)* invertible, and *(c)* has efficiently computable Jacobians $\partial f_k / \partial x_k$.

> For example, a linear mapping $f(x) = Ax + b$ can easily satisfy *(b)* and *(c)*, but is not suffciently expressive.

[2]Typically, we use a standard Gaussian $p_0(x_0) = \mathcal{N}(0, I)$ as the prior distribution.

Often times, we parametrize such learnable mappings f_k using purposefully designed neural networks that are non-linear (expressive), yet invertible and has easily computable Jacobians. Here we provide a few (opinionated) pointers to recent works:

- Planar and radial flows (Rezende & Mohamed, 2015);
- Coupling flows (Dinh et al., 2017)
- Block neural autoregressive flows (De Cao et al., 2020)
- Transformer autoregressive flows (Zhai et al., 2025)

References

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