Likelihood based Generative Modeling:

Variational Autoencoders and Normalizing Flows

Seminar on Scientific Machine Learning, Talk 5

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Introduction

Introduction

How can one turn an apple into a banana?

Likelihood based Generative modeling

Likelihood based Generative modeling:
Learn a probability distribution from data, and sample from it.

Problem Setup

Let:

- $\mathbf{X} = (\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n)$ be observed data.
- $p_\theta(\mathbf{x})$ be a probability density.
- θ be a parameter vector to estimate.

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Objective: Find θ, $p_\theta(\mathbf{x})$ that model the observed data the best.

Why?

- generate new samples distributed like $p_\theta(\mathbf{x})$
- evaluate data using $p_\theta(\mathbf{x})$.

Likelihood-based Models

Approach

Given data $\mathbf{x}_1, \cdots, \mathbf{x}_n$, we find $p_\theta(x)$ by maximizing the likelihood.

Likelihood:

$$\mathcal{L}(\theta) = \prod_{i=1}^{n} p_\theta(\mathbf{x}_i)$$

In practice, we minimize the negative log-likelihood:

$$\hat{\theta}_{MLE} = \arg\min_\theta J(\theta, \mathbf{x}^{(1)}, \cdots, \mathbf{x}^{(n)}) = \frac{1}{n}\sum_{i=1}^{n} -\log p_\theta(\mathbf{x}^{(i)})$$

How?

Key Principle

- We model $p_\theta(\mathbf{x})$ using Neural Networks
- Find optimal θ with Gradient Descent

Generative Modeling

What is Generative Modeling?

Use learned probability density $p_\theta(\mathbf{x})$ to generate new samples
$\rightarrow$ These have same characteristics

Applications:

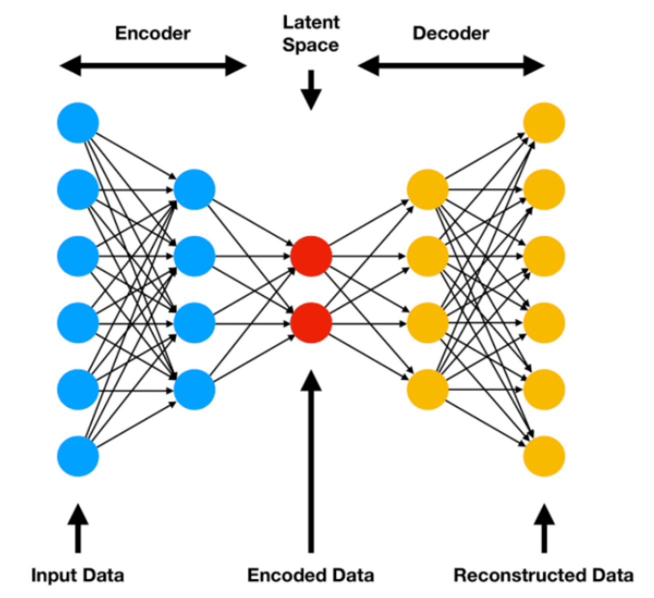
- Image/Video Generation
- Text-to-Anything
- Drug Discovery

Key Approaches:

- Variational Autoencoders (VAEs)
- Normalizing flows

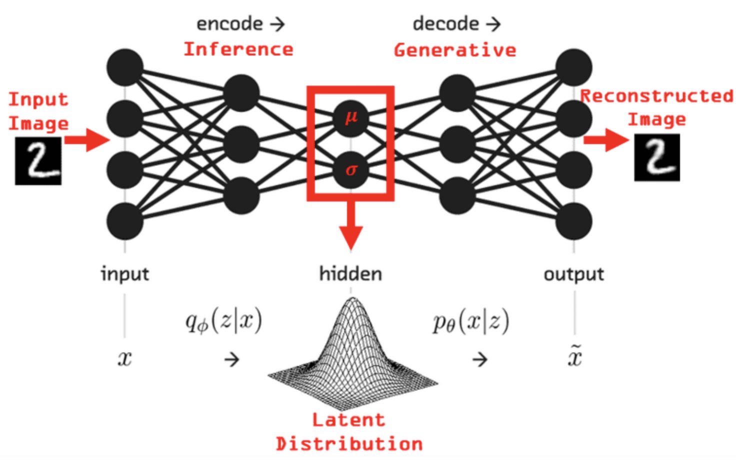
Variational Autoencoders

Variational Autoencoders



https://www.geeksforgeeks.org/numpy-types-of-autoencoders/

Variational Autoencoders



https://theaisummer.com/Autoencoder/

Variational Autoencoders

- Generate $\hat{x}$ following a distribution $p(x)$
- We sample a simple Latent distribution p(z).
  1. $p(x|z)$ as decoder for generation
  2. $p(z|x)$ as encoder for learning latent distribution

VAE Main Idea:

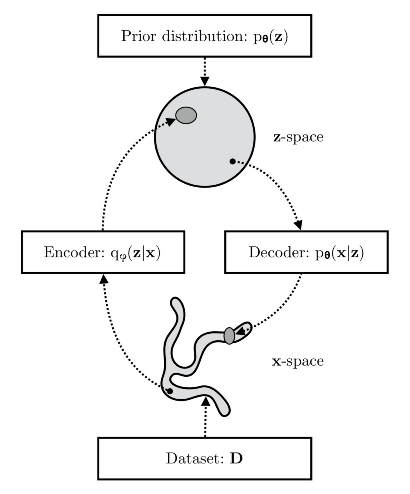
Use a easy to sample from latent distribution $p(z)$ (often Gaussian). To generate new samples $\sim p(x)$. Using approximations of the conditional distributions.

Variational Autoencoders

$\rightarrow$ Why "Variational" AE?

- Not a fixed encoding z, but a distribution over possible z's.
    1. $p(z|x)$ is intractable, so we approximate: $p(z|x) \approx q_\phi(z|x)$.
    2. $p(x|z) \approx p_\theta(x|z)$.
        - Approximate $p_\theta(x|z)$ and $q_\phi(z|x)$ using neural networks.

Variational Autoencoders



[Kingma & Welling, 2019]

vanilla VAE

Main Assumptions:

- latent distribution prior $p(z) \sim \mathcal{N}(0, I)$
- $q_\phi(z|x) \sim \mathcal{N}(\mu_\phi, \sigma_\phi)$. $\rightarrow$ outputs μ_ϕ, σ_ϕ
- $p_\theta(x|z) \sim \mathcal{N}(\mu, \sigma), \text{Bernoulli}(\hat{x})$

VAE objective ELBO

$\rightarrow$ What should our loss function be such that the NNs can approximate the conditional probabilities?

ELBO: Log Likelihood maximization/(minimization)

Maximise $\log p(x) \geq$ Evidence Lower Bound

ELBO

$$
\begin{aligned}
\text{ELBO}(x) &:= \mathbb{E}_{q(z|x)}\left[\log \frac{p(x,z)}{q(z|x)}\right] \\
&= \mathbb{E}_{q(z|x)}\left[\log p(x|z)\right] - D_{\text{KL}}(q(z|x) \,\|\, p(z))
\end{aligned}
$$

Understanding the ELBO

$$\mathrm{ELBO}(x) = \mathbb{E}_{q_\phi(z|x)}\left[\log \frac{p_\theta(x,z)}{q_\phi(z|x)}\right]$$

$$= \underbrace{\mathbb{E}_{q_\phi(z|x)}\left[\log p_\theta(x|z)\right]}_{\text{Reconstruction}} - \underbrace{D_{\mathrm{KL}}(q_\phi(z|x) \,\|\, p(z))}_{\text{Regularizing}}$$

Understand the ELBO

1. Approximation of the $\log p(x) \rightarrow$ Lower bound

2. $\text{ELBO(x)} = \underbrace{\mathbb{E}_{q_\phi(z|x)}\left[\log p_\theta(x|z)\right]}_{\text{Reconstruction}} - \underbrace{D_{\mathrm{KL}}(q_\phi(z|x) \parallel p(z))}_{\text{Regularizing}}$

ELBO in practice

$$\mathrm{ELBO}(x) = \underbrace{\mathbb{E}_{q_\phi(z|x)}\left[\log p_\theta(x|z)\right]}_{\text{Reconstruction}} - \underbrace{D_{\mathrm{KL}}(q_\phi(z|x) \,\|\, p(z))}_{\text{Regularizing}}$$

$$\underbrace{D_{\mathrm{KL}}(q_\phi(z|x) \,\|\, p(z))}_{\text{Has analytical form.}} \approx \frac{1}{L}\sum_{\ell=1}^{L} \log \frac{q_\phi(z^{(\ell)} \mid x)}{p(z^{(\ell)})}, \quad z^{(\ell)} \sim q_\phi(z \mid x)$$

$$\mathbb{E}_{q_\phi(z|x)}\left[\log p_\theta(x \mid z)\right] \approx \frac{1}{L}\sum_{\ell=1}^{L} \log p_\theta(x \mid z^{(\ell)}), \quad z^{(\ell)} \sim q_\phi(z \mid x)$$

Gradients of the ELBO

$$\mathbb{E}_{q_\phi(z|x)}\left[\log p_\theta(x \mid z)\right] \approx \frac{1}{L}\sum_{\ell=1}^{L} \log p_\theta(x \mid z^{(\ell)}), \quad z^{(\ell)} \sim q_\phi(z \mid x)$$

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$z^{(\ell)} = q_\phi(z|x) \sim \mathcal{N}(\mu_\phi, \sigma_\phi)$. The sampling is not differentiable w.r.t ϕ.

$\rightarrow$ We reparameterization in terms of a noise parameter $\epsilon \sim \mathcal{N}(0, I)$: $z = g_\phi(\epsilon)$. s.t. it is differential w.r.t ϕ

$\rightarrow z = \mu_\phi + \sigma_\phi \odot \epsilon,$

Gradients of the ELBO: Reparameterization trick

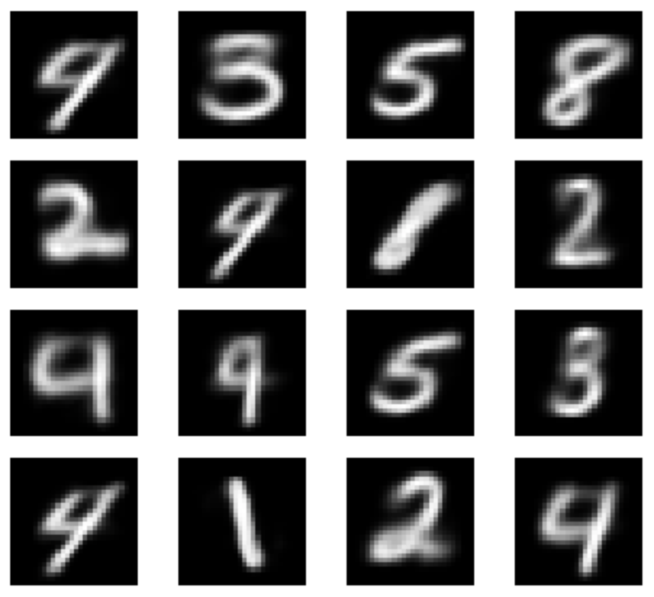
$$\mathbb{E}_{q_\phi(z|x)}\left[\log p_\theta(x \mid z)\right] \approx \frac{1}{L}\sum_{\ell=1}^{L} \log p_\theta(x \mid z^{(\ell)}), \quad z^{(\ell)} \sim q_\phi(z \mid x)$$

$$z = \mu_\phi(x) + \sigma_\phi(x) \odot \epsilon, \quad \epsilon \sim \mathcal{N}(0, I)$$

$\rightarrow$ To clarify: We move the sampling to $p(\epsilon) \sim \mathcal{N}(0, I)$ such that

$q_\phi(z = \mu_\phi + \sigma_\phi \odot \epsilon|x)$ is differentiable w.r.t μ_ϕ, σ_ϕ.

VAE example MNIST



VAE: Initialization (Encoder, Decoder)

```python
class VAE(nn.Module):
    def __init__(self, input_dim, encoder_hidden_dims, latent_dim, decoder_hidden_dims):
    ↪  (...)
    # === Encoder Part ===
    encoder_layers = []
    in_dim = input_dim
    for h_dim in encoder_hidden_dims:
        encoder_layers.append(nn.Linear(in_dim, h_dim))
        encoder_layers.append(nn.ReLU())
        in_dim = h_dim
    self.encoder_net = nn.Sequential(*encoder_layers)

    self.fc_mu = nn.Linear(in_dim, latent_dim)
    self.fc_log_var = nn.Linear(in_dim, latent_dim)

    # === Decoder Part ===
    decoder_layers = []
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VAE: encode and decode Methods

```python
def encode(self, x):
    h_encoder = self.encoder_net(x)
    mu = self.fc_mu(h_encoder)
    log_var = self.fc_log_var(h_encoder)
    return mu, log_var

def decode(self, z):
    h_decoder = self.decoder_net(z)
    recon_x = torch.sigmoid(self.fc_output(h_decoder))
    return recon_x
```

VAE: reparameterize and forward Methods

```python
def reparameterize(self, mu, log_var):
    std = torch.exp(0.5 * log_var)
    eps = torch.randn_like(std)
    return mu + eps * std

def forward(self, x):
    x_flat = x.view(-1, self.input_dim)
    mu, log_var = self.encode(x_flat)
    z = self.reparameterize(mu, log_var)
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VAE: Loss

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def loss_function(recon_x, x, mu, log_var):
    # 1. Reconstruction Loss
    BCE = F.binary_cross_entropy(recon_x,
    x.view(-1, INPUT_DIM), reduction='sum')

    # 2. KL Divergence
    KLD = -0.5 * torch.sum(1 + log_var - mu.pow(2) - log_var.exp())

    # Total loss
    return BCE + KLD
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Summary

- VAE $\rightarrow$ AE with latent distribution (easy sampling).
- More continuous latent space than AE
- ELBO loss.
- Reparameterization trick for gradients.
- Gaussian assumption for the prior $p(z)$, and the encoder $q_\phi(z|x)$
- Decoder $p_\theta(x|z)$ assumption based on data.
- [Kingma & Welling, 2019]

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$\rightarrow$ one Limitation

- inflexibility of gaussian assumption on $q_\phi(z|x)$

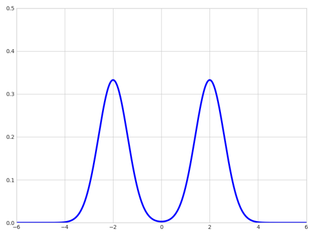
Extensions: more flexible/expressive $q_\phi(z|x)$

1. Normalizing flows
    - More flexible $q(z|x)$ by reparameterization via flows.

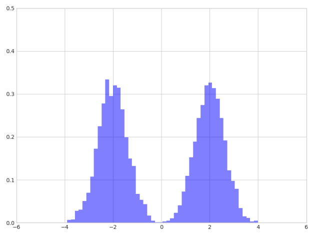
Normalizing flows

Introductory Problem

$p_X(x)$



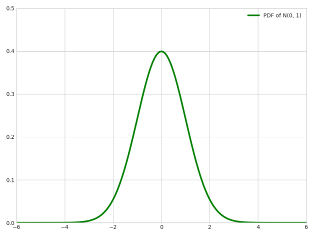
Data following $p_X(x)$



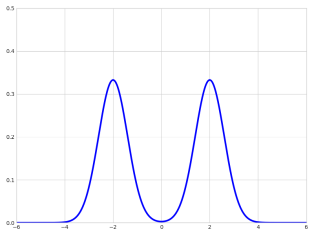
$\rightarrow$ How do we sample or evaluate from p_X?

Introductory Problem

Base distribution: $p_Z(z)$



Target distribution: $p_X(x)$



Idea: Change of variables

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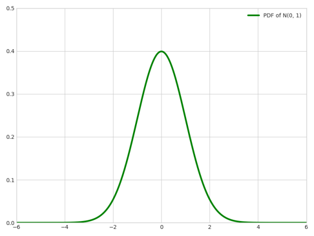

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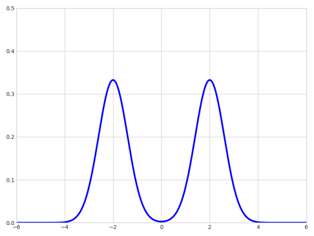

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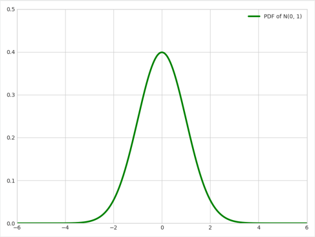

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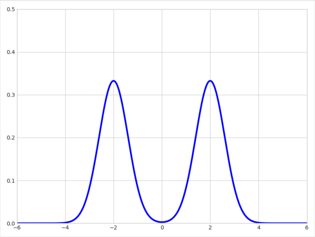

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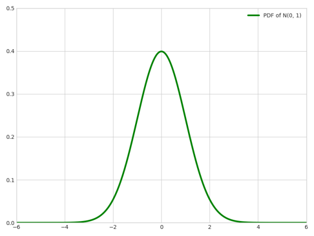

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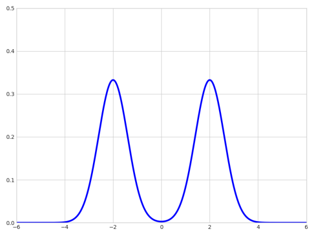

Idea: Change of variables

Solution:

1. Sample from base distribution (e.g., Gaussian) $z \sim p_Z(z)$
2. Apply transformation $x = f^{-1}(z)$
3. Learn f such that x follows desired distribution

Formal Problem Statement

Given:

- A Base distribution $p_Z(\mathbf{z})$ with $\mathbf{z} \in \mathbb{R}^d$
- Data that follows the target $\sim p_X(\mathbf{x})$, with $\mathbf{x} \in \mathbb{R}^d$

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Goal:

Find bijective transformation $f : \mathbb{R}^d \to \mathbb{R}^d$, such that

$$p_X(\mathbf{x}) = p_Z(f(\mathbf{x})) \left|\det J_f(\mathbf{x})\right|^{-1}$$

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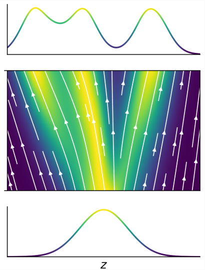
Then:

- evaluate the probability $p_X(\mathbf{x})$
- generate new samples $\mathbf{x} = f^{-1}(\mathbf{z}) \sim p_X(x)$

Designing Neural Networks for Normalizing flows

Idea:

Learn $f(z)$ with Neural Networks.
$\rightarrow$ We don't learn the distribution, **but** the transformation



[Grathwohl et al., 2018]

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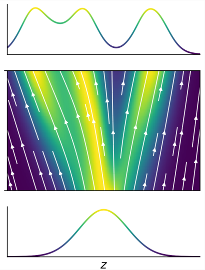

[Grathwohl et al., 2018]

Key considerations:

We need to be able to compute

- $\mathbf{x} = f^{-1}(\mathbf{z})$
- $|\det J_f(\mathbf{x})|^{-1}$

Designing Neural Networks for Normalizing flows

The Neural Network

- must be invertible and differentiable
- has an efficiently computable inverse and Jacobian determinant

Designing Neural Networks for Normalizing flows

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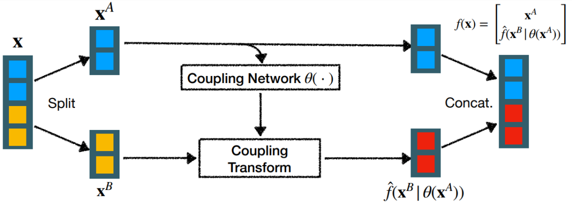
We trade-off between:

- Expressivity
- Computational speed

Coupling Flows: Partition-based Invertible Transformations

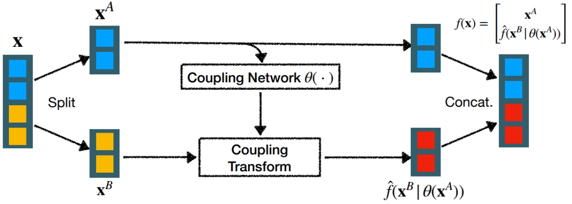
Key Idea: Split input $\mathbf{x} = [\mathbf{x}_A, \mathbf{x}_B]$ and transform only one part



[Brubaker and Köthe, 2021]

Coupling Flows: Partition-based Invertible Transformations

Key Idea: Split input $\mathbf{x} = [\mathbf{x}_A, \mathbf{x}_B]$ and transform only one part



[Brubaker and Köthe, 2021]

$$J_f(\mathbf{x}) = \begin{bmatrix} I & 0 \\ \frac{\partial}{\partial \mathbf{x}_A} \hat{f}(\mathbf{x}_B \mid \theta(\mathbf{x}_A)) & D\hat{f}(\mathbf{x}_B \mid \theta(\mathbf{x}_A)) \end{bmatrix}$$

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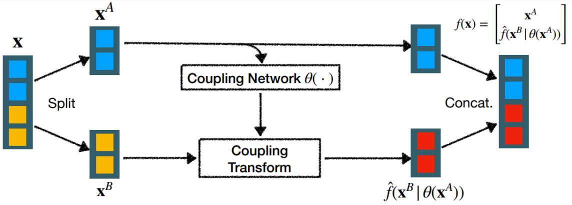

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Advantages:

- Efficient Jacobian, Determinant computation

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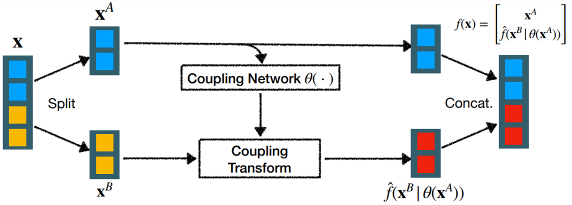

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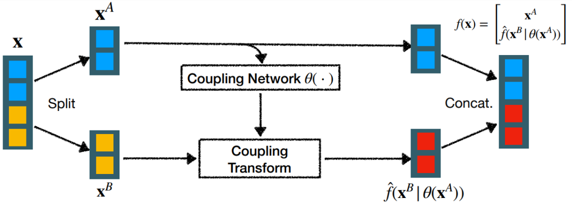

$\rightarrow$ What about the first dimensions?

Composing flows

We can compose flows:

$$f = f_K \circ f_{K-1} \circ \cdots \circ f_1$$

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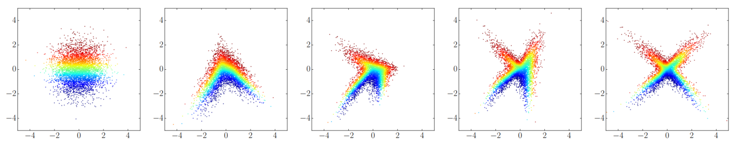

[Papamakarios et al., 2021]

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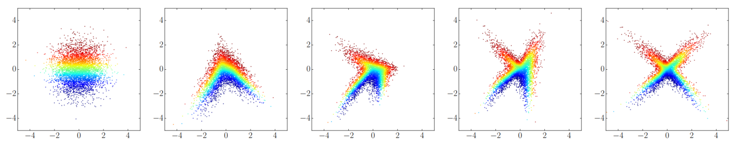

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The determinant then yields:

$$\det J_f = \det J_{f_K} \cdot \det J_{f_{K-1}} \cdots \det J_{f_1} = \prod_{k=1}^{K} \det J_{f_k}$$

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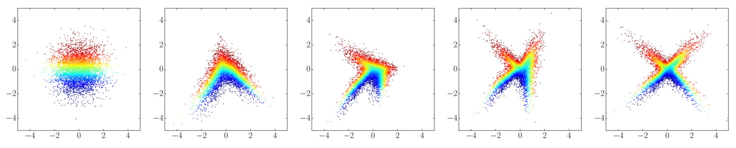

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$\rightarrow$ Transform different dimensions during each subflow

Training Normalizing Flows

- Typically trained via maximum likelihood:

$$\mathcal{L}(\theta) = -\mathbb{E}_{\mathbf{x} \sim p_{data}}[\log p_\theta(\mathbf{x})]$$

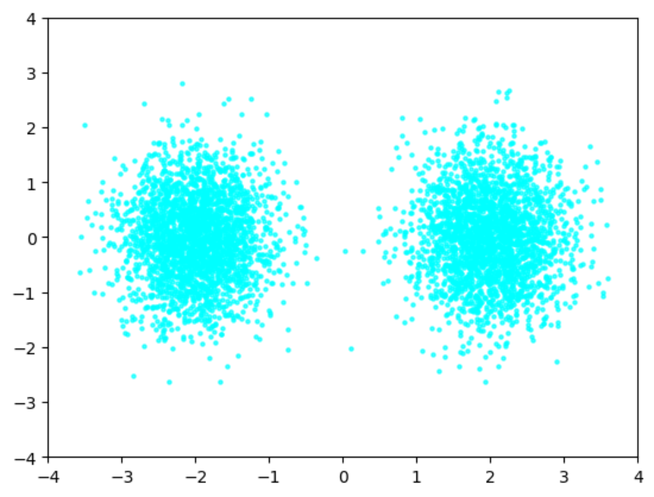
- For flows, this becomes:

$$\mathcal{L}(\theta) = -\mathbb{E}_{\mathbf{x} \sim p_{data}}[\log(\underbrace{p_Z(f^{-1}(\mathbf{x};\theta)}_{\text{Transformation error}})) + \log \underbrace{|\det J_{f^{-1}}(\mathbf{x};\theta)|}_{\text{Normalization}}]$$

Summary Normalizing Flows

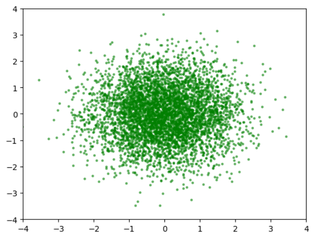
- Use Neural Networks to learn transforms between distributions
- From simple to complicated distribution
- NN has to be invertible, differentiable

Example: Learn a double Gaussian distribution flow

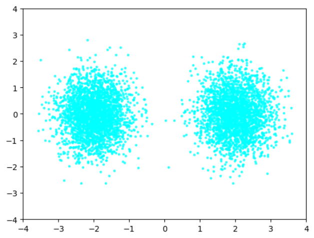


Example: Learn a double Gaussian distribution flow

Base distribution: $p_Z(z)$



Target distribution: $p_X(x)$



Example: Learn a double Gaussian distribution flow

```python
def create_normalizing_flow(num_layers=8, hidden_features=128):
    base_dist = StandardNormal(shape=[2])
    transforms = []
    for i in range(num_layers):
        mask = torch.zeros(2); mask[i % 2] = 1
        transforms.append(
            AffineCouplingTransform(
                mask=mask,
                transform_net_create_fn=lambda in_feat, out_feat: ContextNet(in_feat, out_feat, hidden_features)
            )
        )
    transform = CompositeTransform(transforms)
    flow = Flow(transform, base_dist)
    return flow
```

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Example: Learn a double Gaussian distribution flow

```python
model.train()
pbar = tqdm(range(num_iter), desc="Training NF")
for i in pbar:
    x = mixture_dist.sample((batch_size,))
    loss = -model.log_prob(inputs=x).mean()
    optimizer.zero_grad()
    loss.backward()
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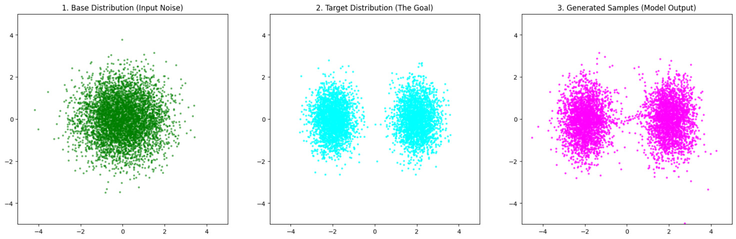


Challenges and Limitations

- Computational cost of Jacobian determinant calculations
- Trade-off between expressiveness and fast Invertability
- Often outperformed by other methods

$\rightarrow$ Can we improve Normalizing Flows?

Continuous Normalizing Flows: From Discrete to Continuous Transformations

Discrete NFs

- K fixed transformations
- $\mathbf{z}_k = f_k(\mathbf{z}_{k-1})$

Continuous NFs

- Continuous trajectory $\mathbf{z}(t)$
- $\frac{d\mathbf{z}}{dt} = f(\mathbf{z}(t), t; \theta)$

Key Insight: Replace discrete steps with continuous-time ODE

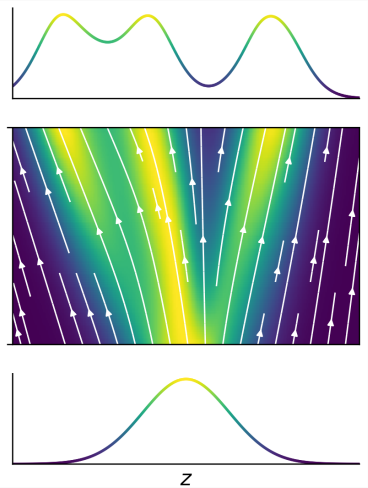
Connection to Neural ODEs

- Dynamics are described by an ODE:

$$\frac{d\mathbf{z}(t)}{dt} = f(\mathbf{z}(t), t; \theta)$$

  where f is a neural network

- Key advantages:
  - no need for matrix inversion
  - more flexible



[Grathwohl et al., 2018]

Example 2: Learn distribution using flow-matching

```
for epoch in tqdm(range(NUM_EPOCHS)):
    model.train()

    # Sample data from base distribution
    x = torch.randn(BATCH_SIZE, 2) * STD
    # Sample from target distribution
    y = qr_dist.sample(BATCH_SIZE)
    t = torch.rand(BATCH_SIZE, 1)

    # Perform flow matching
    psi_t = (1 - t) * x + t * y
    v_pred = model(psi_t, t.squeeze())
    v_true = y - x

    # Loss and backprop
    loss = criterion(v_pred, v_true)
    optimizer.zero_grad()
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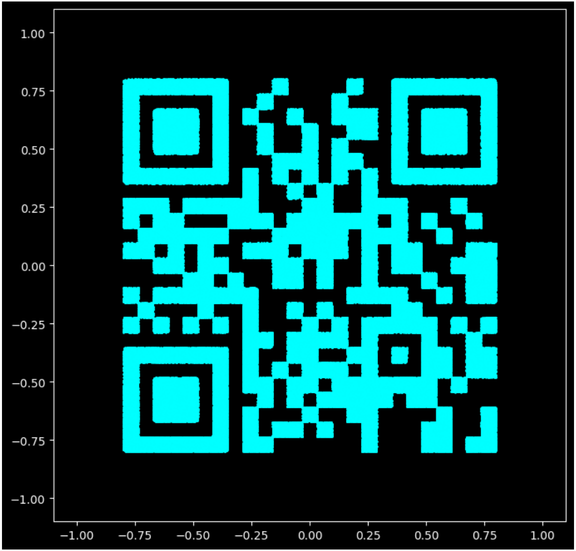
Example: Learn a QR-Code distribution flow

```
# Initialize from Gaussian prior
x = torch.randn(current_batch_size, 2, device=device) * BASE_DISTRIBUTION_STD

# Euler integration
for step in range(num_steps):
    t = torch.full((current_batch_size,), step/num_steps)
    dx = model(x, t) / num_steps
    x = x + dx
```

Example 2: Learn distribution using flow-matching



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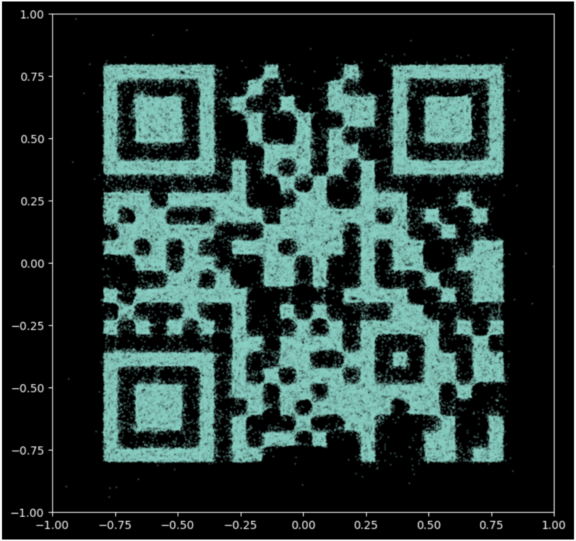


Applications in Physics

General Application Fields

Both architectures can be used in two ways:

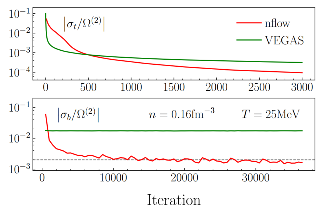
- backward (computing the likelihood of a sample)
- forward (sampling from the modeled distribution)

- **Generative modeling**: High-quality image generation
- **Density estimation**: Anomaly detection, Monte Carlo sampling

Normalizing Flows in Physics: Example

Application in Monte Carlo Sampling:

- Perform Monte Carlo importance sampling for high-dimensional integrals
- The flow learns the probability distribution necessary for MC integration, enabling more precise and efficient sampling



[Roggero et al., 2021]

VAEs in Physics

- Galaxy generation for calibration [Ravanbakhsh et al., 2016]
- Chemical design [Gomez-Bombarelli et al., 2018]
- Anomaly detection at LHC [Pol et al., 2020]
- Multimodal data integration Time Series [Brenner et al., 2024]

The Banana Problem

But how do we turn an apple into a banana?

The Banana Problem

1. Get Fruit dataset

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2. Use VAE to learn Fruit distributions
    - Optimize ELBO
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5. Decode alongside the latent space path

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6. enjoy!

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Backup slides

Other flows

Most Widely Used Flow Types

Coupling Flows:

- split data to ensure a triangular Jacobian matrix

Autoregressive Flows:

- Each input dimension is transformed, only depending on the previous ones, making the Jacobian triangular by design

Spline-based Flows:

- Use piecewise polynomial functions
- More expressive than affine transformations

Extra slide: Understanding the ELBO

$$\mathrm{ELBO}(x,z) = \mathbb{E}_{q(z|x)}\left[\log \frac{p(x,z)}{q(z|x)}\right] = \mathbb{E}_{q(z|x)}\left[\log \frac{p(z|x)p(x)}{q(z|x)}\right]$$

$$= \underbrace{\mathbb{E}_{q(z|x)}\left[\log p(x)\right]}_{\text{Estimate of log likelihood.}} - D_{\mathrm{KL}}(q(z|x) \parallel p(z|x))$$

$$\mathrm{ELBO}(x,z) \leq \log p(x)$$

Extra slide: More details on Reparameterization trick

$$\mathbb{E}_{q_\phi(z|x)}\left[\log p_\theta(x \mid z)\right] \approx \frac{1}{L}\sum_{\ell=1}^{L} \log p_\theta(x \mid z^{(\ell)}), \quad z^{(\ell)} \sim q_\phi(z \mid x)$$

$z^{(\ell)} = q_\phi(z|x) \sim \mathcal{N}(\mu_\phi, \sigma_\phi)$. The sampling is not differentiable w.r.t ϕ.

$\rightarrow$ We reparameterize in terms of a noise parameter $\epsilon \sim \mathcal{N}(0, I)$:

$z = g_\phi(\epsilon)$. s.t. it is differential w.r.t ϕ

$$\rightarrow z = \mu_\phi + \sigma_\phi \odot \epsilon,$$

$$q_\phi(z \mid x) = p(g_\phi^{-1}(z)) \cdot \left|\det\left(\frac{\partial g_\phi(\epsilon)}{\partial \epsilon}\right)\right|^{-1}$$

$$\log q_\phi(z \mid x) = \log p(\epsilon) - \log\left|\det\left(\frac{\partial z}{\partial \epsilon}\right)\right|$$

Extra Slide: More in depth example: VAEs DSR

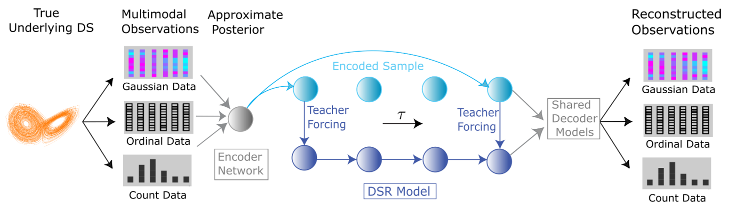

Figure 1. MTF setup. Multimodal observations are translated via an encoder into a common latent representation, which is used for sparse TF in the DSR model's latent space. The latent trajectory is then mapped back into observation space via modality-specific decoder models, which are shared between the MVAE and DSR model.

[Brenner et al., 2024]