Normalizing Flow Models

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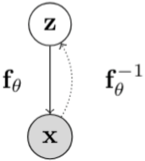
Lecture 8

Normalizing flow models

- Consider a directed, latent-variable model over observed variables X and latent variables Z
- In a **normalizing flow model**, the mapping between Z and X, given by $\mathbf{f}_\theta : \mathbb{R}^n \mapsto \mathbb{R}^n$, is deterministic and invertible such that $X = \mathbf{f}_\theta(Z)$ and $Z = \mathbf{f}_\theta^{-1}(X)$



- Using change of variables, the marginal likelihood $p(\mathbf{x})$ is given by

$$p_X(\mathbf{x};\theta) = p_Z\left(\mathbf{f}_\theta^{-1}(\mathbf{x})\right)\left|\det\left(\frac{\partial \mathbf{f}_\theta^{-1}(\mathbf{x})}{\partial \mathbf{x}}\right)\right|$$

- Note: $\mathbf{x}, \mathbf{z}$ need to be continuous and have the same dimension.

A Flow of Transformations

Normalizing: Change of variables gives a normalized density after applying an invertible transformation
Flow: Invertible transformations can be composed with each other

$$\mathbf{z}_m = \mathbf{f}_\theta^m \circ \cdots \circ \mathbf{f}_\theta^1(\mathbf{z}_0) = \mathbf{f}_\theta^m(\mathbf{f}_\theta^{m-1}(\cdots(\mathbf{f}_\theta^1(\mathbf{z}_0)))) \triangleq \mathbf{f}_\theta(\mathbf{z}_0)$$

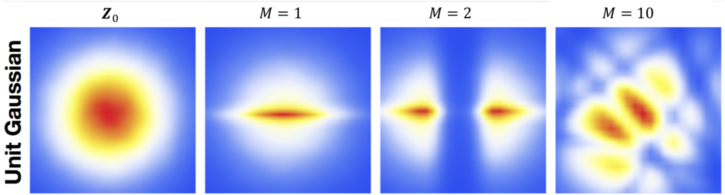
- Start with a simple distribution for $\mathbf{z}_0$ (e.g., Gaussian)
- Apply a sequence of M invertible transformations to finally obtain $\mathbf{x} = \mathbf{z}_M$
- By change of variables

$$p_X(\mathbf{x};\theta) = p_Z\left(\mathbf{f}_\theta^{-1}(\mathbf{x})\right) \prod_{m=1}^{M} \left|\det\left(\frac{\partial(\mathbf{f}_\theta^m)^{-1}(\mathbf{z}_m)}{\partial \mathbf{z}_m}\right)\right|$$

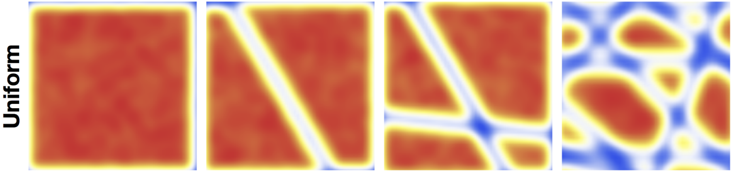
(Note: determininant of product equals product of determinants)

Planar flows (Rezende & Mohamed, 2016)

- Base distribution: Gaussian



- Base distribution: Uniform



- 10 planar transformations can transform simple distributions into a more complex one

Learning and Inference

- Learning via **maximum likelihood** over the dataset $\mathcal{D}$

$$\max_{\theta} \log p_X(\mathcal{D}; \theta) = \sum_{\mathbf{x} \in \mathcal{D}} \log p_Z\left(\mathbf{f}_\theta^{-1}(\mathbf{x})\right) + \log \left| \det\left(\frac{\partial \mathbf{f}_\theta^{-1}(\mathbf{x})}{\partial \mathbf{x}} \right) \right|$$

- **Exact likelihood evaluation** via inverse tranformation $\mathbf{x} \mapsto \mathbf{z}$ and change of variables formula
- **Sampling** via forward transformation $\mathbf{z} \mapsto \mathbf{x}$

$$\mathbf{z} \sim p_Z(\mathbf{z}) \quad \mathbf{x} = \mathbf{f}_\theta(\mathbf{z})$$

- **Latent representations** inferred via inverse transformation (no inference network required!)

$$\mathbf{z} = \mathbf{f}_\theta^{-1}(\mathbf{x})$$

Desiderata for flow models

- Simple prior $p_Z(\mathbf{z})$ that allows for efficient sampling and tractable likelihood evaluation. E.g., isotropic Gaussian
- Invertible transformations with tractable evaluation:
  - Likelihood evaluation requires efficient evaluation of $\mathbf{x} \mapsto \mathbf{z}$ mapping
  - Sampling requires efficient evaluation of $\mathbf{z} \mapsto \mathbf{x}$ mapping
- Computing likelihoods also requires the evaluation of determinants of $n \times n$ Jacobian matrices, where n is the data dimensionality
  - Computing the determinant for an $n \times n$ matrix is $O(n^3)$: prohibitively expensive within a learning loop!
  - **Key idea**: Choose tranformations so that the resulting Jacobian matrix has special structure. For example, the determinant of a triangular matrix is the product of the diagonal entries, i.e., an $O(n)$ operation

Triangular Jacobian

$$\mathbf{x} = (x_1, \cdots, x_n) = \mathbf{f}(\mathbf{z}) = (f_1(\mathbf{z}), \cdots, f_n(\mathbf{z}))$$

$$J = \frac{\partial \mathbf{f}}{\partial \mathbf{z}} = \begin{pmatrix} \frac{\partial f_1}{\partial z_1} & \cdots & \frac{\partial f_1}{\partial z_n} \\ \cdots & \cdots & \cdots \\ \frac{\partial f_n}{\partial z_1} & \cdots & \frac{\partial f_n}{\partial z_n} \end{pmatrix}$$

Suppose $x_i = f_i(\mathbf{z})$ only depends on $\mathbf{z}_{\leq i}$. Then

$$J = \frac{\partial \mathbf{f}}{\partial \mathbf{z}} = \begin{pmatrix} \frac{\partial f_1}{\partial z_1} & \cdots & 0 \\ \cdots & \cdots & \cdots \\ \frac{\partial f_n}{\partial z_1} & \cdots & \frac{\partial f_n}{\partial z_n} \end{pmatrix}$$

has lower triangular structure. Determinant can be computed in **linear time**. Similarly, the Jacobian is upper triangular if x_i only depends on $\mathbf{z}_{\geq i}$

Recap of normalizing flow models

So far

- Transform simple to complex distributions via sequence of invertible transformations
- Directed latent variable models with marginal likelihood given by the change of variables formula
- Triangular Jacobian permits efficient evaluation of log-likelihoods

Plan for today

- Invertible transformations with diagonal Jacobians (NICE, Real-NVP)
- Autoregressive Models as Normalizing Flow Models
- Invertible CNNs (MintNet)
- Gaussianization flows
- Case Study: Probability density distillation for efficient learning and inference in Parallel Wavenet

Designing invertible transformations

- NICE or Nonlinear Independent Components Estimation (Dinh et al., 2014) composes two kinds of invertible transformations: additive coupling layers and rescaling layers
- Real-NVP (Dinh et al., 2017)
- Inverse Autoregressive Flow (Kingma et al., 2016)
- Masked Autoregressive Flow (Papamakarios et al., 2017)
- I-resnet (Behrmann et al, 2018)
- Glow (Kingma et al, 2018)
- MintNet (Song et al., 2019)
- And many more

NICE - Additive coupling layers

Partition the variables $\mathbf{z}$ into two disjoint subsets, say $\mathbf{z}_{1:d}$ and $\mathbf{z}_{d+1:n}$ for any $1 \leq d < n$

- Forward mapping $\mathbf{z} \mapsto \mathbf{x}$:
  - $\mathbf{x}_{1:d} = \mathbf{z}_{1:d}$ (identity transformation)
  - $\mathbf{x}_{d+1:n} = \mathbf{z}_{d+1:n} + m_\theta(\mathbf{z}_{1:d})$ ($m_\theta(\cdot)$ is a neural network with parameters θ, d input units, and $n-d$ output units)
- Inverse mapping $\mathbf{x} \mapsto \mathbf{z}$:
  - $\mathbf{z}_{1:d} = \mathbf{x}_{1:d}$ (identity transformation)
  - $\mathbf{z}_{d+1:n} = \mathbf{x}_{d+1:n} - m_\theta(\mathbf{x}_{1:d})$
- Jacobian of forward mapping:

$$J = \frac{\partial \mathbf{x}}{\partial \mathbf{z}} = \begin{pmatrix} I_d & 0 \\ \frac{\partial \mathbf{x}_{d+1:n}}{\partial \mathbf{z}_{1:d}} & I_{n-d} \end{pmatrix}$$

$$\det(J) = 1$$

- **Volume preserving transformation** since determinant is 1.

NICE - Rescaling layers

- Additive coupling layers are composed together (with arbitrary partitions of variables in each layer)
- Final layer of NICE applies a rescaling transformation
- Forward mapping $\mathbf{z} \mapsto \mathbf{x}$:

$$x_i = s_i z_i$$

  where $s_i > 0$ is the scaling factor for the i-th dimension.
- Inverse mapping $\mathbf{x} \mapsto \mathbf{z}$:

$$z_i = \frac{x_i}{s_i}$$

- Jacobian of forward mapping:

$$J = \mathrm{diag}(\mathbf{s})$$

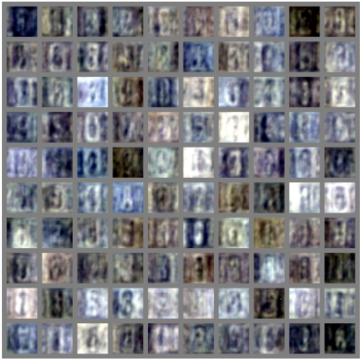
$$\det(J) = \prod_{i=1}^{n} s_i$$

Samples generated via NICE

(a) Model trained on MNIST

(b) Model trained on TFD

Samples generated via NICE



(c) Model trained on SVHN

(d) Model trained on CIFAR-10

Real-NVP: Non-volume preserving extension of NICE

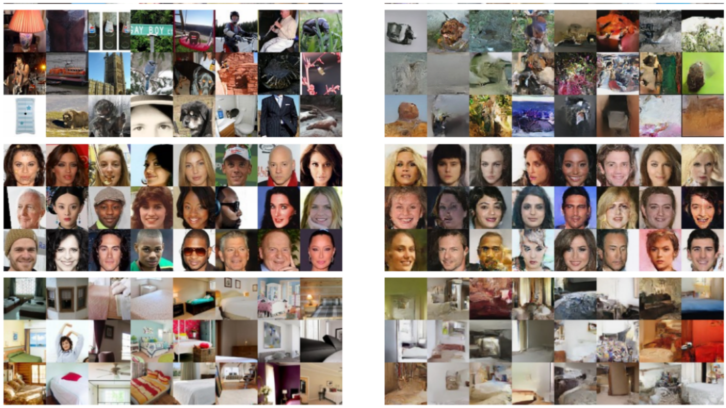
- Forward mapping $\mathbf{z} \mapsto \mathbf{x}$:
  - $\mathbf{x}_{1:d} = \mathbf{z}_{1:d}$ (identity transformation)
  - $\mathbf{x}_{d+1:n} = \mathbf{z}_{d+1:n} \odot \exp(\alpha_\theta(\mathbf{z}_{1:d})) + \mu_\theta(\mathbf{z}_{1:d})$
  - $\mu_\theta(\cdot)$ and $\alpha_\theta(\cdot)$ are both neural networks with parameters θ, d input units, and $n - d$ output units [$\odot$ denotes elementwise product]
- Inverse mapping $\mathbf{x} \mapsto \mathbf{z}$:
  - $\mathbf{z}_{1:d} = \mathbf{x}_{1:d}$ (identity transformation)
  - $\mathbf{z}_{d+1:n} = (\mathbf{x}_{d+1:n} - \mu_\theta(\mathbf{x}_{1:d})) \odot (\exp(-\alpha_\theta(\mathbf{x}_{1:d})))$
- Jacobian of forward mapping:

$$J = \frac{\partial \mathbf{x}}{\partial \mathbf{z}} = \begin{pmatrix} I_d & 0 \\ \frac{\partial \mathbf{x}_{d+1:n}}{\partial \mathbf{z}_{1:d}} & \mathrm{diag}(\exp(\alpha_\theta(\mathbf{z}_{1:d}))) \end{pmatrix}$$

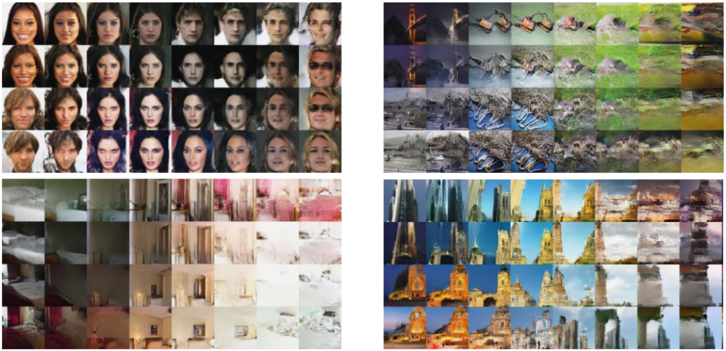
$$\det(J) = \prod_{i=d+1}^{n} \exp(\alpha_\theta(\mathbf{z}_{1:d})_i) = \exp\left(\sum_{i=d+1}^{n} \alpha_\theta(\mathbf{z}_{1:d})_i\right)$$

- **Non-volume preserving transformation** in general since determinant can be less than or greater than 1

Samples generated via Real-NVP



Latent space interpolations via Real-NVP



Using with four validation examples $\mathbf{z}^{(1)}, \mathbf{z}^{(2)}, \mathbf{z}^{(3)}, \mathbf{z}^{(4)}$, define interpolated $\mathbf{z}$ as:

$$\mathbf{z} = cos\phi(\mathbf{z}^{(1)} cos\phi' + \mathbf{z}^{(2)} sin\phi') + sin\phi(\mathbf{z}^{(3)} cos\phi' + \mathbf{z}^{(4)} sin\phi')$$

with manifold parameterized by ϕ and ϕ'.

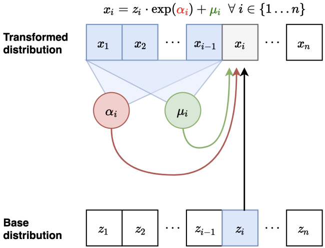
Continuous Autoregressive models as flow models

- Consider a Gaussian autoregressive model:

$$p(\mathbf{x}) = \prod_{i=1}^{n} p(x_i | \mathbf{x}_{<i})$$

  such that $p(x_i \mid \mathbf{x}_{<i}) = \mathcal{N}(\mu_i(x_1, \cdots, x_{i-1}), \exp(\alpha_i(x_1, \cdots, x_{i-1}))^2)$. Here, $\mu_i(\cdot)$ and $\alpha_i(\cdot)$ are neural networks for $i > 1$ and constants for $i = 1$.
- Sampler for this model:
  - Sample $z_i \sim \mathcal{N}(0, 1)$ for $i = 1, \cdots, n$
  - Let $x_1 = \exp(\alpha_1)z_1 + \mu_1$. Compute $\mu_2(x_1), \alpha_2(x_1)$
  - Let $x_2 = \exp(\alpha_2)z_2 + \mu_2$. Compute $\mu_3(x_1, x_2), \alpha_3(x_1, x_2)$
  - Let $x_3 = \exp(\alpha_3)z_3 + \mu_3$. ...
- **Flow interpretation:** transforms samples from the standard Gaussian $(z_1, z_2, \ldots, z_n)$ to those generated from the model $(x_1, x_2, \ldots, x_n)$ via invertible transformations (parameterized by $\mu_i(\cdot), \alpha_i(\cdot)$)

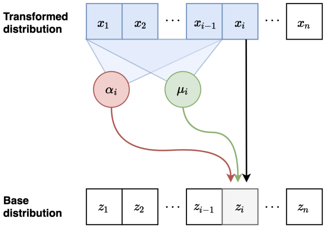
Masked Autoregressive Flow (MAF)



- Forward mapping from $\mathbf{z} \mapsto \mathbf{x}$:
  - Let $x_1 = \exp(\alpha_1)z_1 + \mu_1$. Compute $\mu_2(x_1), \alpha_2(x_1)$
  - Let $x_2 = \exp(\alpha_2)z_2 + \mu_2$. Compute $\mu_3(x_1, x_2), \alpha_3(x_1, x_2)$
- Sampling is sequential and slow (like autoregressive): $O(n)$ time

Figure adapted from Eric Jang's blog

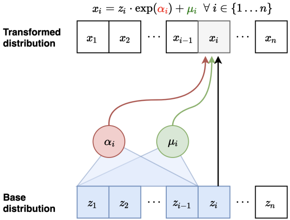
Masked Autoregressive Flow (MAF)



- Inverse mapping from $\mathbf{x} \mapsto \mathbf{z}$:
  - Compute **all** μ_i, α_i (can be done in parallel using e.g., MADE)
  - Let $z_1 = (x_1 - \mu_1)/\exp(\alpha_1)$ (scale and shift)
  - Let $z_2 = (x_2 - \mu_2)/\exp(\alpha_2)$
  - Let $z_3 = (x_3 - \mu_3)/\exp(\alpha_3)$ ...
- Jacobian is lower diagonal, hence efficient determinant computation
- Likelihood evaluation is easy and parallelizable (like MADE)
- Layers with different variable orderings can be stacked

Figure adapted from Eric Jang's blog

Inverse Autoregressive Flow (IAF)



- Forward mapping from $\mathbf{z} \mapsto \mathbf{x}$ (parallel):
  - Sample $z_i \sim \mathcal{N}(0, 1)$ for $i = 1, \cdots, n$
  - Compute all μ_i, α_i (can be done in parallel)
  - Let $x_1 = \exp(\alpha_1) z_1 + \mu_1$
  - Let $x_2 = \exp(\alpha_2) z_2 + \mu_2$ ...
- Inverse mapping from $\mathbf{x} \mapsto \mathbf{z}$ (sequential):
  - Let $z_1 = (x_1 - \mu_1)/\exp(\alpha_1)$. Compute $\mu_2(z_1), \alpha_2(z_1)$
  - Let $z_2 = (x_2 - \mu_2)/\exp(\alpha_2)$. Compute $\mu_3(z_1, z_2), \alpha_3(z_1, z_2)$
- Fast to sample from, slow to evaluate likelihoods of data points (train)
- Note: Fast to evaluate likelihoods of a generated point (cache $z_1, z_2, \dots, z_n$)

Figure adapted from Eric Jang's blog

IAF is inverse of MAF

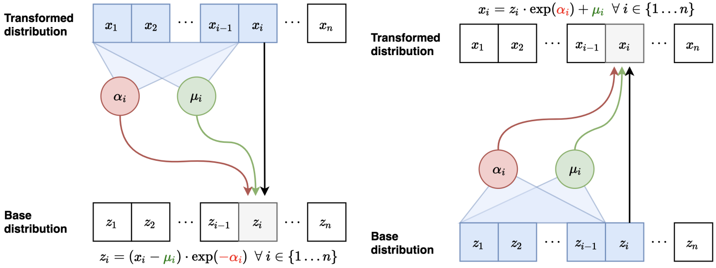


Figure: Inverse pass of MAF (**left**) vs. Forward pass of IAF (**right**)

- Interchanging **z** and **x** in the inverse transformation of MAF gives the forward transformation of IAF
- Similarly, forward transformation of MAF is inverse transformation of IAF

Figure adapted from Eric Jang's blog

IAF vs. MAF

- Computational tradeoffs
  - MAF: Fast likelihood evaluation, slow sampling
  - IAF: Fast sampling, slow likelihood evaluation
- MAF more suited for training based on MLE, density estimation
- IAF more suited for real-time generation
- Can we get the best of both worlds?

Parallel Wavenet

- Two part training with a teacher and student model
- Teacher is parameterized by MAF. Teacher can be efficiently trained via MLE
- Once teacher is trained, initialize a student model parameterized by IAF. Student model cannot efficiently evaluate density for external datapoints but allows for efficient sampling
- **Key observation**: IAF can also efficiently evaluate densities of its own generations (via caching the noise variates $z_1, z_2, \ldots, z_n$)

Parallel Wavenet

- **Probability density distillation**: Student distribution is trained to minimize the KL divergence between student (s) and teacher (t)

$$D_{\mathrm{KL}}(s,t) = E_{\mathbf{x}\sim s}[\log s(\mathbf{x}) - \log t(\mathbf{x})]$$

- Evaluating and optimizing Monte Carlo estimates of this objective requires:
  - Samples $\mathbf{x}$ from student model (IAF)
  - Density of $\mathbf{x}$ assigned by student model
  - Density of $\mathbf{x}$ assigned by teacher model (MAF)
- All operations above can be implemented efficiently

Parallel Wavenet: Overall algorithm

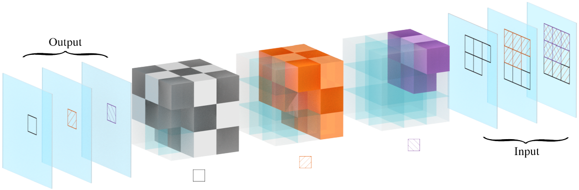
- Training
  - Step 1: Train teacher model (MAF) via MLE
  - Step 2: Train student model (IAF) to minimize KL divergence with teacher
- Test-time: Use student model for testing
- Improves sampling efficiency over original Wavenet (vanilla autoregressive model) by 1000x!

MintNet (Song et al., 2019)

- MintNet: Building invertible neural networks with masked convolutions.
- A regular convolutional neural network is powerful, but it is not invertible and its Jacobian determinant is expensive.
- We can instead use masked convolutions like in autoregressive models to enforce ordering (like PixelCNN)
- Because of the ordering, the Jacobian matrix is triangular and the determinant is efficient to compute.
- If all the diagonal elements of the Jacobian matrix are (strictly) positive, the transformation is invertible.

MintNet (Song et al., 2019)

- Illustration of a masked convolution with 3 filters and kernel size 3×3.



- Solid checkerboard cubes inside each filter represent unmasked weights, while the transparent blue blocks represent the weights that have been masked out.
- The receptive field of each filter on the input feature maps is indicated by regions shaded with the pattern (the colored square) below the corresponding filter.

MintNet (Song et al., 2019)

- Uncurated samples on MNIST, CIFAR-10, and ImageNet 32x32 datasets

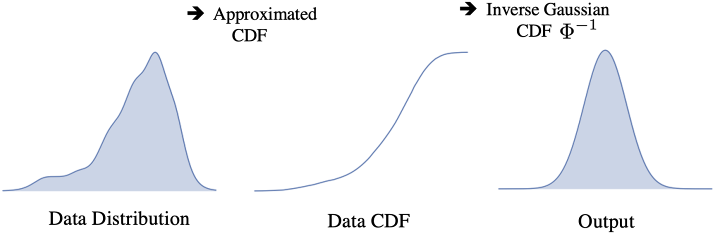
(a) MNIST (b) CIFAR-10 (c) ImageNet-32×32

Gaussianization Flows (Meng et al., 2020)

- Let $X = f_\theta(Z)$ be a flow model with Gaussian prior $Z \sim \mathcal{N}(0, I) = p_Z$, and let $\tilde{X} \sim p_{data}$ be a random vector distributed according to the true data distribution.
- Flow models are trained with maximum likelihood to minimize the KL divergence $D_{\mathrm{KL}}\left(p_{data} \,\|\, p_\theta(x)\right) = D_{\mathrm{KL}}\left(p_{\tilde{X}} \,\|\, p_X\right)$. Gaussian samples transformed through f_θ should be distributed as the data.
- It can be shown that $D_{\mathrm{KL}}\left(p_{\tilde{X}} \,\|\, p_X\right) = D_{\mathrm{KL}}\left(p_{f_\theta^{-1}(\tilde{X})} \,\middle\|\, p_{f_\theta^{-1}(X)}\right) = D_{\mathrm{KL}}\left(p_{f_\theta^{-1}(\tilde{X})} \,\middle\|\, p_Z\right)$. Data samples transformed through f_θ^{-1} should be distributed as Gaussian
- How can we achieve this?

Gaussianization Flows (Meng et al., 2020)

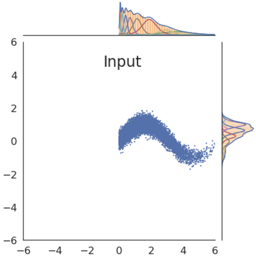
- Let's start with a 1D example. Let the data $\tilde{X}$ have density p_{data} and cumulative density function (CDF) $F_{data}(a) = \int_{-\infty}^{a} p_{data}$.
- **Inverse CDF trick**: If F_{data} is known, we can sample from p_{data} via $\tilde{X} = F_{data}^{-1}(U)$ where $U \in [0, 1]$ is a uniform random variable.



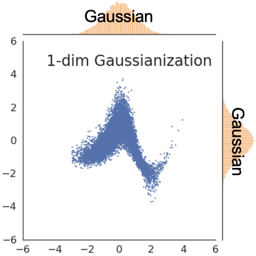
- This means that $U = F_{data}(\tilde{X})$ is uniform. We can transform U into a Gaussian using the inverse CDF trick: $\Phi^{-1}(U) = \Phi^{-1}(F_{data}(\tilde{X}))$.
- The invertible transformation $\Phi^{-1} \circ F_{data}$ Gaussianizes the data!

Gaussianization Flows (Meng et al., 2020)

- Step 1: Dimension-wise Gaussianization (Jacobian is a diagonal matrix and is tractable)



Input data

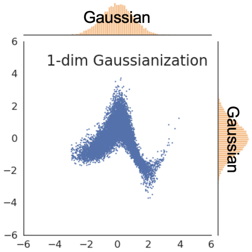


Dimension-wise Gaussianization

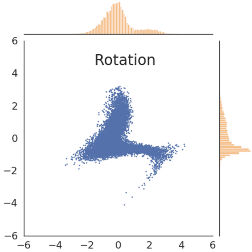
Note: Even though each dimension is marginally Gaussian, they are **not** jointly Gaussian. Aside: Approximating this with a Gaussian prior is a shallow flow model known as a copula model (Sklar, 1959).

Gaussianization Flows (Meng et al., 2020)

- Step 2: apply a rotation matrix to the transformed data (Jacobian is an orthogonal matrix and is tractable)



Input

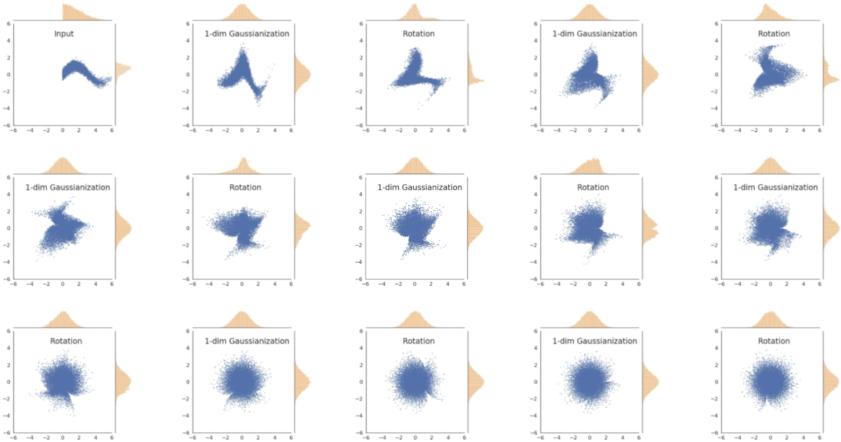


After rotation

- Note: $\mathcal{N}(\mathbf{0}, \mathbf{I})$ is rotationally invariant

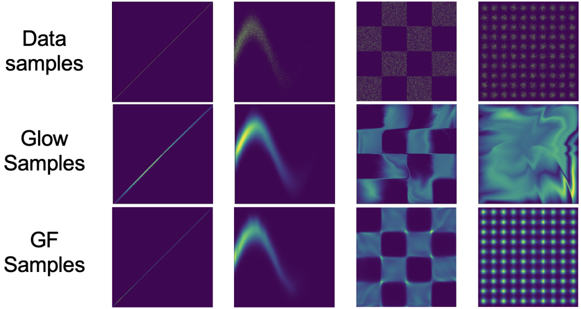
Gaussianization Flows (Meng et al., 2020)

- Gaussianization flow: repeat Step 1 and Step 2 (stacking learnable Gaussian copula). Transform data into a normal distribution.



Experiments: Density Estimation

- Density estimation on 2D datasets



Summary of Normalizing Flow Models

- Transform simple distributions into more complex distributions via change of variables
- Jacobian of transformations should have tractable determinant for efficient learning and density estimation
- Computational tradeoffs in evaluating forward and inverse transformations