From Zero to Generative

Learning Generative Modelling from scratch

Carolina Cuesta-Lazaro

Flatiron Institute
Institute for Advanced Studies

Art: "The art of painting" by Johannes Vermeer

Probabilistic ML has made ***high dimensional inference tractable***

$$p(\text{World}|\text{Prompt})$$

["Genie 2: A large-scale foundation model"
Parker-Holder et al (2024)]

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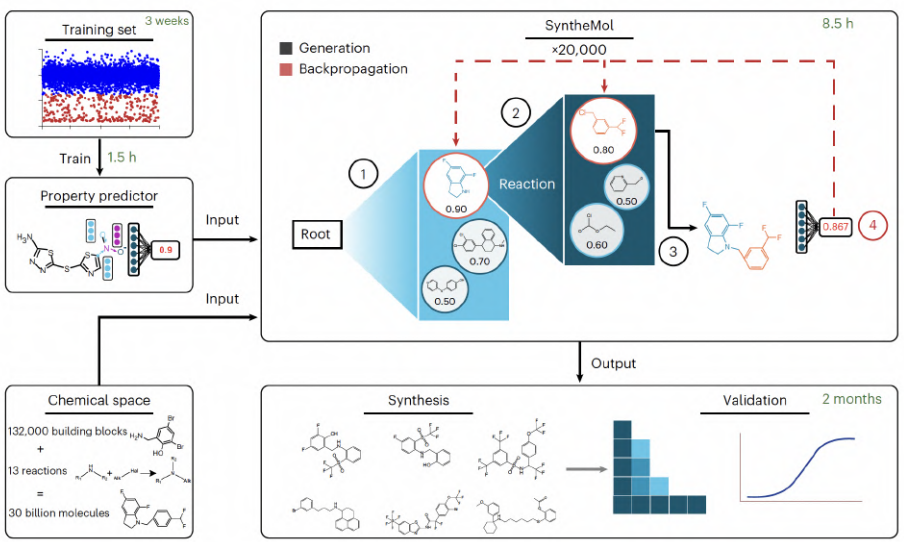
Probabilistic ML has made ***high dimensional inference tractable***

$$p(\text{World}|\text{Prompt})$$

$$p(\text{Drug}|\text{Properties})$$



["Genie 2: A large-scale foundation model"
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["Genie 3: A new frontier for world models"
Parker-Holder et al (2025)]

["Generative AI for designing and validating easily synthesizable and structurally novel antibiotics"
Swanson et al]

Parti-350M

A portrait photo of a kangaroo wearing an orange hoodie and blue sunglasses standing on the grass in front of the Sydney Opera House holding a sign on the chest that says Welcome Friends!

https://parti.research.google

Parti-350M

Parti-750M

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Parti-350M **Parti-750M** **Parti-3B**

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Parti-350M	Parti-750M	Parti-3B	Parti-20B
			

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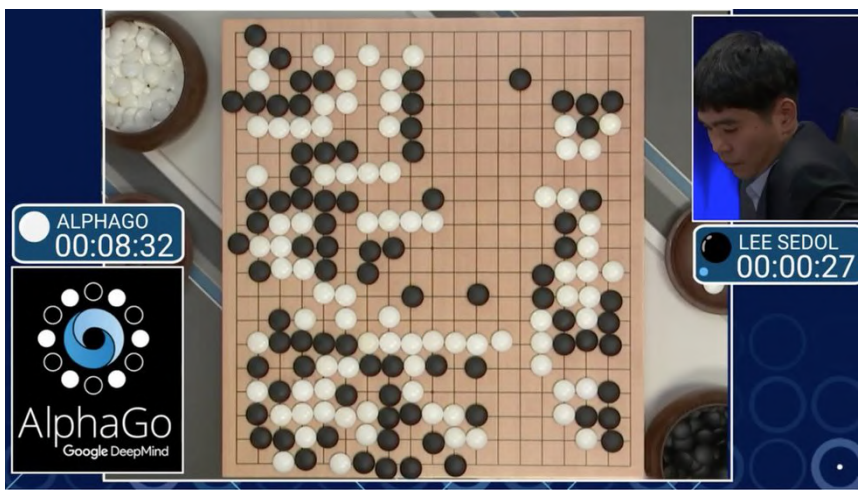
Artificial General Intelligence?

BEFORE



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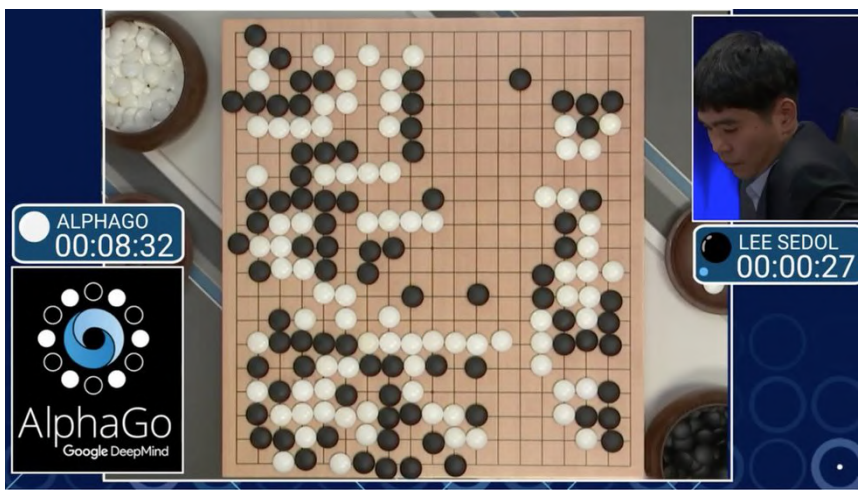

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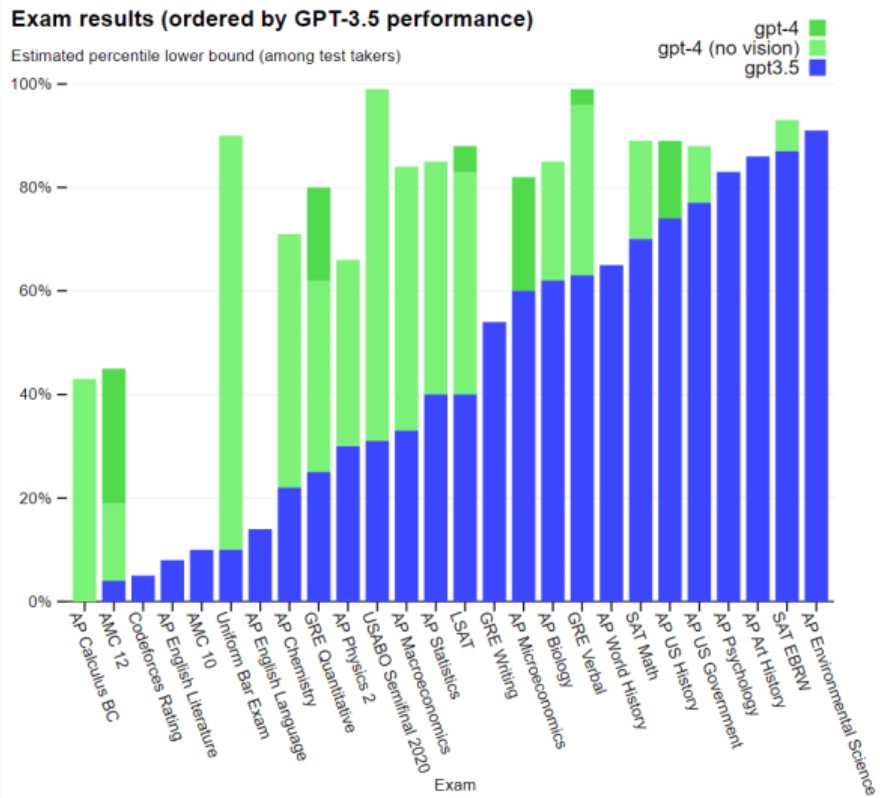

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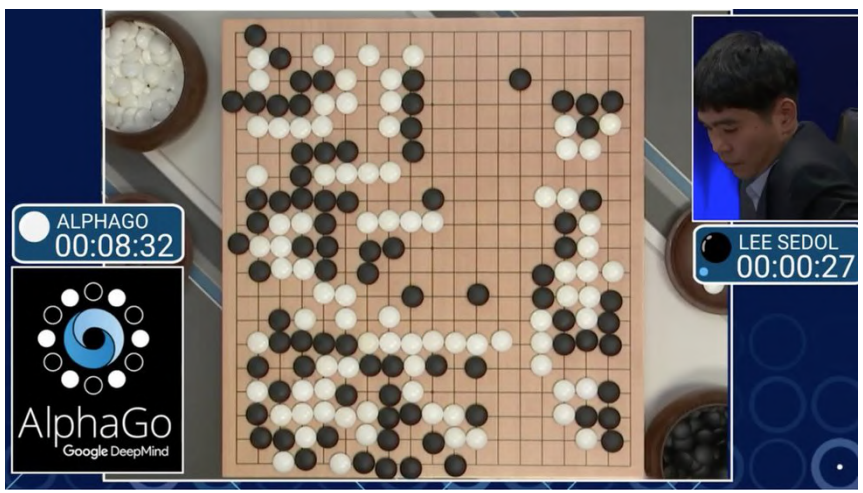

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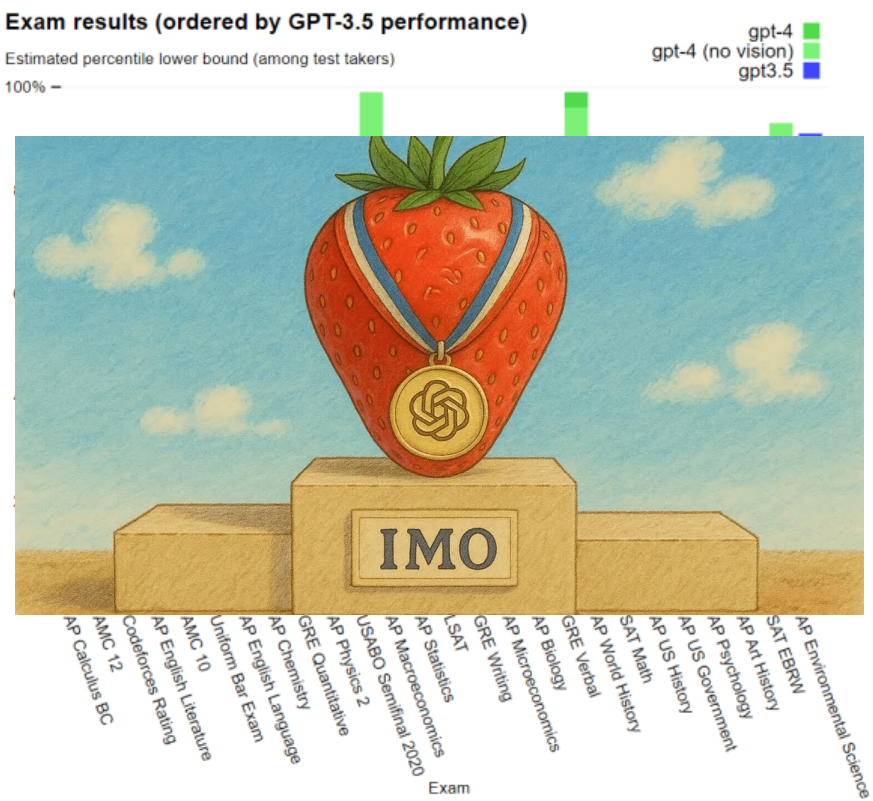
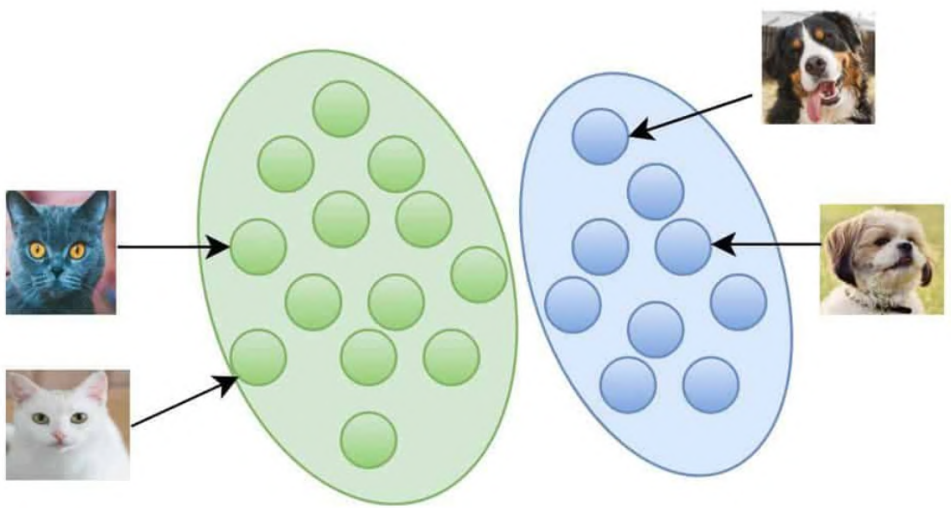


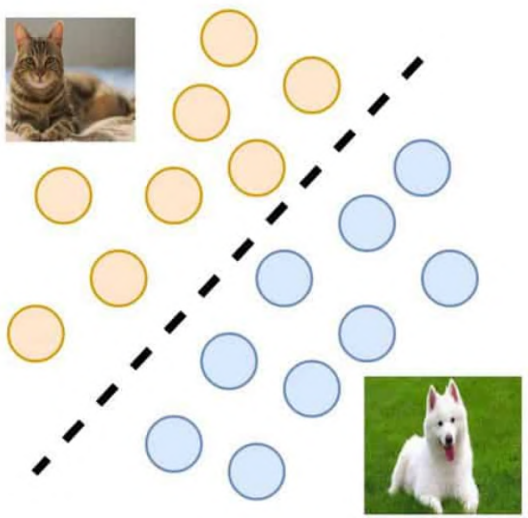
Generation vs Discrimination

$p(x)$

$p(y|x)$



Generative



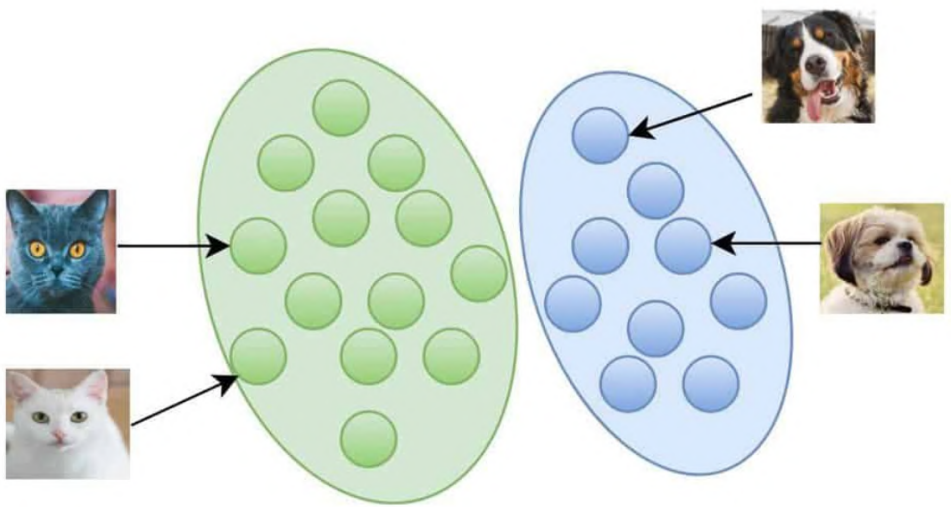
Discriminative

$p(x|y)$

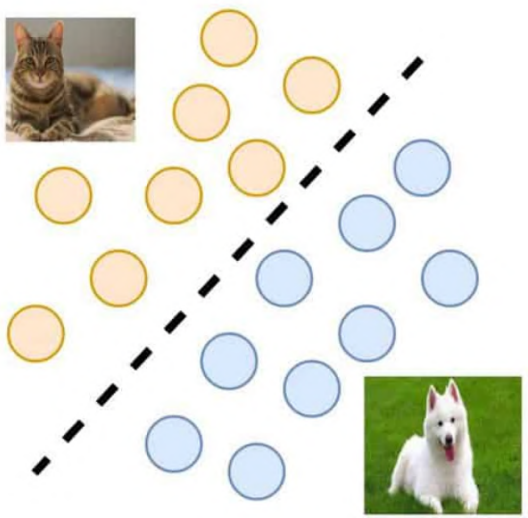
Generation vs Discrimination

$p(x)$

$p(y|x)$



Generative



Discriminative

$p(x|y)$

$$p(x|y) = \frac{p(y|x)p(x)}{p(y)}$$

Generative Models

$$p_\phi(x)$$

Generative Models

Data

$$p_\phi(x)$$

Generative Models

Data

$$p_\phi(x)$$

A PDF that we can optimize

Generative Models

Maximize the likelihood of the data

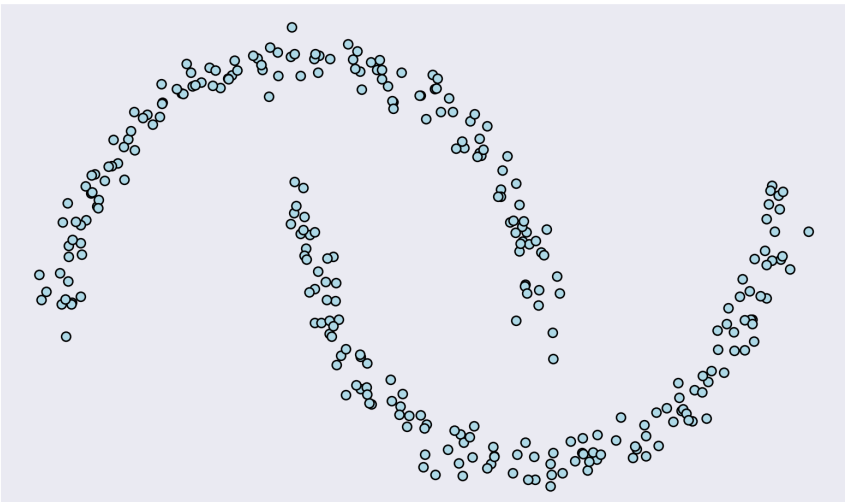
Data

$$p_\phi(x)$$

A PDF that we can optimize

Generative Models 101

Training Samples x_{train}



Generative Models 101

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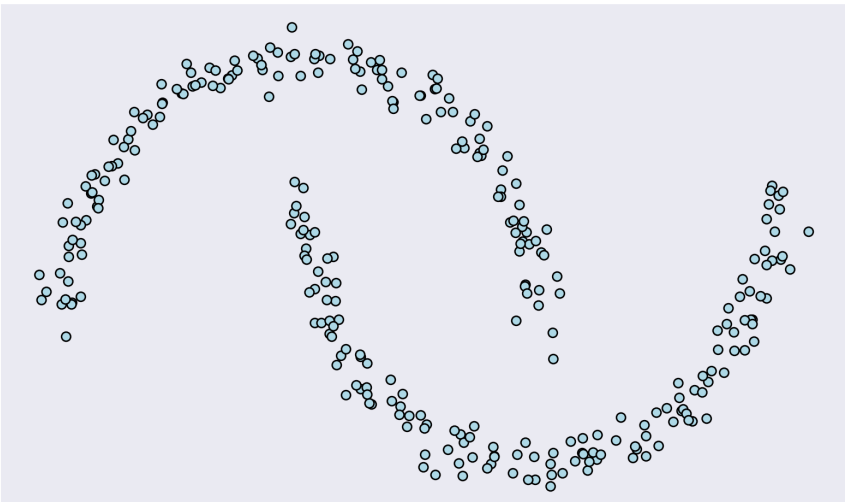
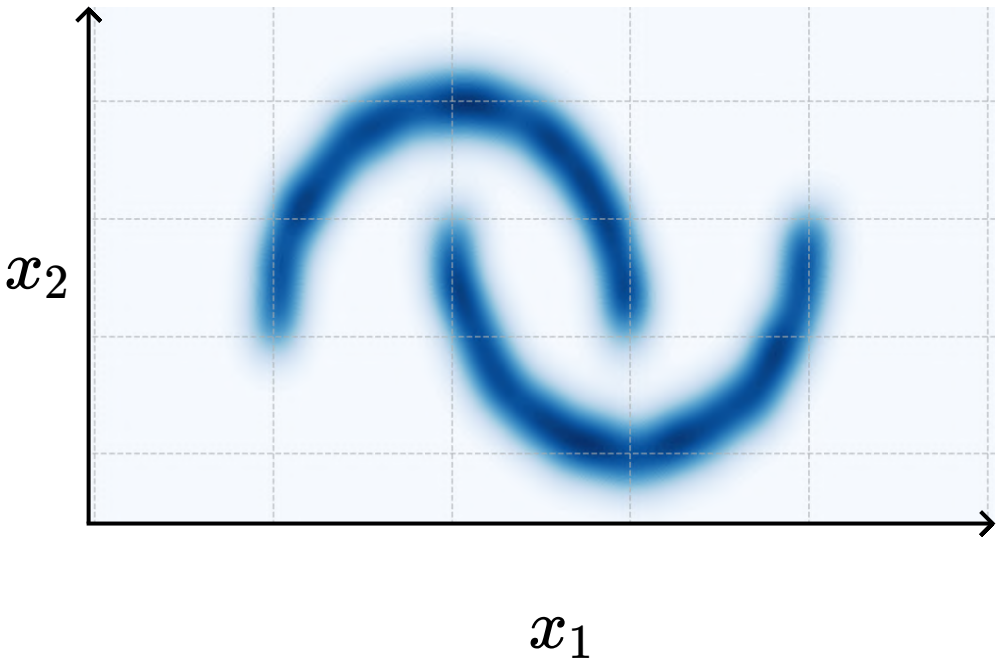


Parametric Model $p_\phi(x)$



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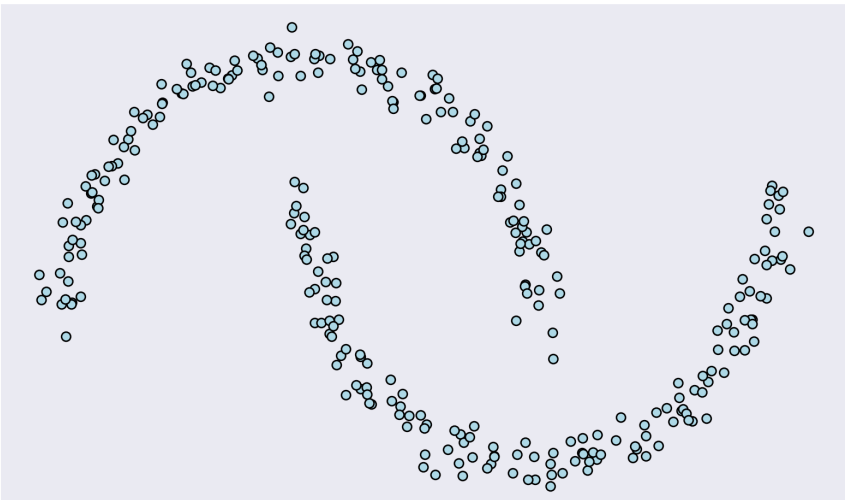

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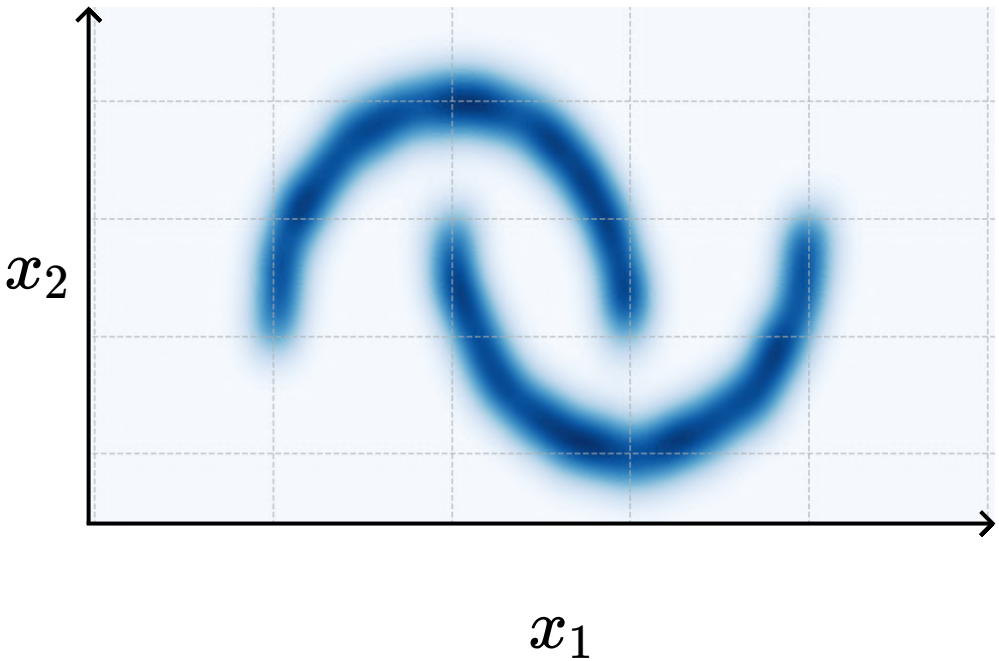

Maximize the likelihood of the training samples

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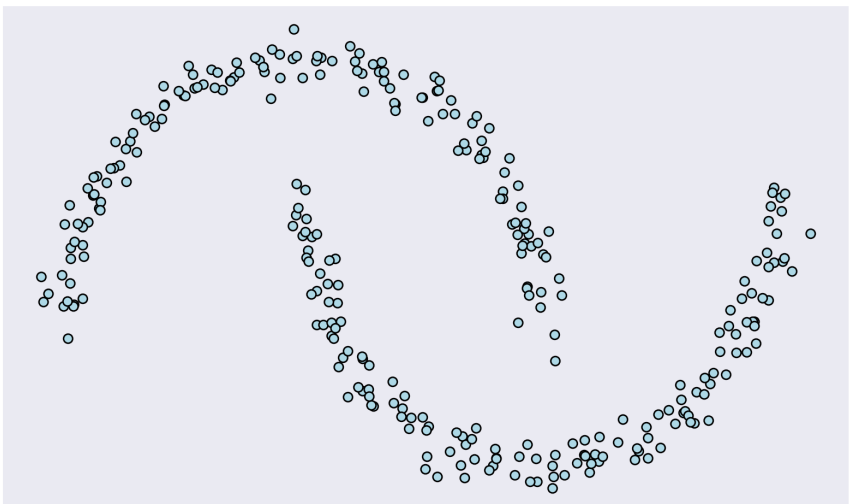

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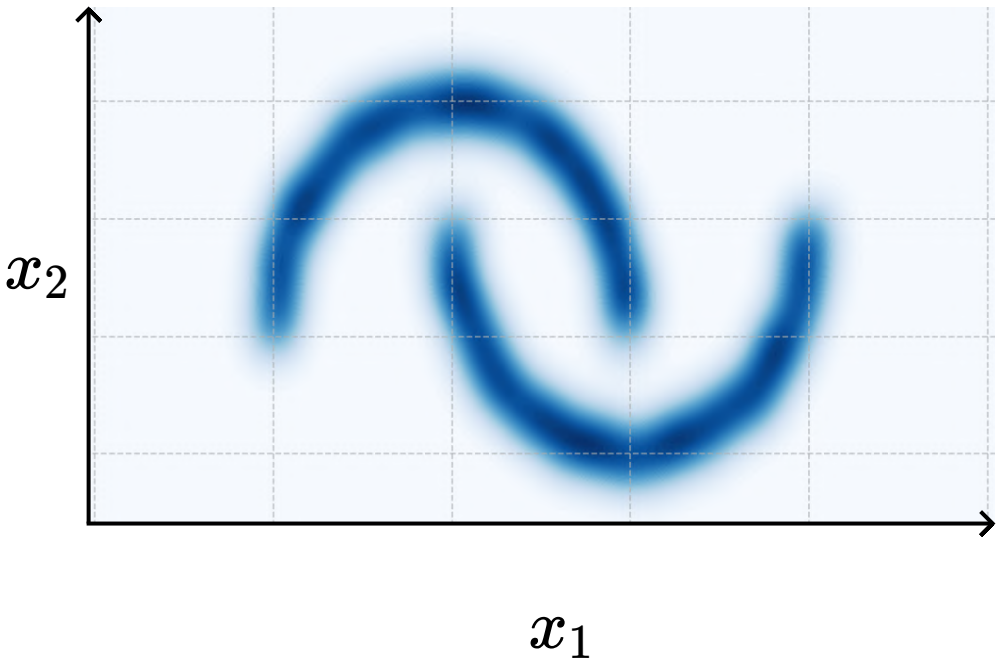
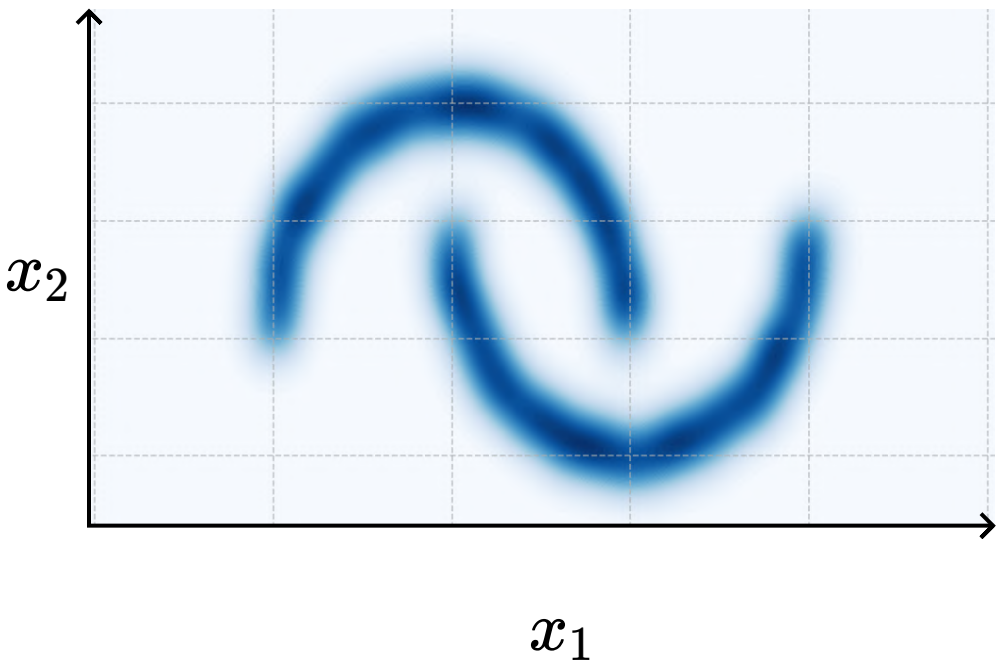


Maximize the likelihood of the training samples

$$\hat{\phi} = \arg\max \left[\log p_\phi(x_{\text{train}})\right]$$

Generative Models: Simulate and Analyze

Trained Model $p_\phi(x)$



Generative Models: Simulate and Analyze

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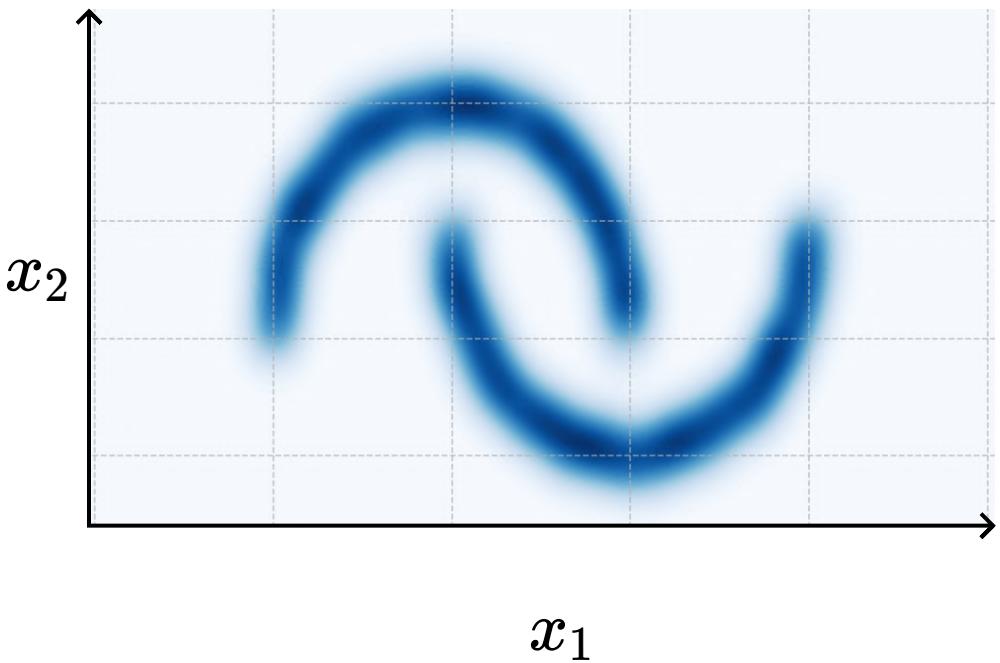
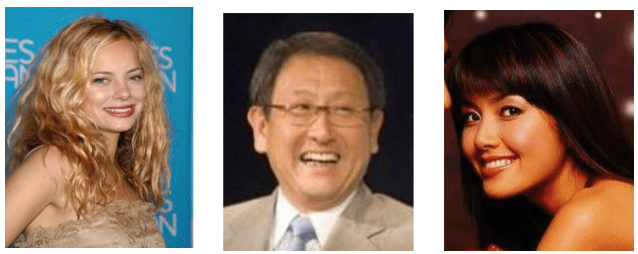


Generate Novel Samples



Generative Models: Simulate and Analyze

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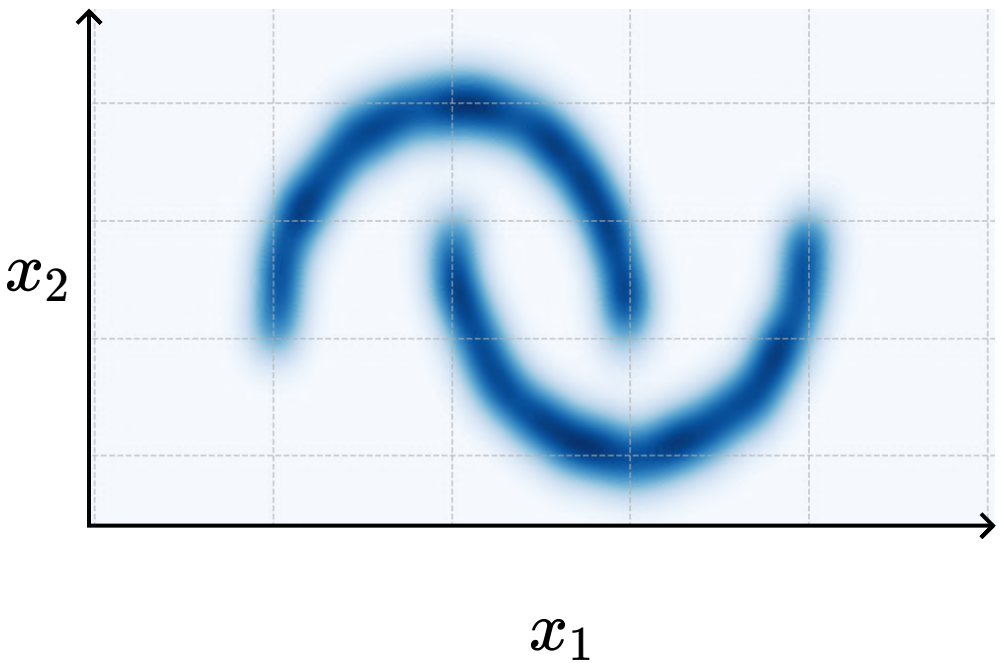

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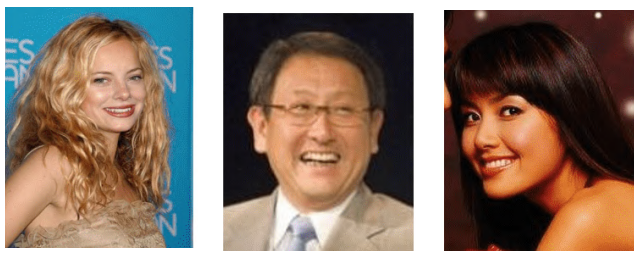
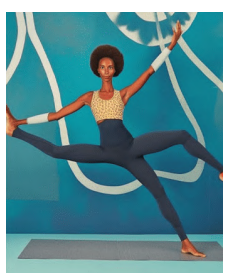


Evaluate probabilities

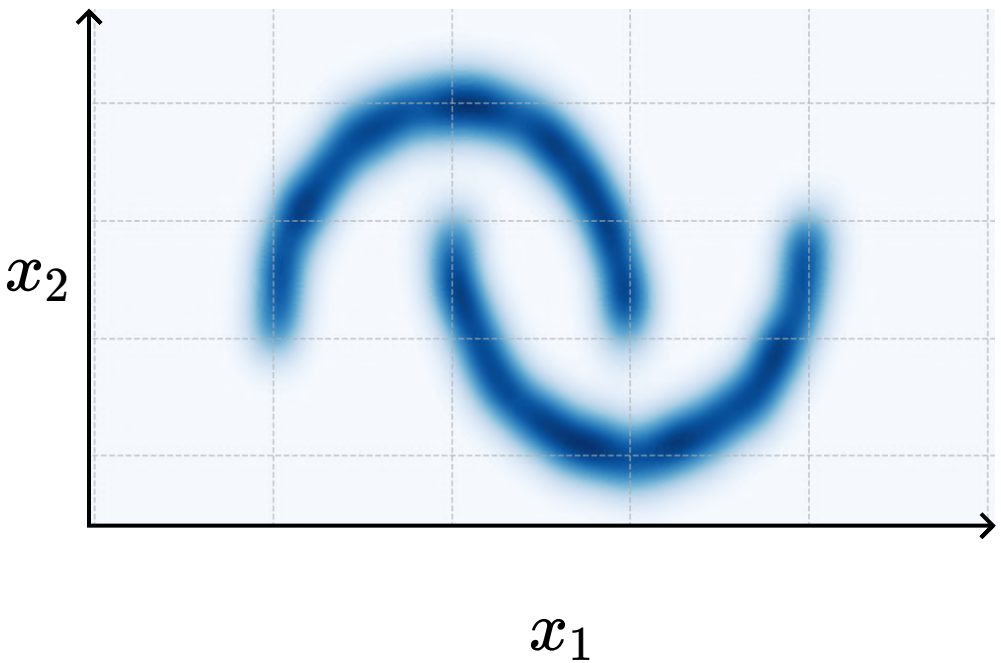
High Probability



Low Probability

Generative Models: Simulate and Analyze

Trained Model $p_\phi(x)$



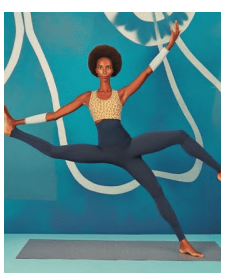
Generate Novel Samples

✅ *Generative Model*

✅ *Simulator*

Evaluate probabilities

High Probability



Low Probability

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Generative Models: Simulate and Analyze

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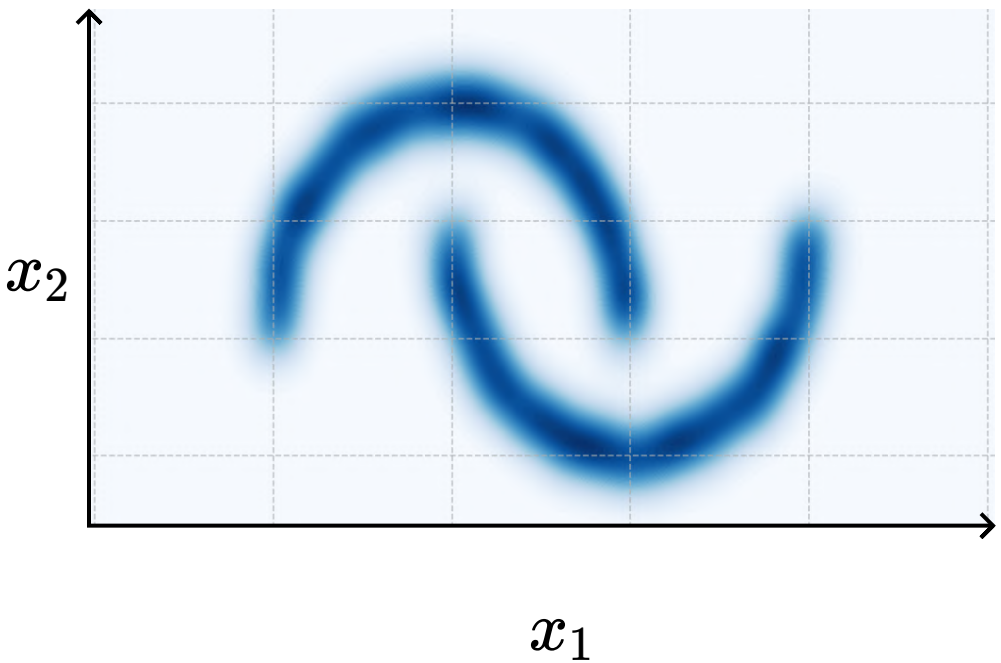


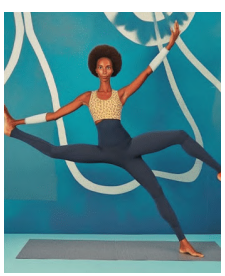
Fast emulators

Generate Novel Samples

- *Generative Model*
- *Simulator*

Evaluate probabilities

High Probability



Low Probability

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Generative Models: Simulate and Analyze

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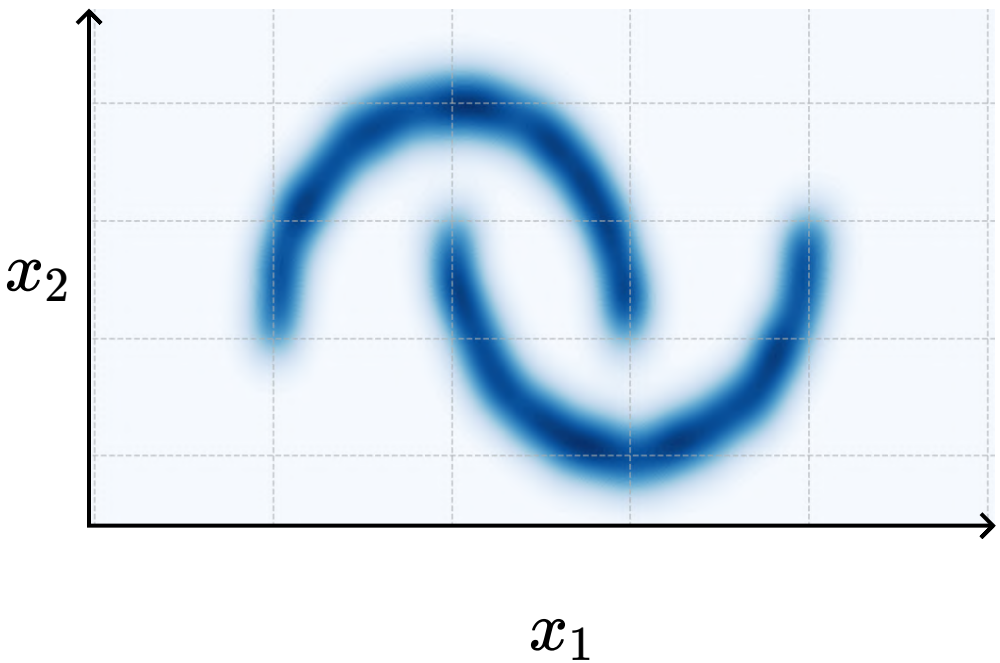

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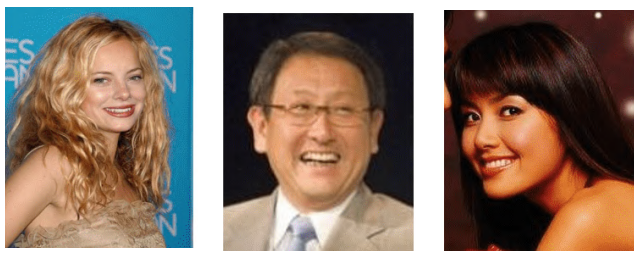


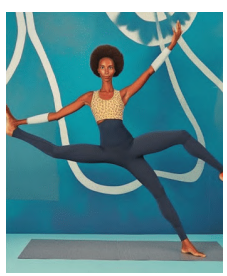
✅ *Generative Model*

✅ *Simulator*

Testing Theories

Evaluate probabilities

High Probability



Low Probability

✅ *Generative Model*

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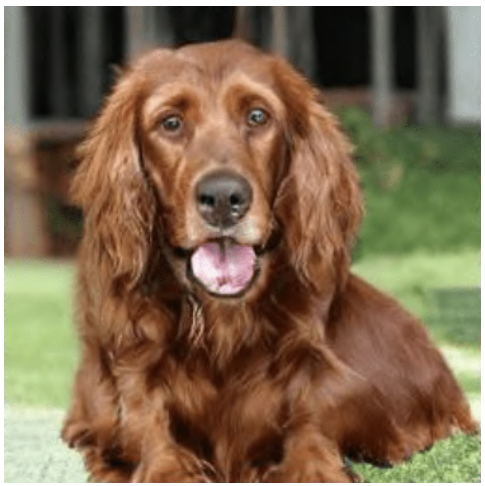
Contrastive Learning

A folk music band of anthropomorphic autumn leaves playing bluegrass instrument

BigGAN

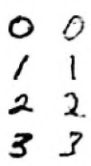


VAEs

GANS

2006 2014 2017 2019 2022 2023

Deep Belief Networks



Normalising Flows

Diffusion Models

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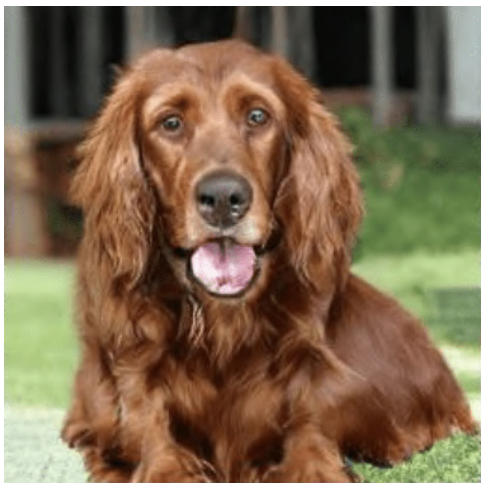

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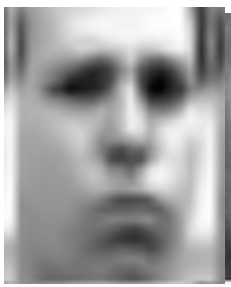

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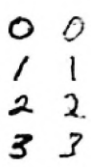
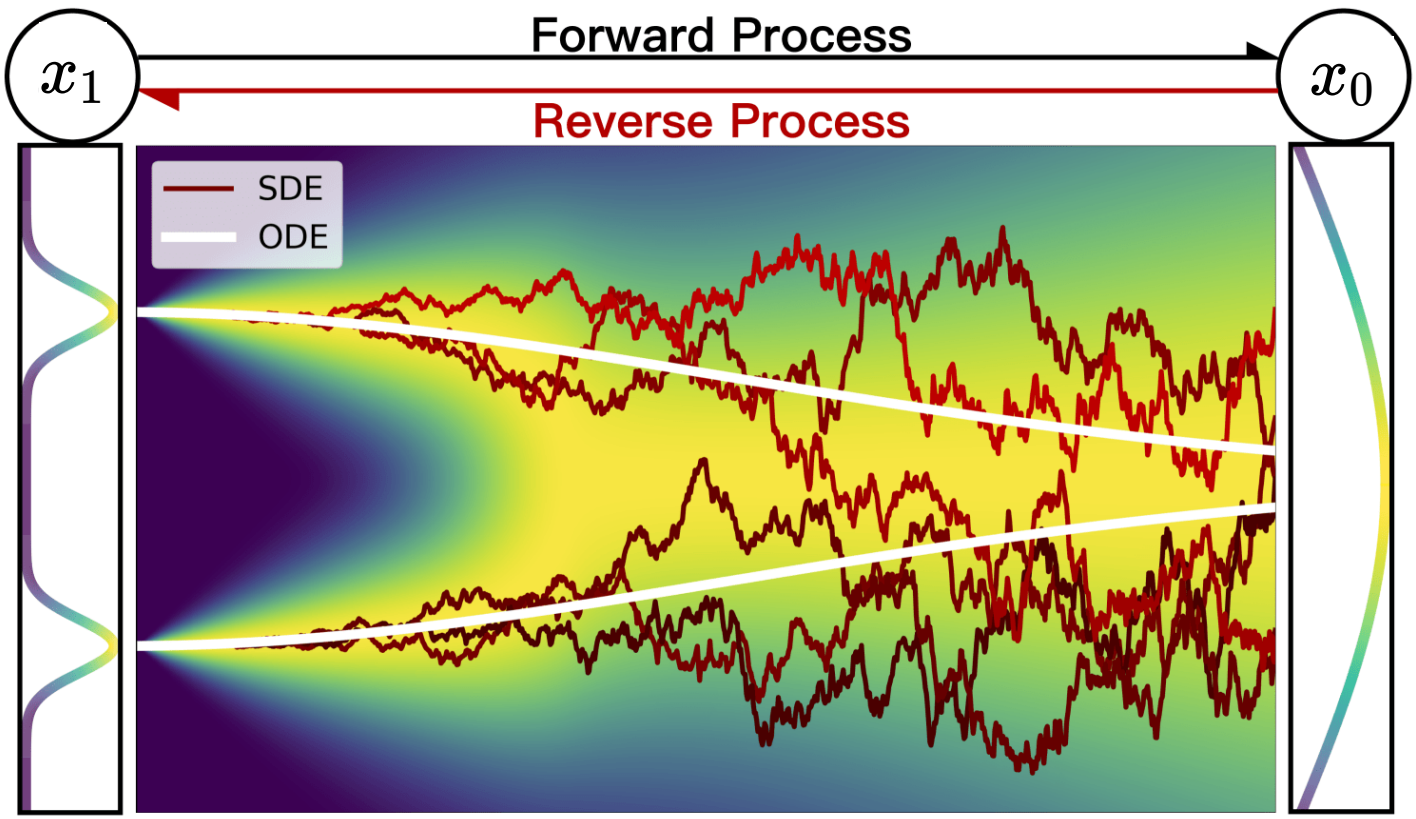


Normalising Flows

Diffusion Models

Bridging two distributions

"Creating noise from data is easy;
creating data from noise is generative modeling."
Yang Song



Data

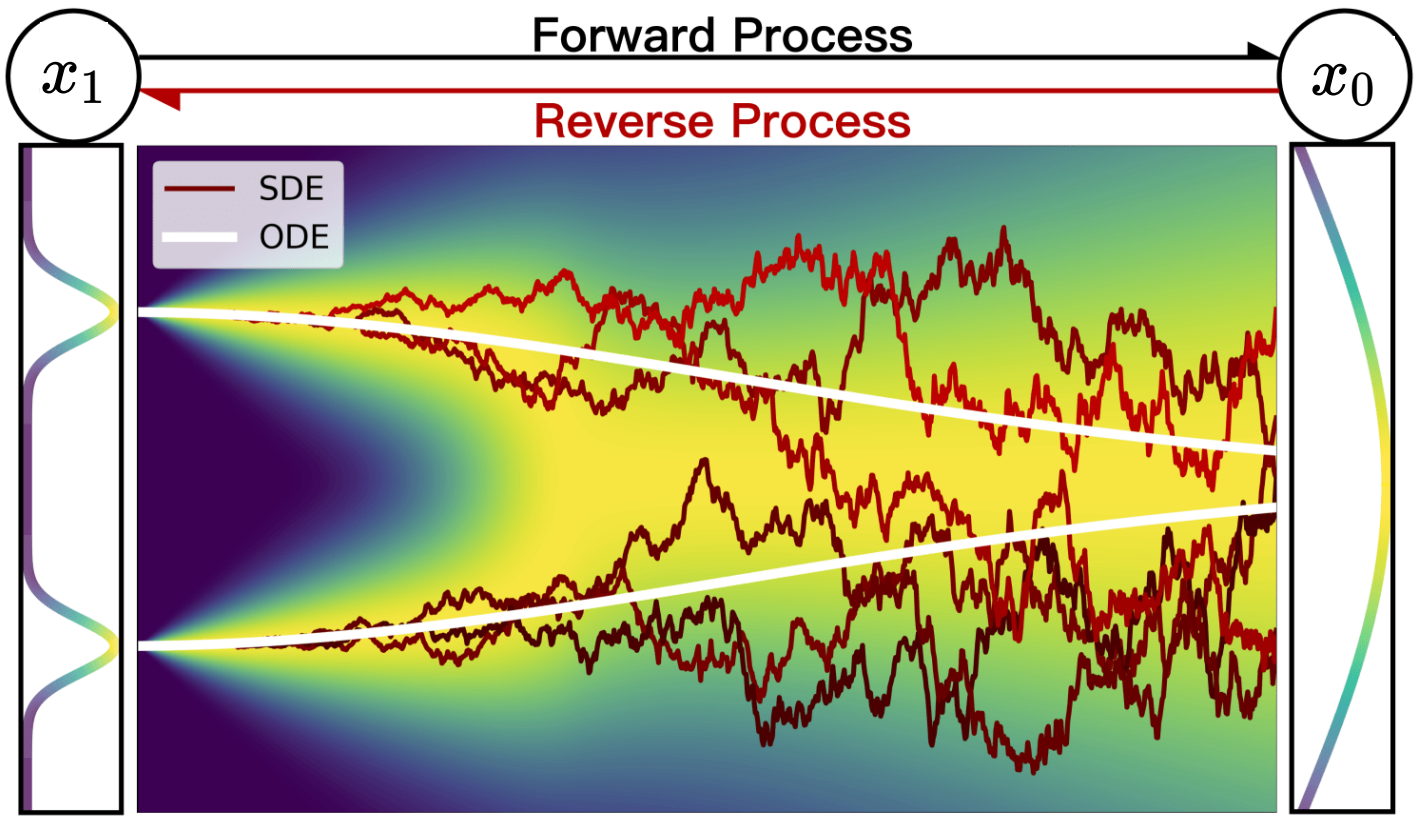
Base

Bridging two distributions

is p(x0) restricted?

Diffusion: p(x0) is Gaussian

Normalising flows: p(x0) can be evaluated



Data

Base

Bridging two distributions

How is the bridge constrained?

Normalizing flows: Reverse = Forward inverse

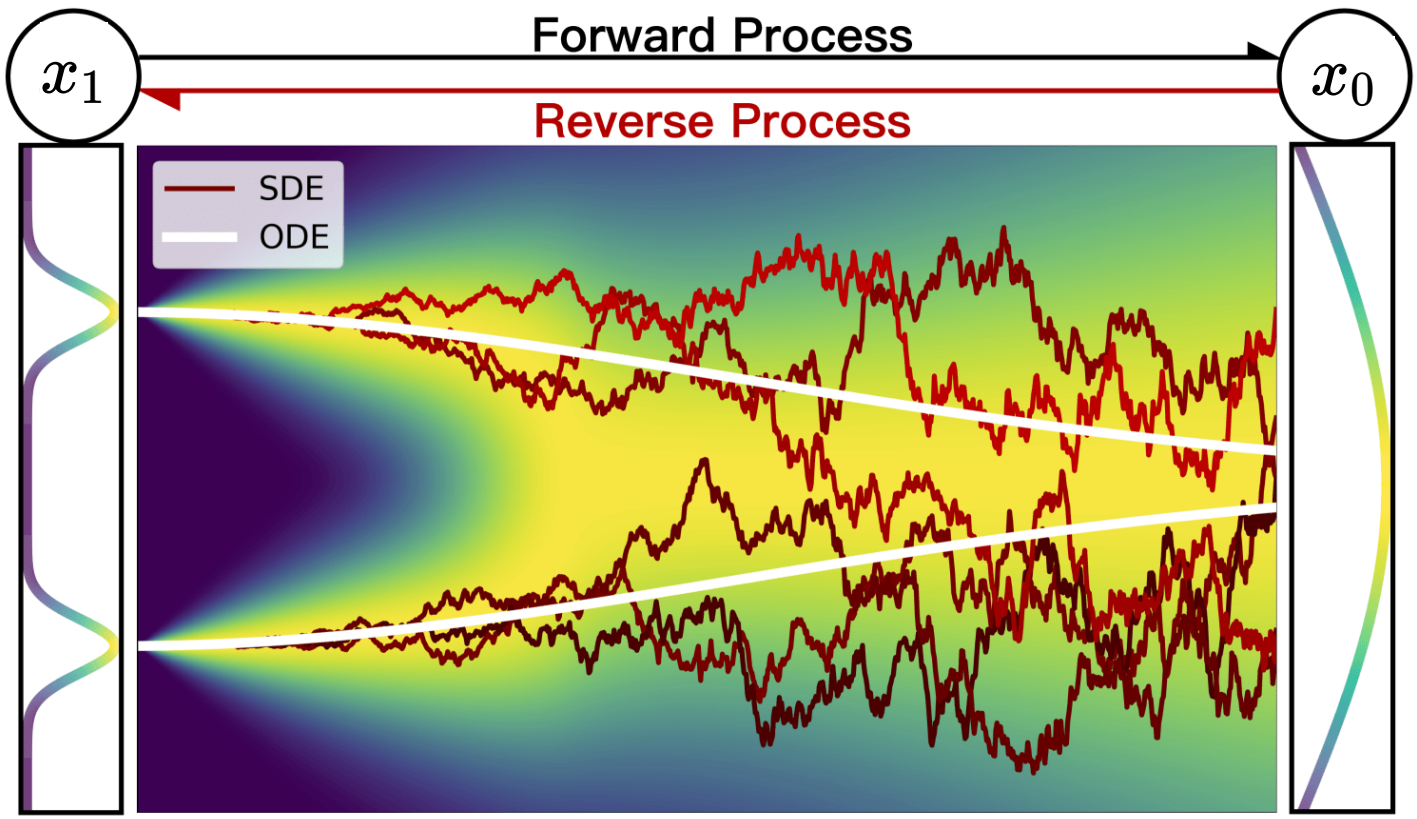
Diffusion: Forward = Gaussian noising

Flow Matching: Forward = Interpolant

is p(x0) restricted?

Diffusion: p(x0) is Gaussian

Normalising flows: p(x0) can be evaluated



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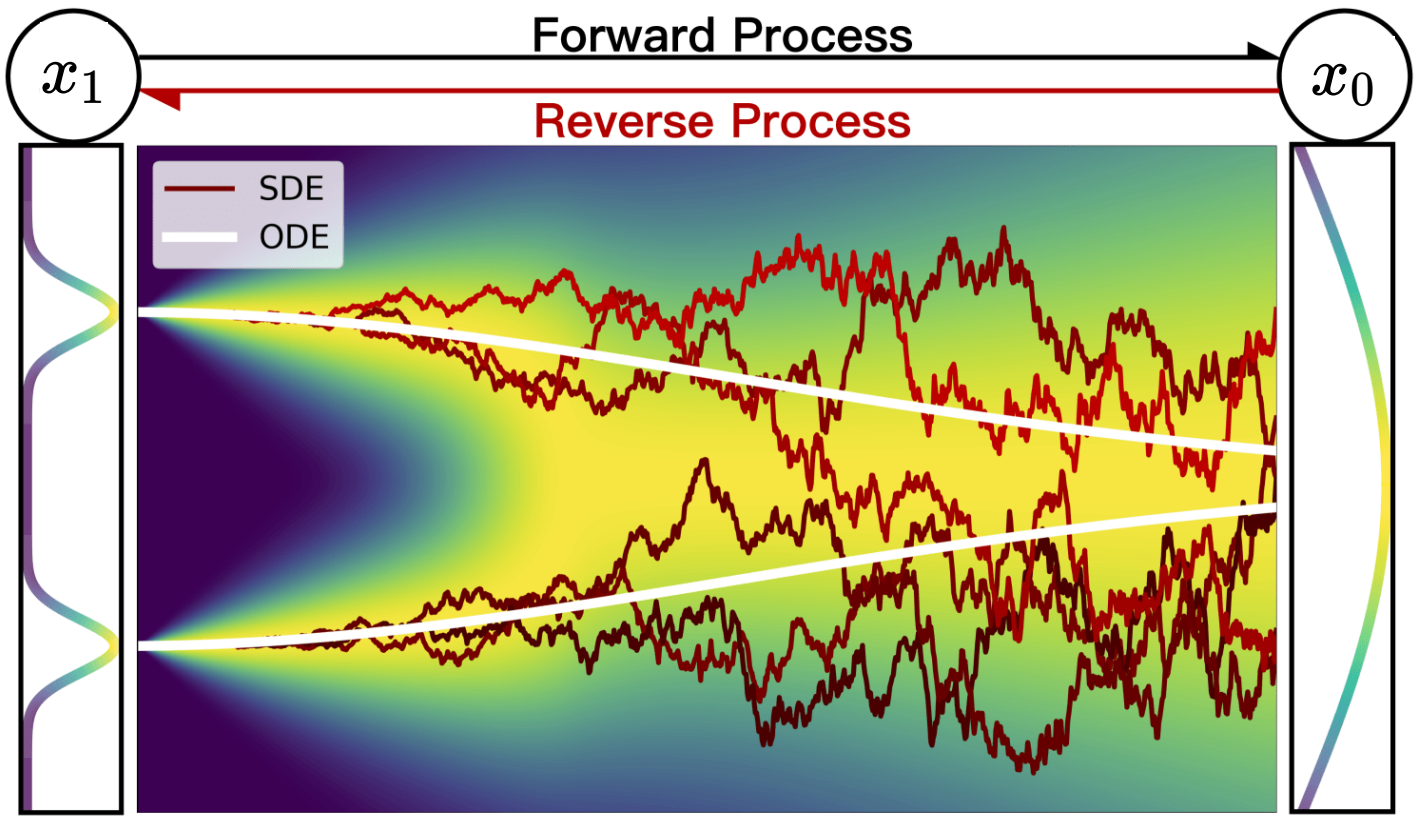

Data

Base

Is bridge stochastic (SDE) or deterministic (ODE)?

Diffusion: Stochastic (SDE) *Normalising flows: Deterministic (ODE)*

Bridging two distributions

How is the bridge constrained?

Normalizing flows: Reverse = Forward inverse

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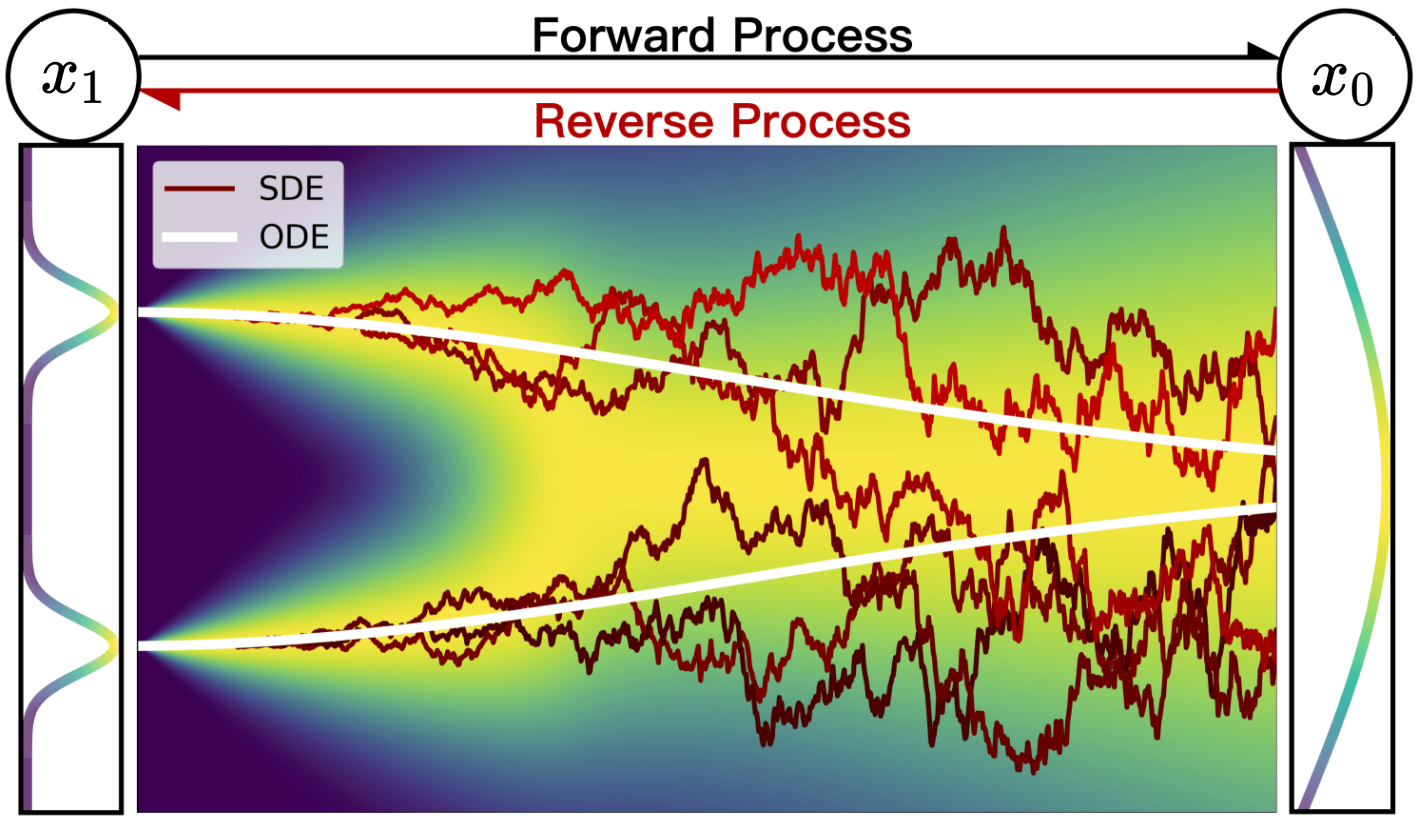


Data

Base

(Exact likelihood evaluation)

Is bridge stochastic (SDE) or deterministic (ODE)?

Diffusion: Stochastic (SDE) *Normalising flows: Deterministic (ODE)*

Flow: Change of Variables

$$X \sim \mathcal{N}(\mu, \sigma)$$

Transformation (flow):

$$Y = g(X) = aX + b$$

How is Y distributed?

Flow: Change of Variables

$$X \sim \mathcal{N}(\mu, \sigma)$$

Transformation (flow):

$$Y = g(X) = aX + b$$

How is Y distributed?

$$Y \sim N(a\mu + b, a^2\sigma^2)$$

Flow: Change of Variables

$$X \sim \mathcal{N}(\mu, \sigma)$$

Transformation (flow):

$$Y = g(X) = aX + b$$

How is Y distributed?

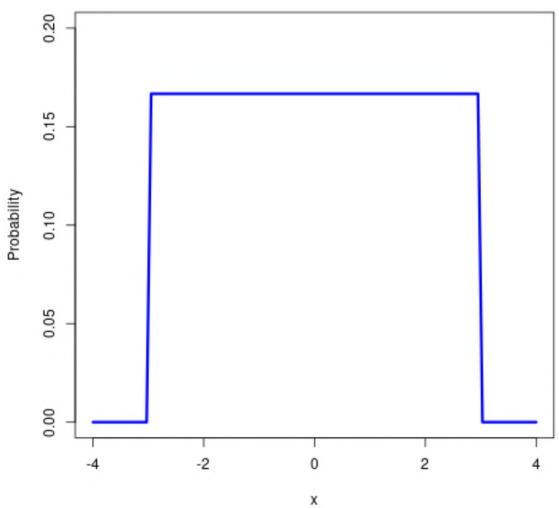
$$Y \sim N(a\mu + b, a^2\sigma^2)$$

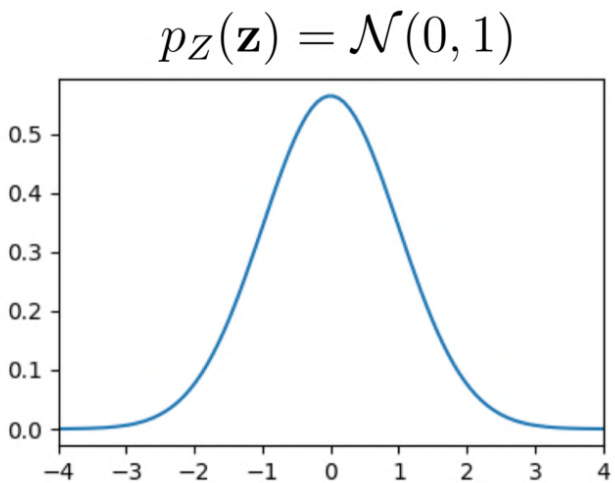
$$p_Y(y) = p_X(g^{-1}(y)) \left| \frac{dg^{-1}(y)}{dy} \right|$$

Box-Muller transform

Normalizing flows in 1934

$$\text{Uniform}(0,1) \rightarrow U_1, U_2$$

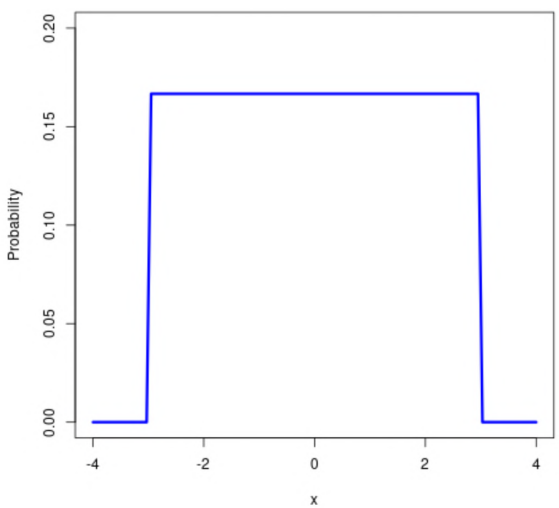


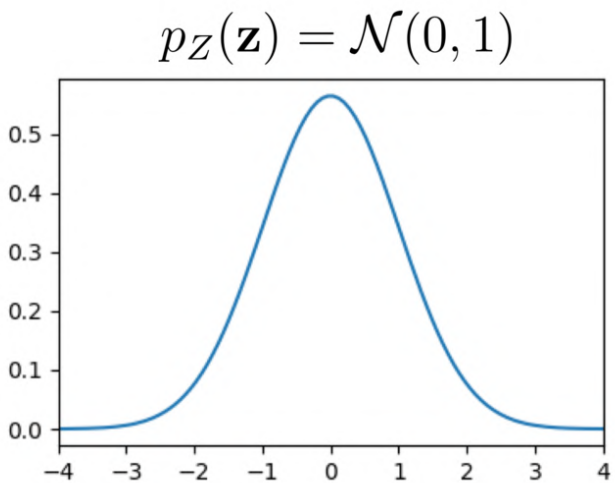


Box-Muller transform

Normalizing flows in 1934

$$\text{Uniform}(0,1) \rightarrow U_1, U_2$$





$$Z_0 = \sqrt{-2\ln U_1}\cos(2\pi U_2)$$

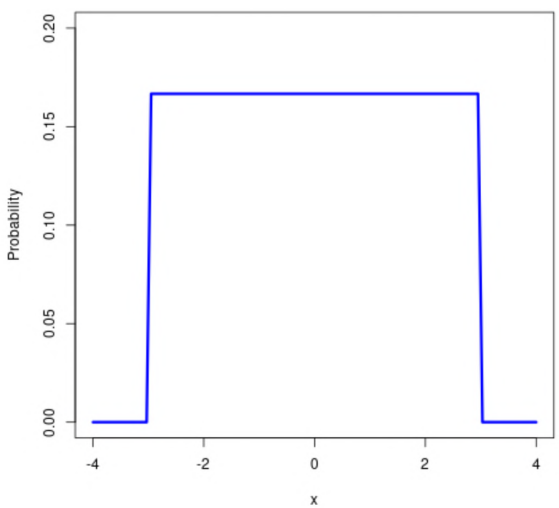
$$Z_1 = \sqrt{-2\ln U_1}\sin(2\pi U_2)$$

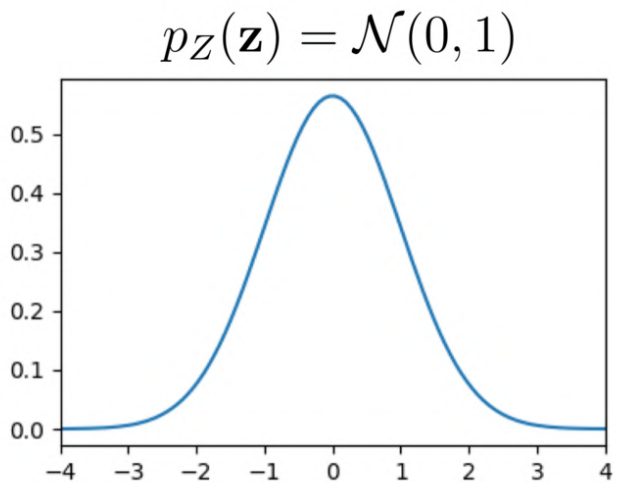
Box-Muller transform

Normalizing flows in 1934

$$\text{Uniform}(0,1) \rightarrow U_1, U_2$$

$$Z_0, Z_2 \leftarrow N(0,1)$$



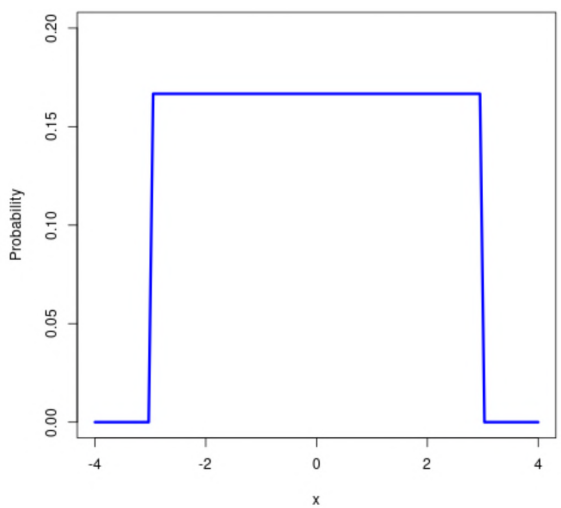


$$Z_0 = \sqrt{-2\ln U_1}\cos(2\pi U_2)$$

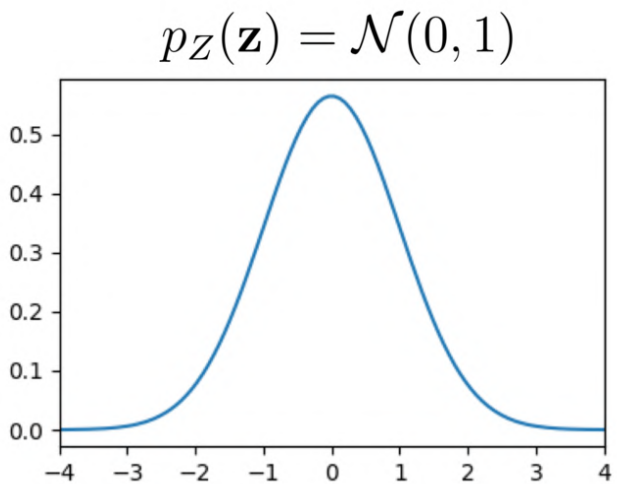
$$Z_1 = \sqrt{-2\ln U_1}\sin(2\pi U_2)$$

Tutorial 1

$$\text{Uniform}(0,1) \rightarrow U_1, U_2$$



$$Z_0, Z_2 \leftarrow N(0,1)$$

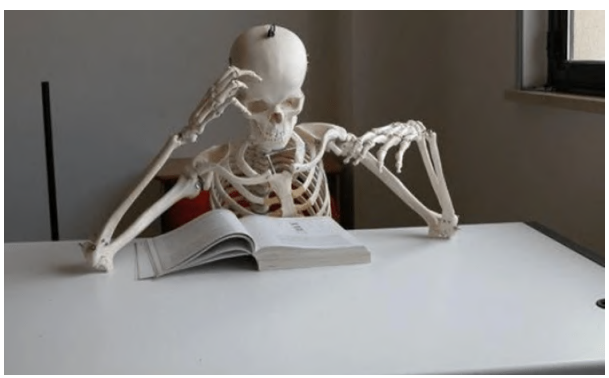


https://tinyurl.com/heidelbergschool

On tutorials

Different people learn differently

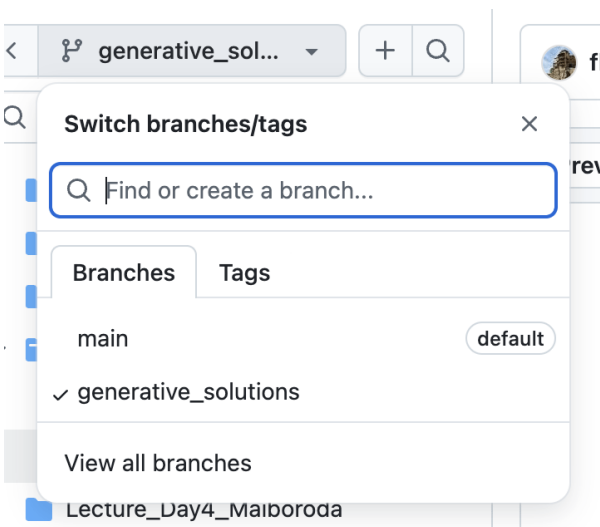
Take the data generator and start from scratch



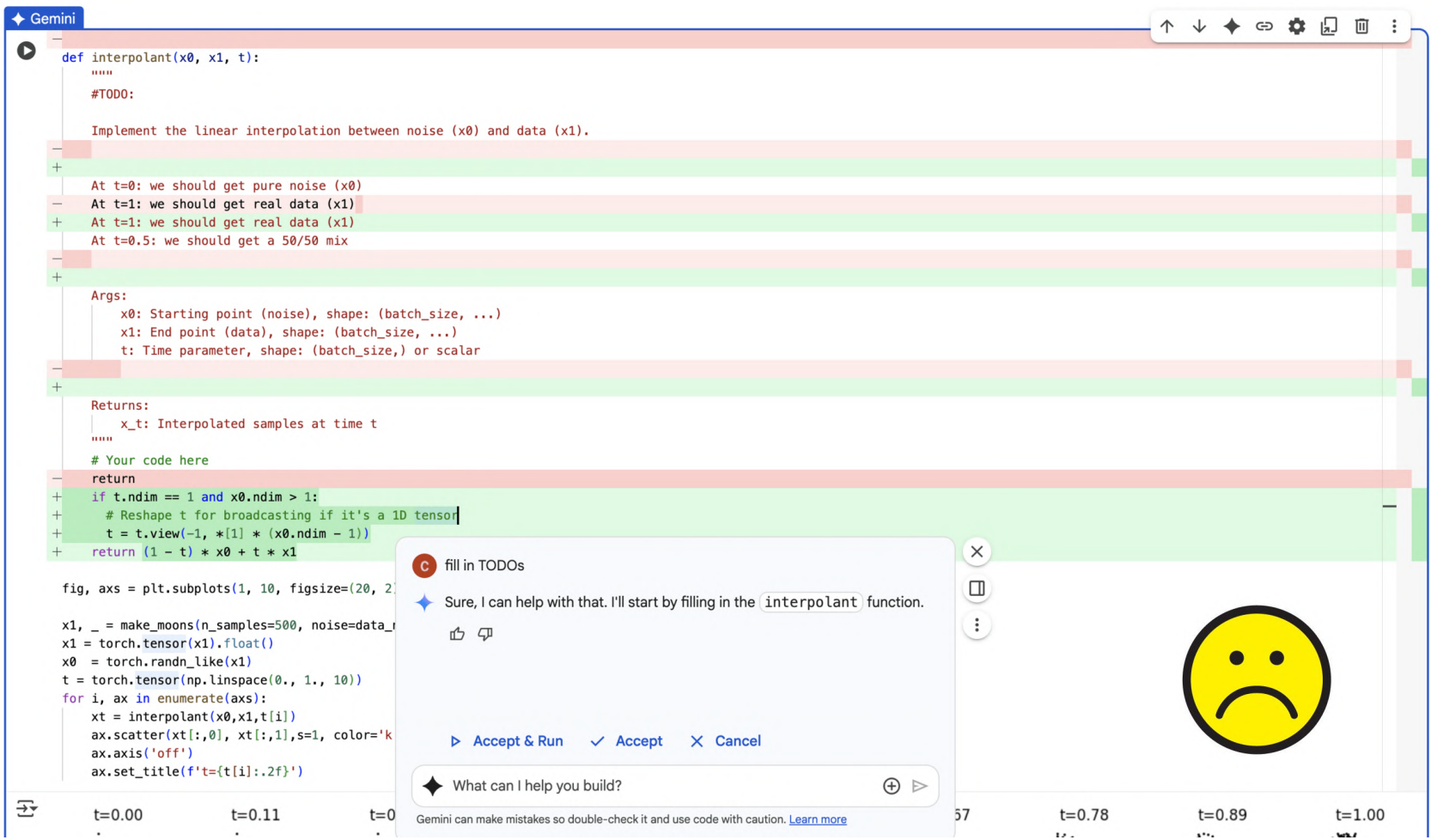
Fill in the gaps

```
In [ ]:
class FlowMatching:
    def __init__(self, velocity_network, device='cuda'):
        self.velocity_net = velocity_network
        self.device = device

    def sample_time(self, batch_size):
        """Sample random time steps between 0 and 1."""
        return torch.rand(batch_size, device=self.device)

    def interpolate(self, x0, x1, t):
        """
        Linear interpolation between noise (x0) and data (x1).
        At t=0: return x0 (noise)
        At t=1: return x1 (data)
        """
        # TODO: fill in the interpolant again

        # Your code here

        return

    def compute_target_velocity(self, x0, x1, t):
        """
        #TODO
        Compute the target velocity field that the neural network should learn.

        Think about this: if we have x_t = (1-t)*x0 + t*x1,
        what is dx_t/dt (the derivative with respect to time)?
        """
        # Your code here
        return # What is dx_t/dt?
```

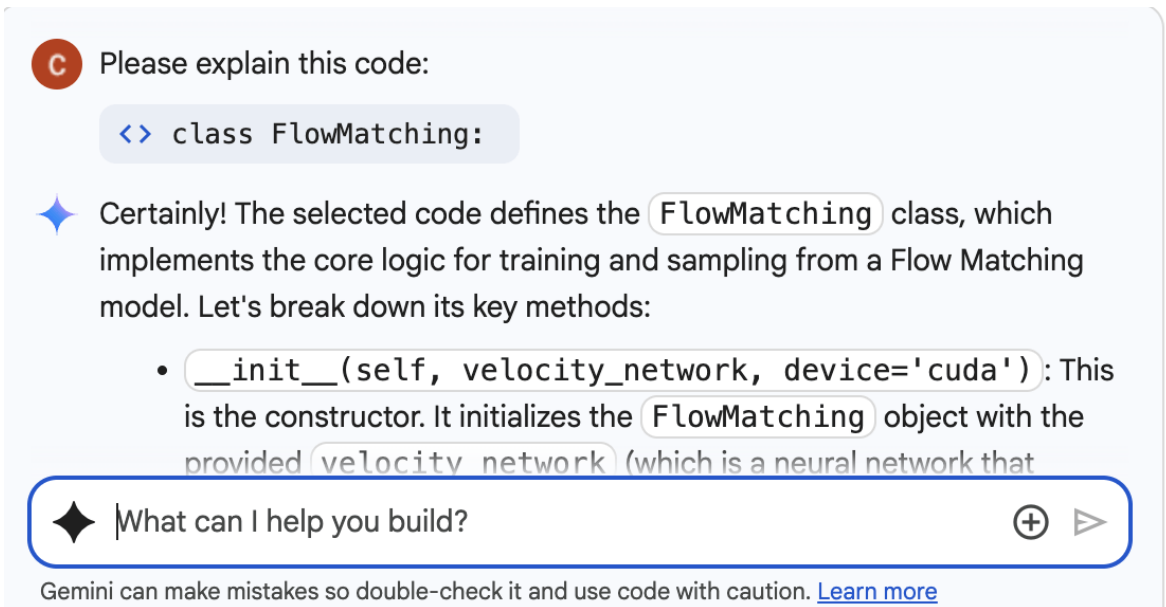
Start from a working solution and play around



On tutorials

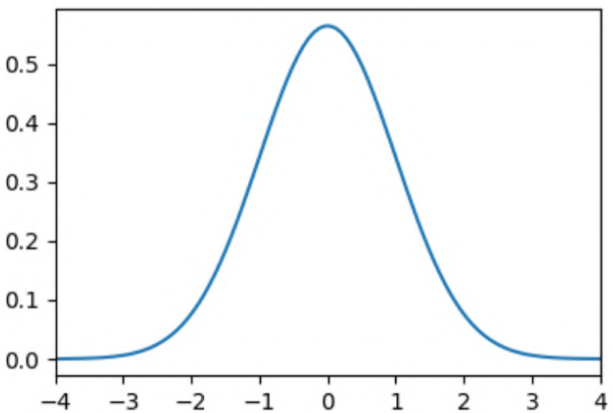


On tutorials



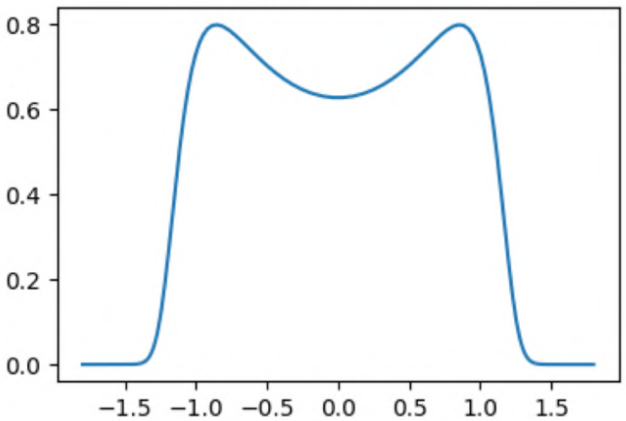
Normalizing flows

$$p_Z(\mathbf{z}) = \mathcal{N}(0, 1)$$



Base distribution

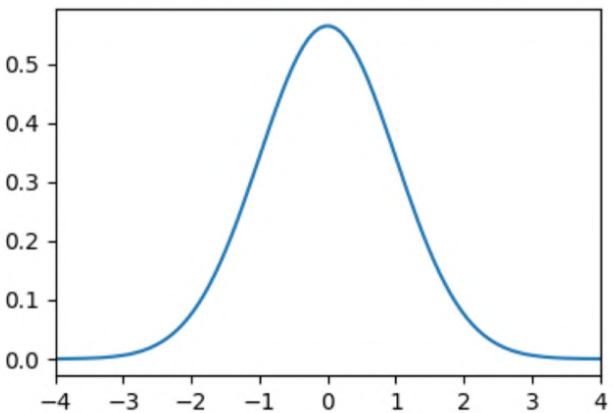
$$p_X(\mathbf{x})$$



Target distribution

Normalizing flows

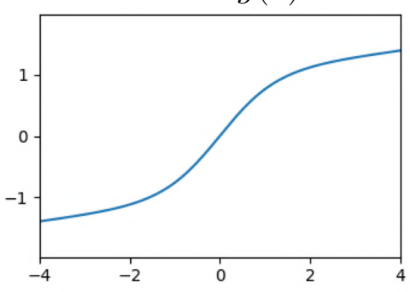
$p_Z(\mathbf{z}) = \mathcal{N}(0, 1)$



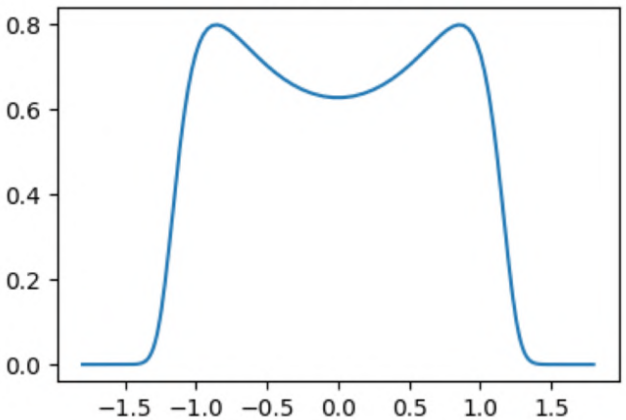
Base distribution

Invertible transformation

$\mathbf{x} = g(\mathbf{z})$



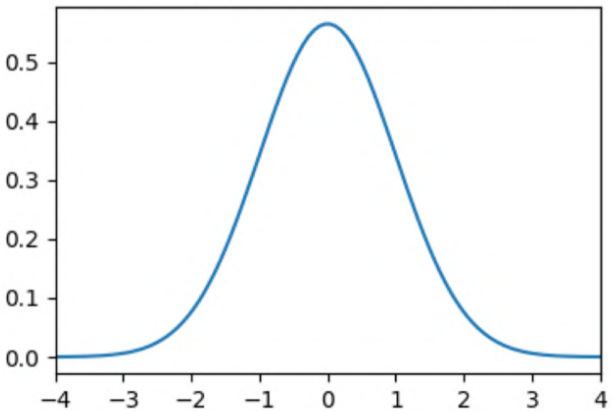
$p_X(\mathbf{x})$



Target distribution

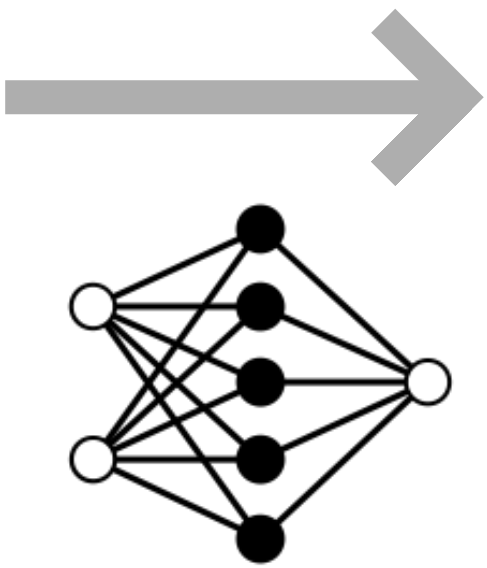
Normalizing flows

$p_Z(\mathbf{z}) = \mathcal{N}(0, 1)$

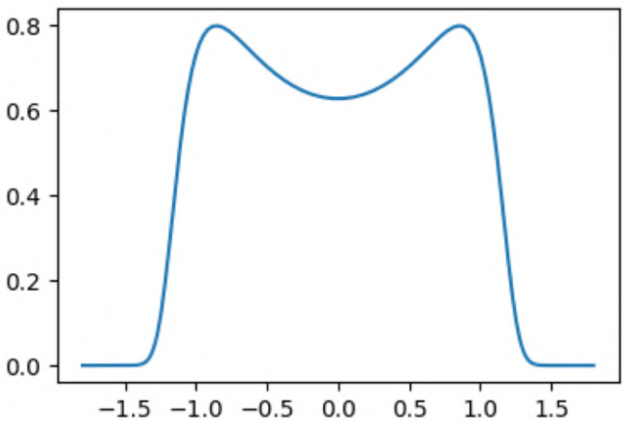


Base distribution

Invertible transformation



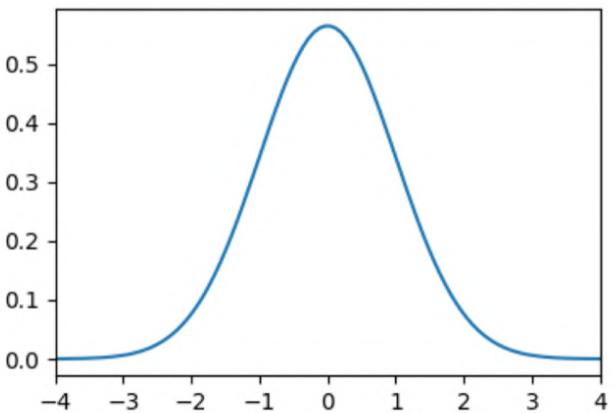
$p_X(\mathbf{x})$



Target distribution

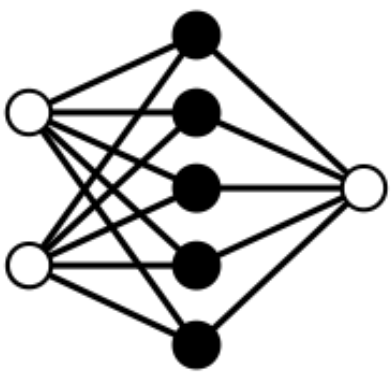
Normalizing flows

$p_Z(\mathbf{z}) = \mathcal{N}(0, 1)$

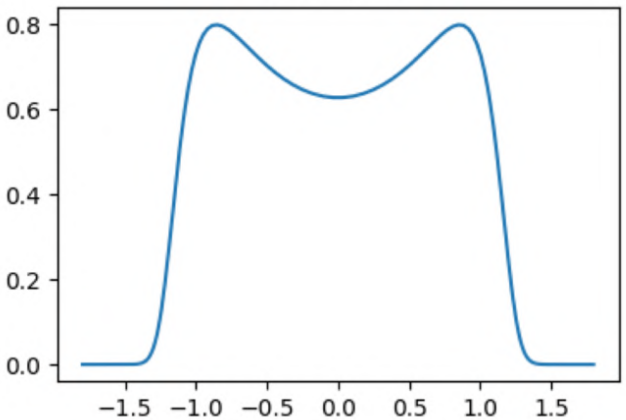


Base distribution

Invertible transformation



$p_X(\mathbf{x})$

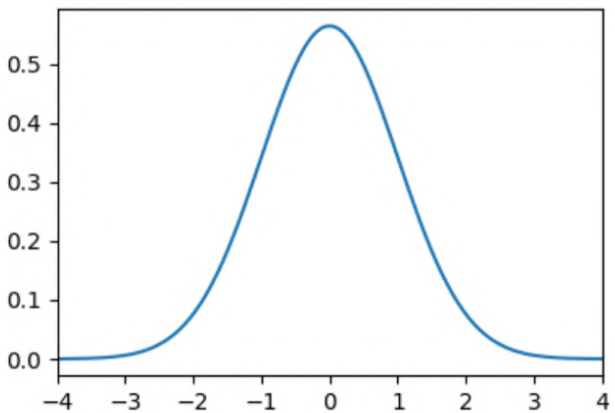


Target distribution

$z \sim p_Z(z)$

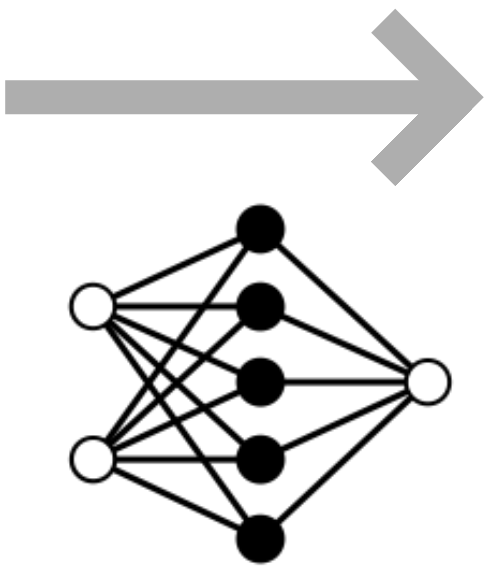
Normalizing flows

$p_Z(\mathbf{z}) = \mathcal{N}(0, 1)$

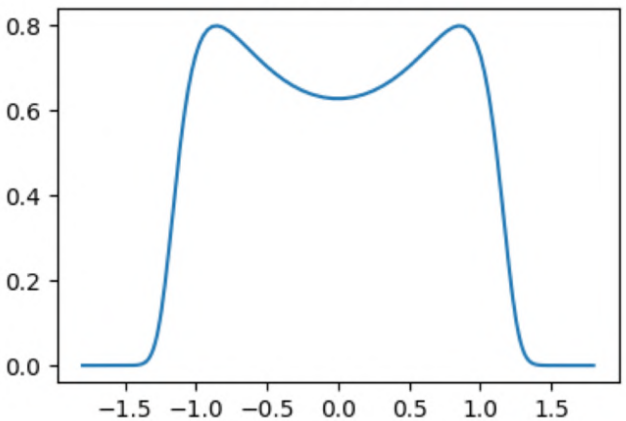


Base distribution

Invertible transformation



$p_X(\mathbf{x})$

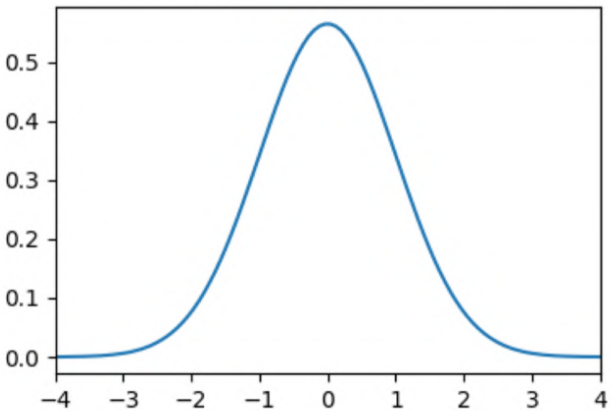


Target distribution

- $z \sim p_Z(z)$
- $p_Z(z)$

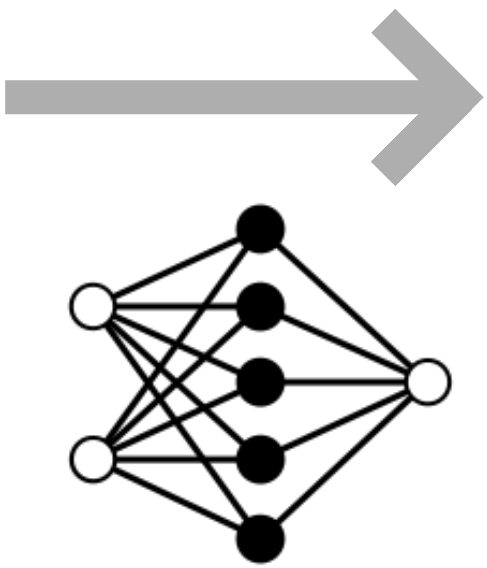
Normalizing flows

$p_Z(\mathbf{z}) = \mathcal{N}(0, 1)$

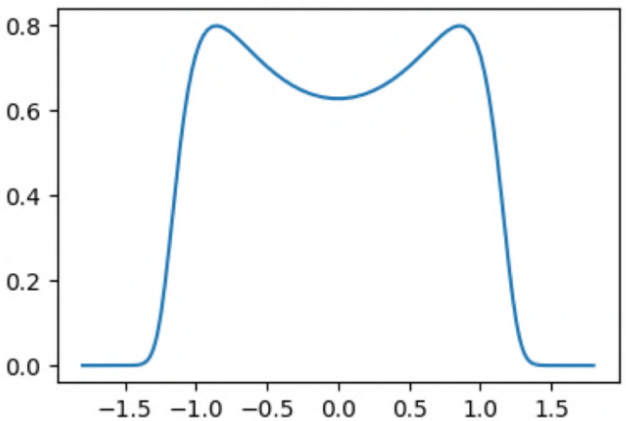


Base distribution

Invertible transformation



$p_X(\mathbf{x})$

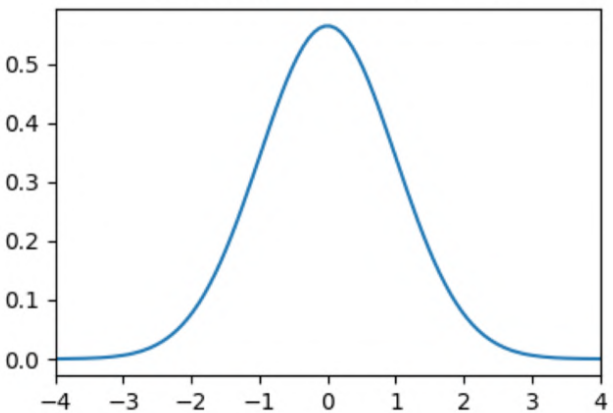


Target distribution

- $z \sim p_Z(z)$
- $p_Z(z)$
- $Z \sim \mathcal{N}(0, 1) \rightarrow g(z) \rightarrow X$

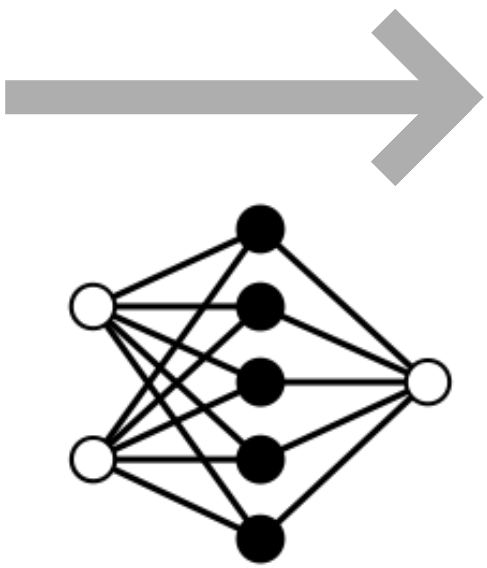
Normalizing flows

$p_Z(\mathbf{z}) = \mathcal{N}(0, 1)$

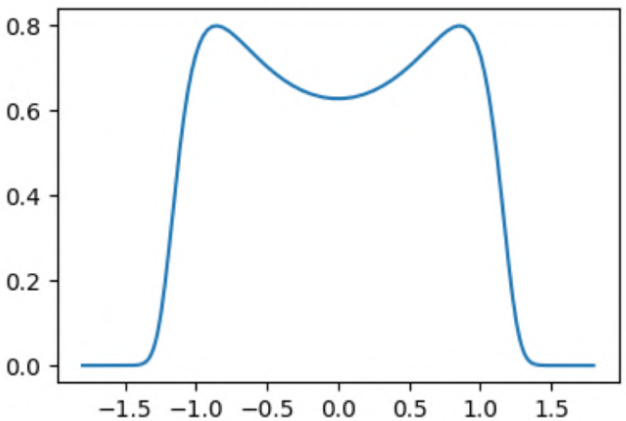


Base distribution

Invertible transformation



$p_X(\mathbf{x})$



Target distribution

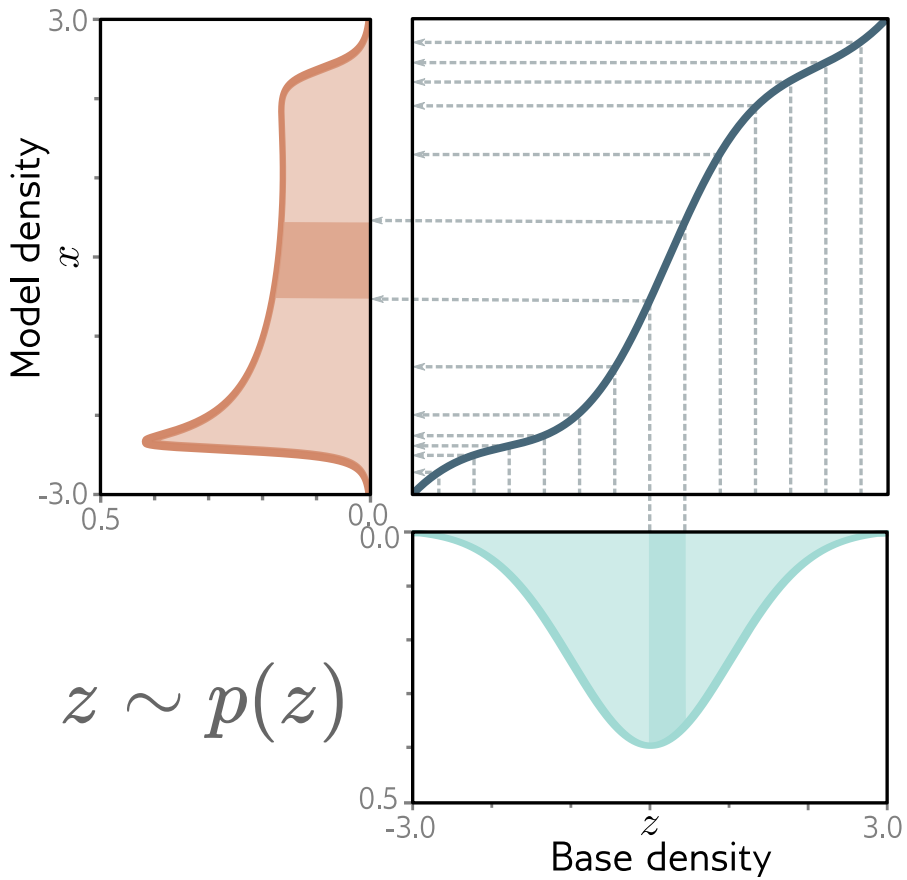
- $z \sim p_Z(z)$
- $p_Z(z)$
- $Z \sim \mathcal{N}(0,1) \rightarrow g(z) \rightarrow X$
- $p_X(x) = p_Z(z) \left| \frac{dz}{dx} \right|$

Normalizing flows

Bijective

$$x = f(z)$$

$$x \sim p(x)$$



$$z \sim p(z)$$

[Image Credit: "Understanding Deep Learning" Simon J.D. Prince]

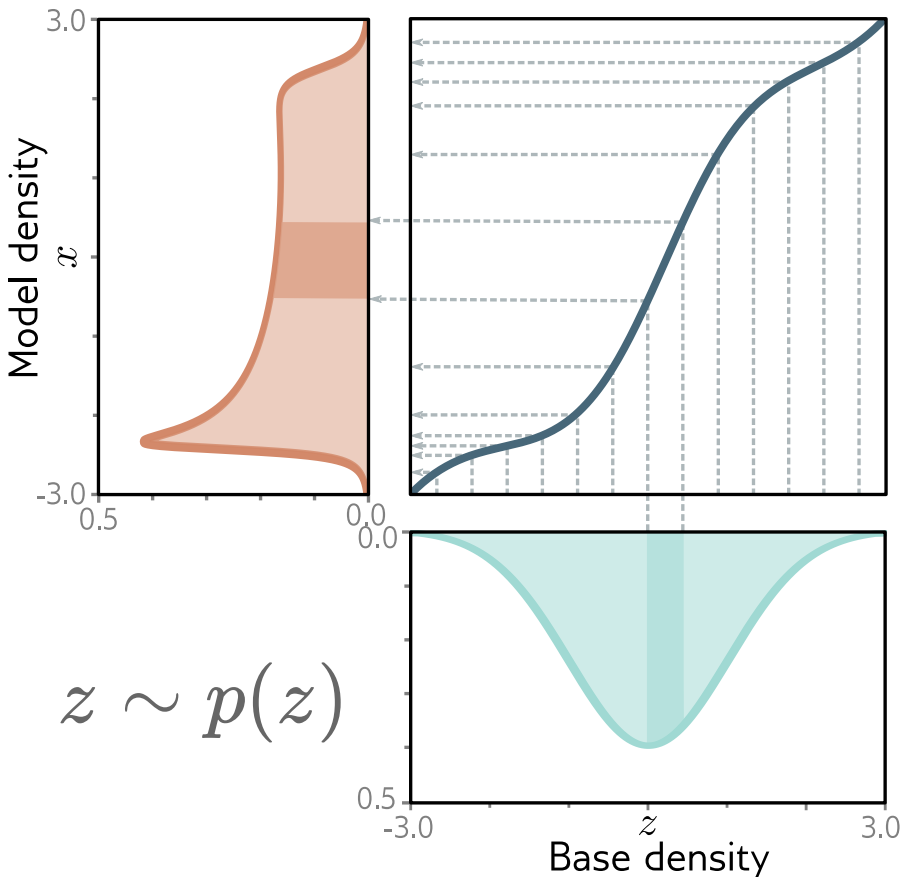
Normalizing flows

Bijective

$$x = f(z)$$

Sample

$$x \sim p(x)$$



$$z \sim p(z)$$

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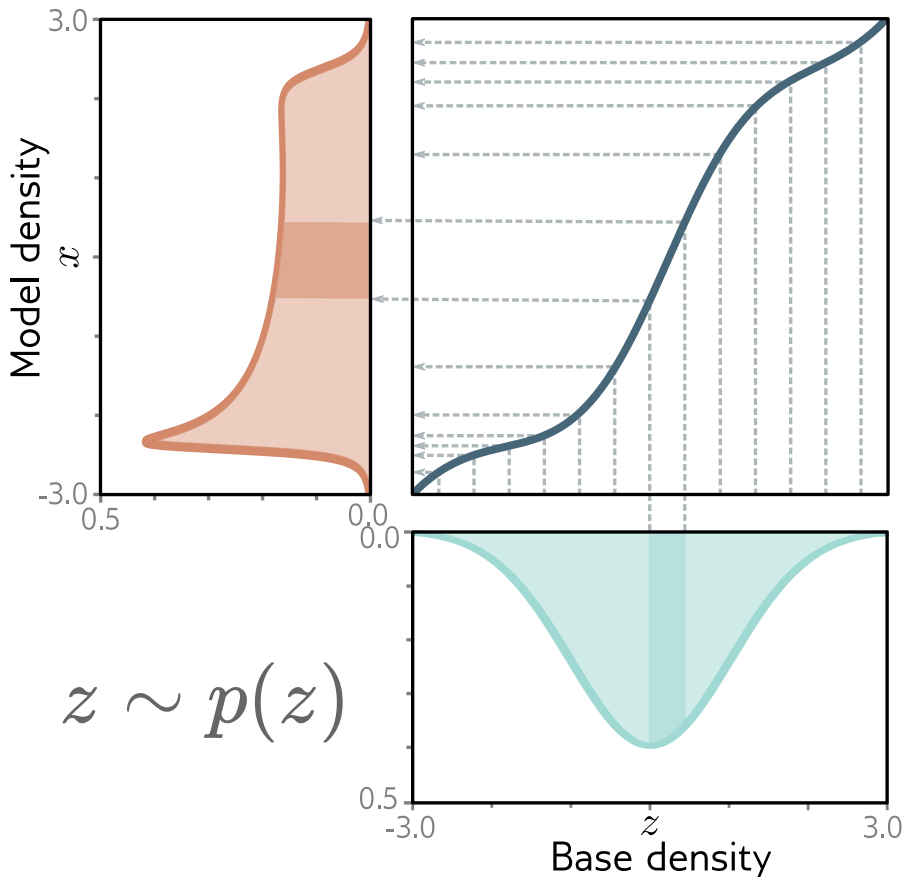
Normalizing flows

Bijective

$$x = f(z)$$

Sample

$$x \sim p(x)$$



$$z \sim p(z)$$

[Image Credit: "Understanding Deep Learning" Simon J.D. Prince]

Probability mass conserved locally

$$p(x) = p(z = f^{-1}(x)) \left| \det J_{f^{-1}}(x) \right|$$

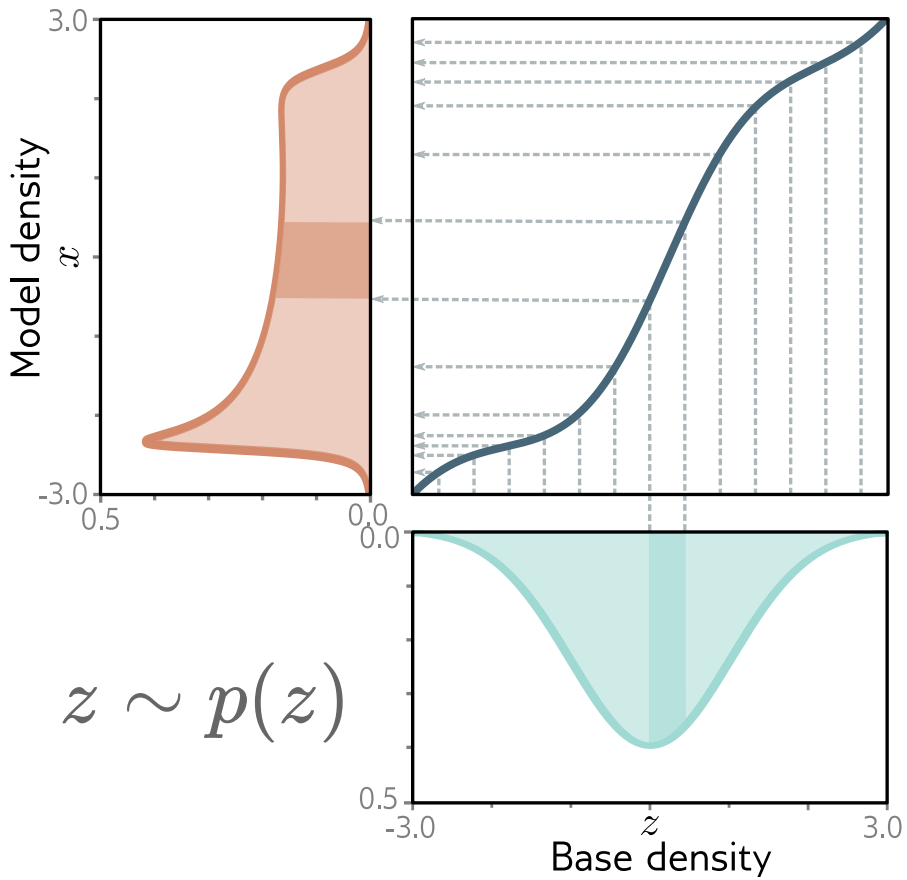
Normalizing flows

Bijective

$$x = f(z)$$

Sample

$$x \sim p(x)$$



$$z \sim p(z)$$

[Image Credit: "Understanding Deep Learning" Simon J.D. Prince]

Probability mass conserved locally

$$p(x) = p(z = f^{-1}(x)) \left| \det J_{f^{-1}}(x) \right|$$

Evaluate probabilities

$$z_0 \sim p(z) \qquad z_k = f_k(z_{k-1})$$

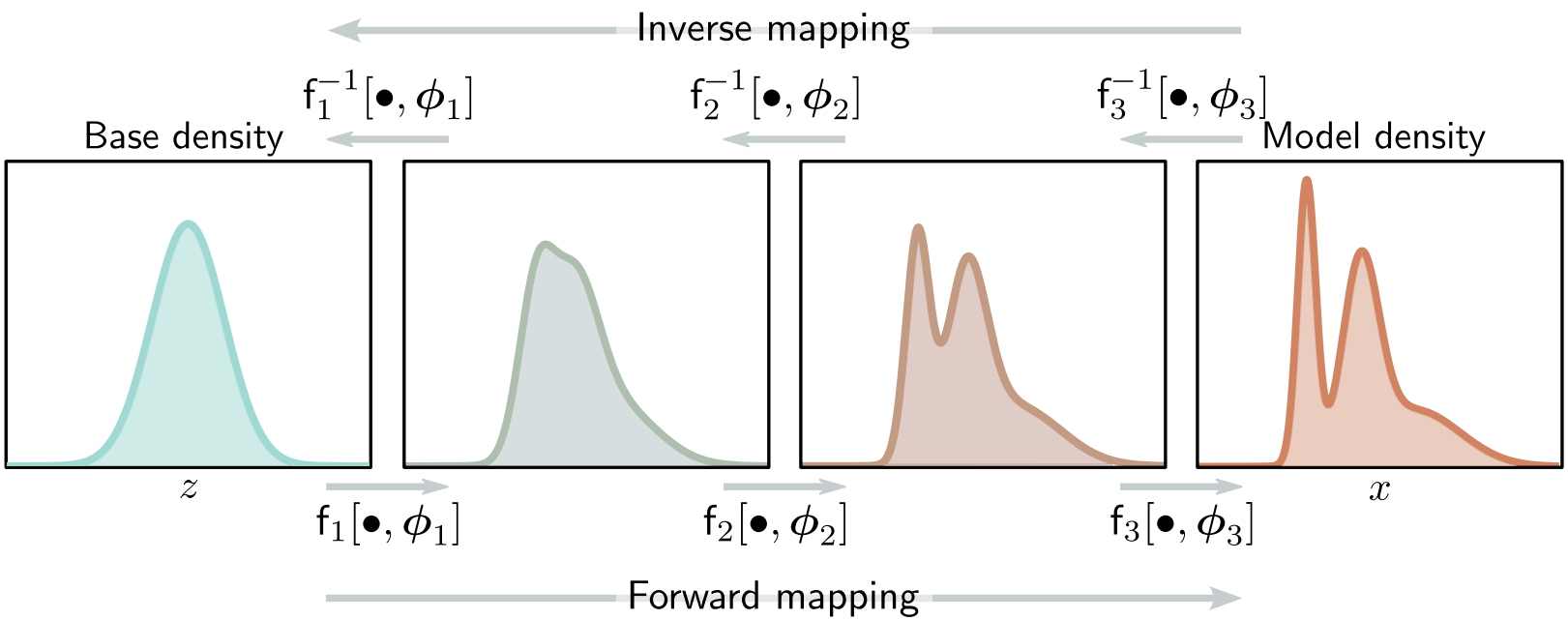
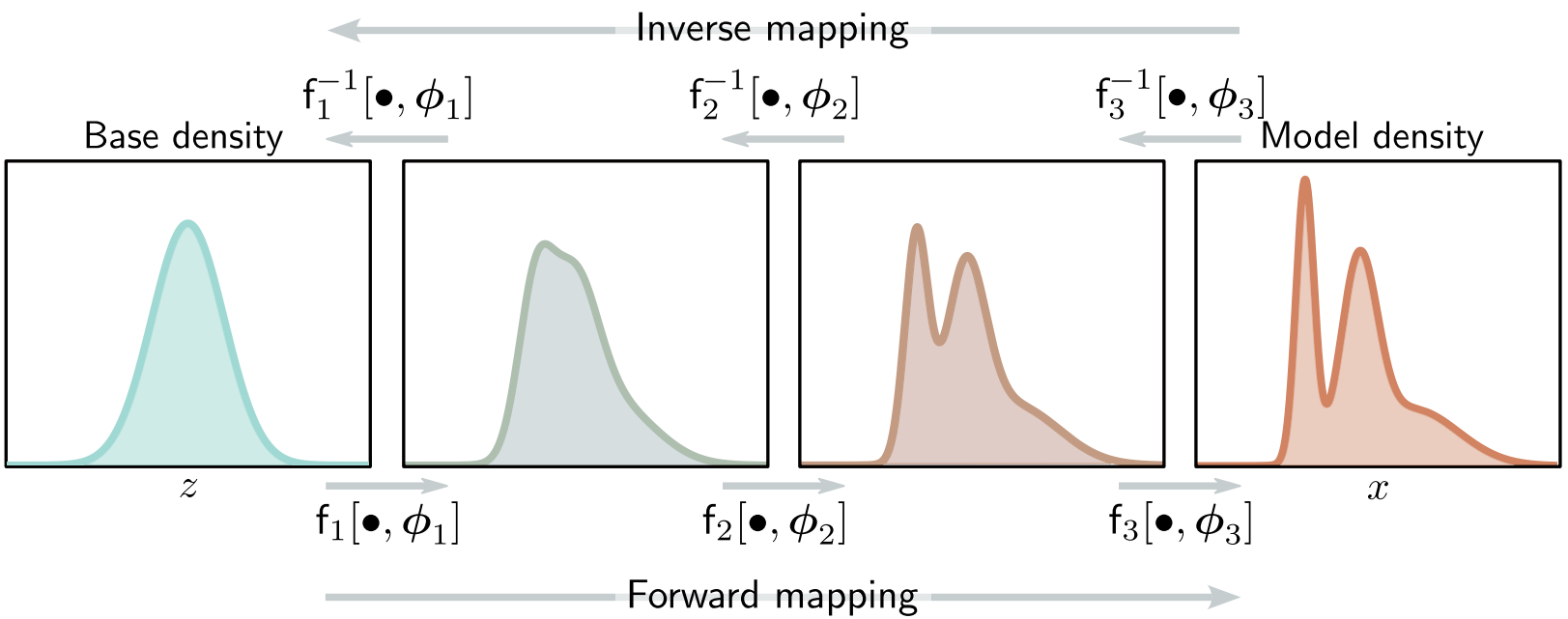


Image Credit: "Understanding Deep Learning" Simon J.D. Prince

$$z_0 \sim p(z) \qquad z_k = f_k(z_{k-1})$$

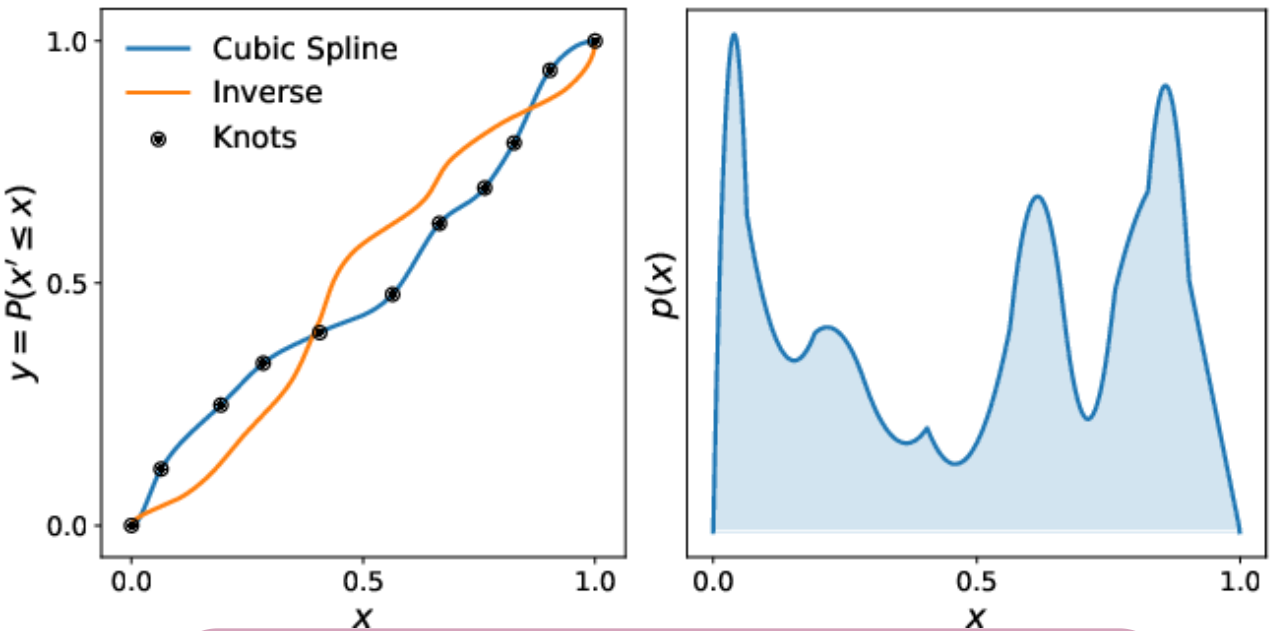


$$\log p(x) = \log p(z_0) - \sum_{k=1}^{K} \log \left| \det J_{f_k}(z_{k-1}) \right|$$

Image Credit: "Understanding Deep Learning" Simon J.D. Prince

Invertible functions aren't that common!

Splines



Issues NFs: **Lack of flexibility**

- Invertible functions
- Tractable Jacobians

Masked Autoregressive Flows

$$p(x) = \prod_i p(x_i \mid x_{1:i-1})$$

Masked Autoregressive Flows

$$p(x) = \prod_i p(x_i \mid x_{1:i-1})$$

$$p(x_i \mid x_{1:i-1}) = \mathcal{N}(x_i \mid \mu_i, (\exp \alpha_i)^2)$$

Masked Autoregressive Flows

$$p(x) = \prod_i p(x_i \mid x_{1:i-1})$$

Neural Network

$$\mu_i, \alpha_i = f_{\phi_i}(x_{1:i-1})$$

$$p(x_i \mid x_{1:i-1}) = \mathcal{N}(x_i \mid \mu_i, (\exp \alpha_i)^2)$$

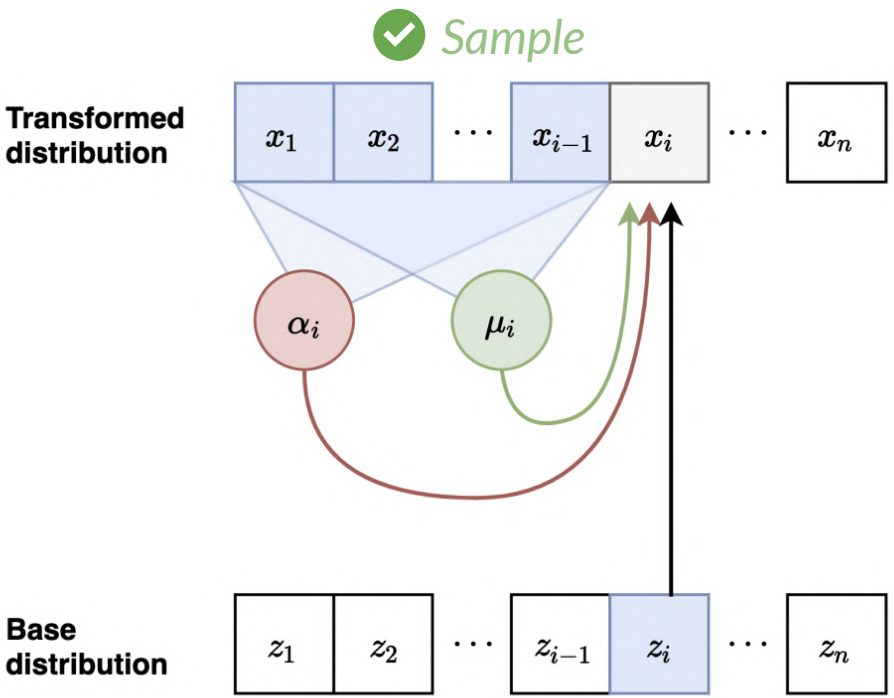
Masked Autoregressive Flows

$$p(x) = \prod_i p(x_i \mid x_{1:i-1})$$

Neural Network

$$\mu_i, \alpha_i = f_{\phi_i}(x_{1:i-1})$$

$$p(x_i \mid x_{1:i-1}) = \mathcal{N}(x_i \mid \mu_i, (\exp \alpha_i)^2)$$



$$x_i = z_i \exp(\alpha_i) + \mu_i$$

Masked Autoregressive Flows

$$p(x) = \prod_i p(x_i \mid x_{1:i-1})$$

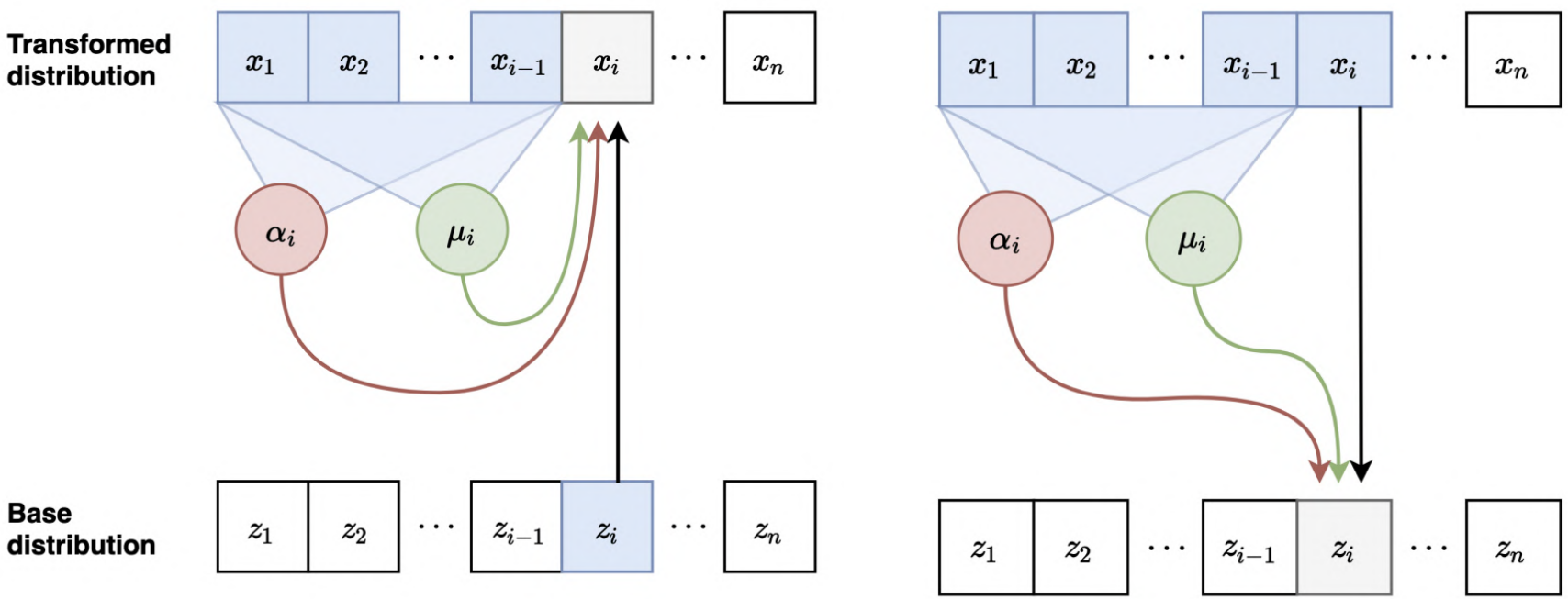
Neural Network

$$\mu_i, \alpha_i = f_{\phi_i}(x_{1:i-1})$$

$$p(x_i \mid x_{1:i-1}) = \mathcal{N}(x_i \mid \mu_i, (\exp \alpha_i)^2)$$

Sample

Evaluate probabilities

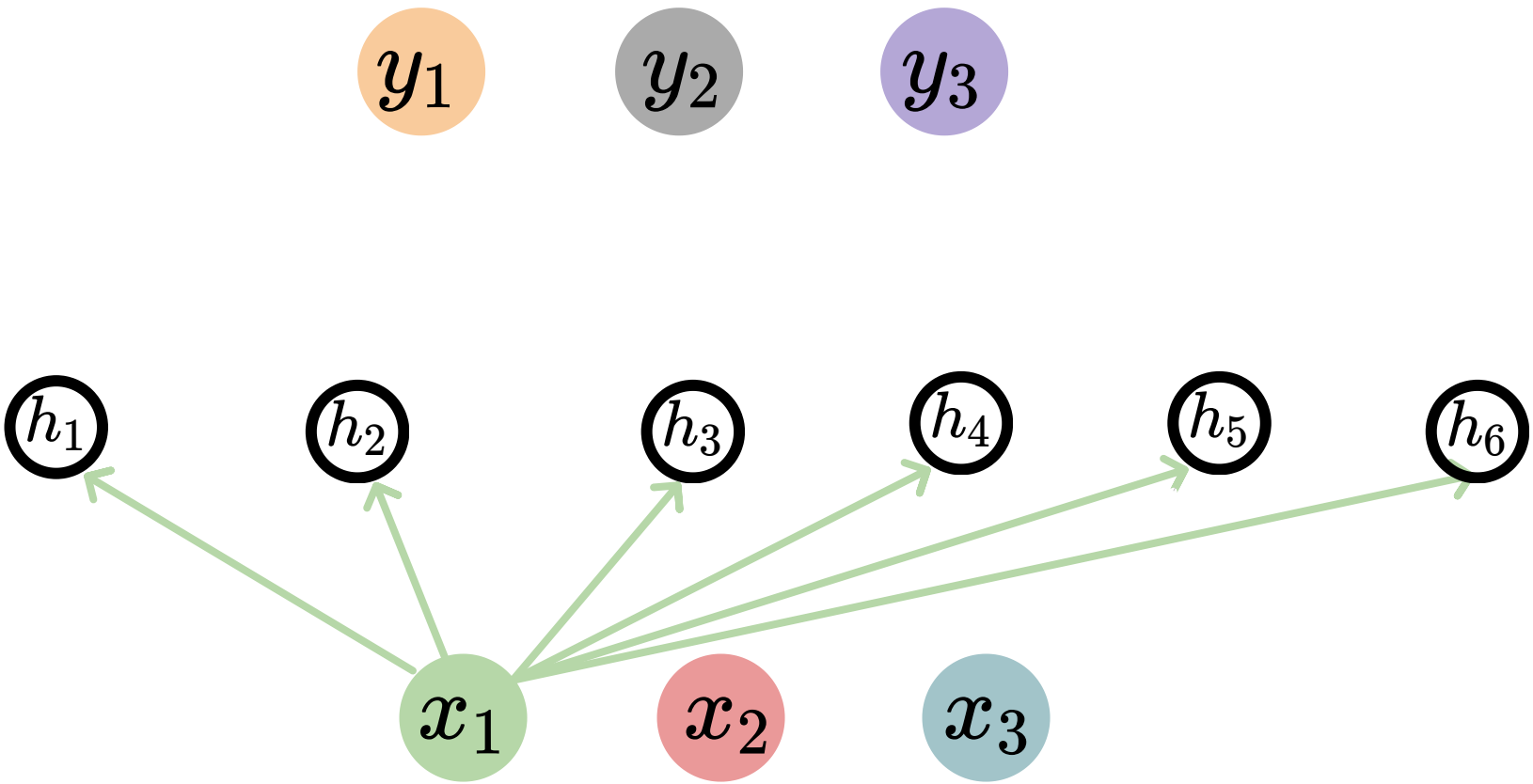


$$x_i = z_i \exp(\alpha_i) + \mu_i$$

$$z_i = (x_i - \mu_i) \exp(-\alpha_i)$$

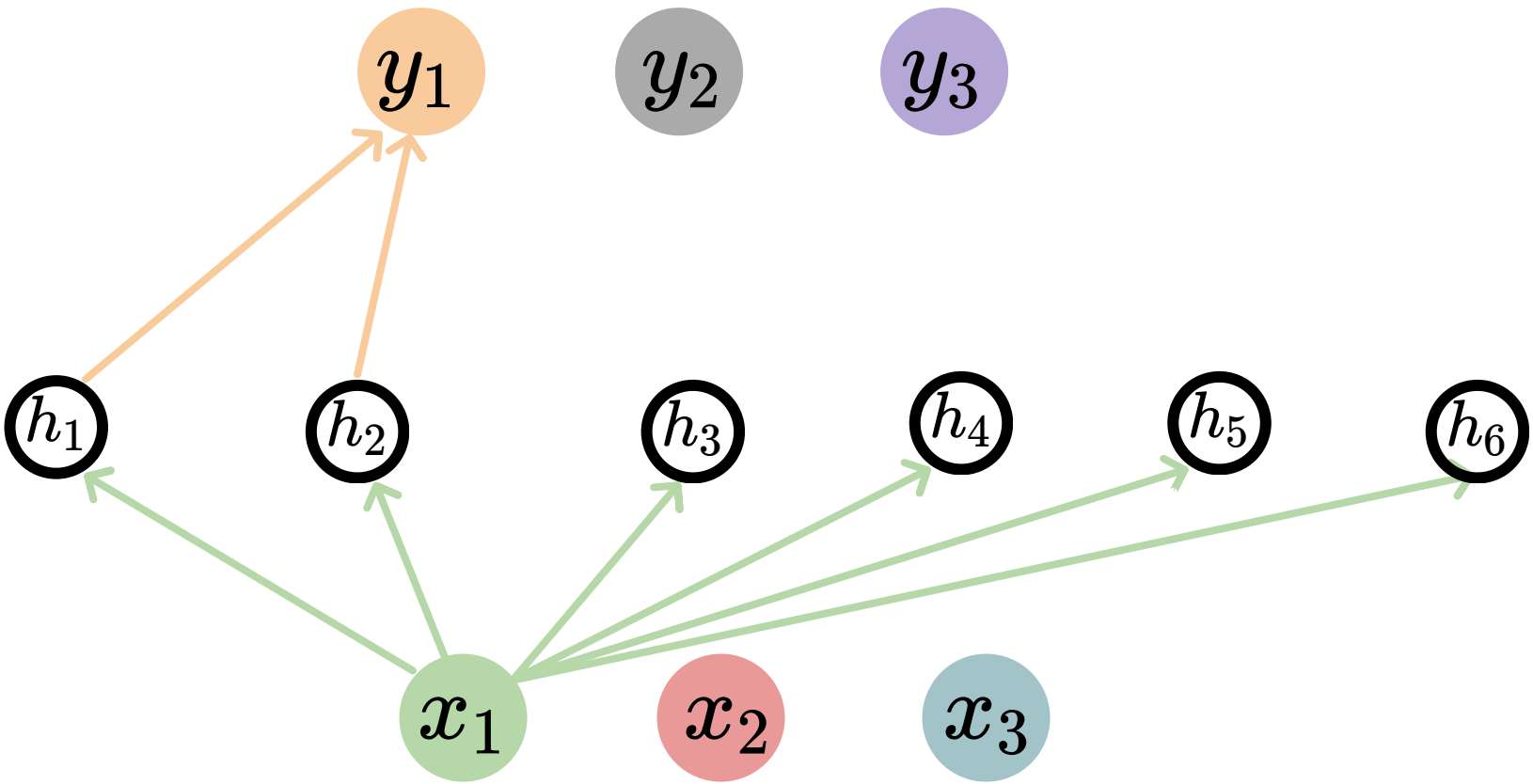
Masked MLP

$$y_i = \mu_i, \alpha_i = f_{\phi_i}(x_{1:i-1})$$



Masked MLP

$$y_i = \mu_i, \alpha_i = f_{\phi_i}(x_{1:i-1})$$



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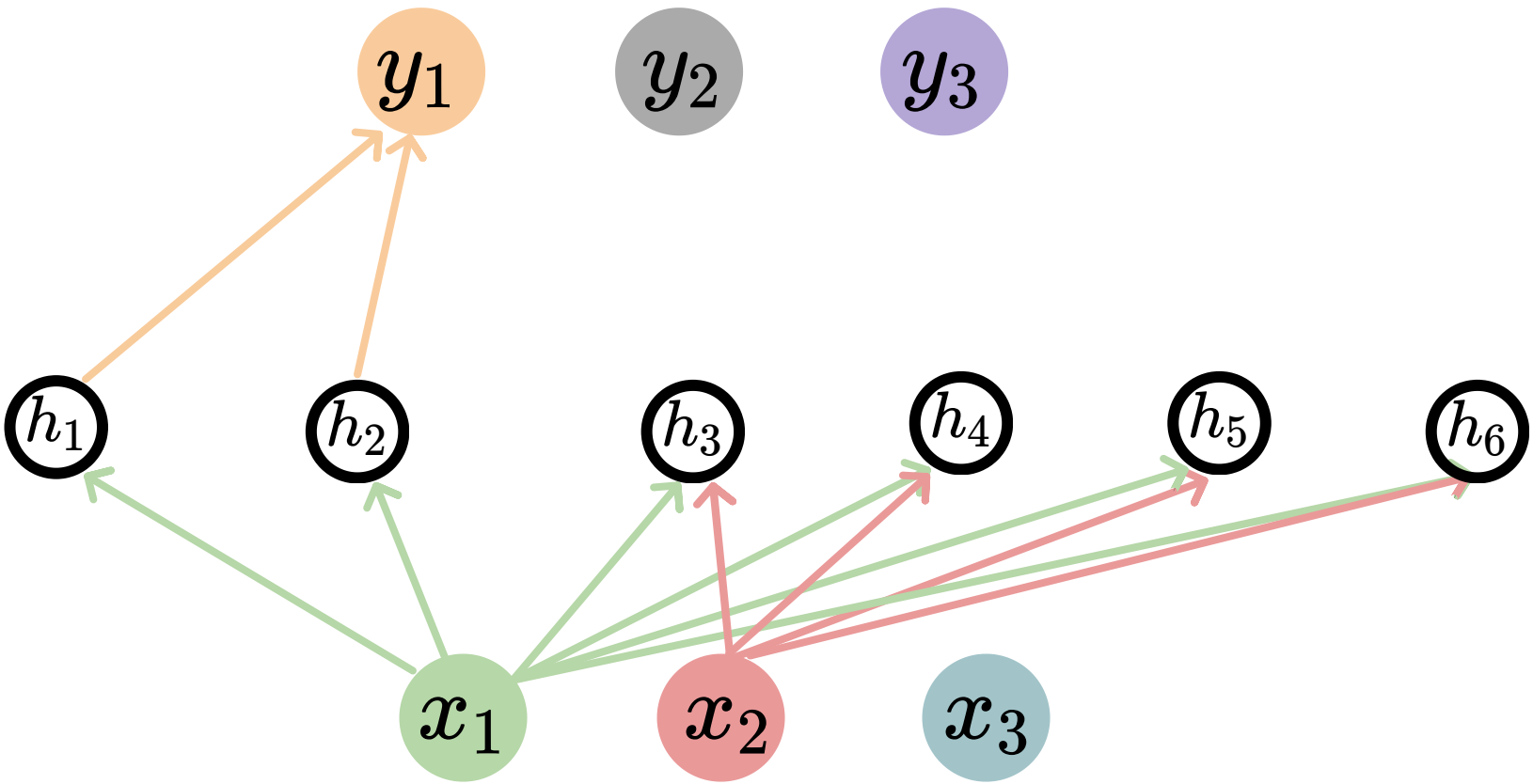
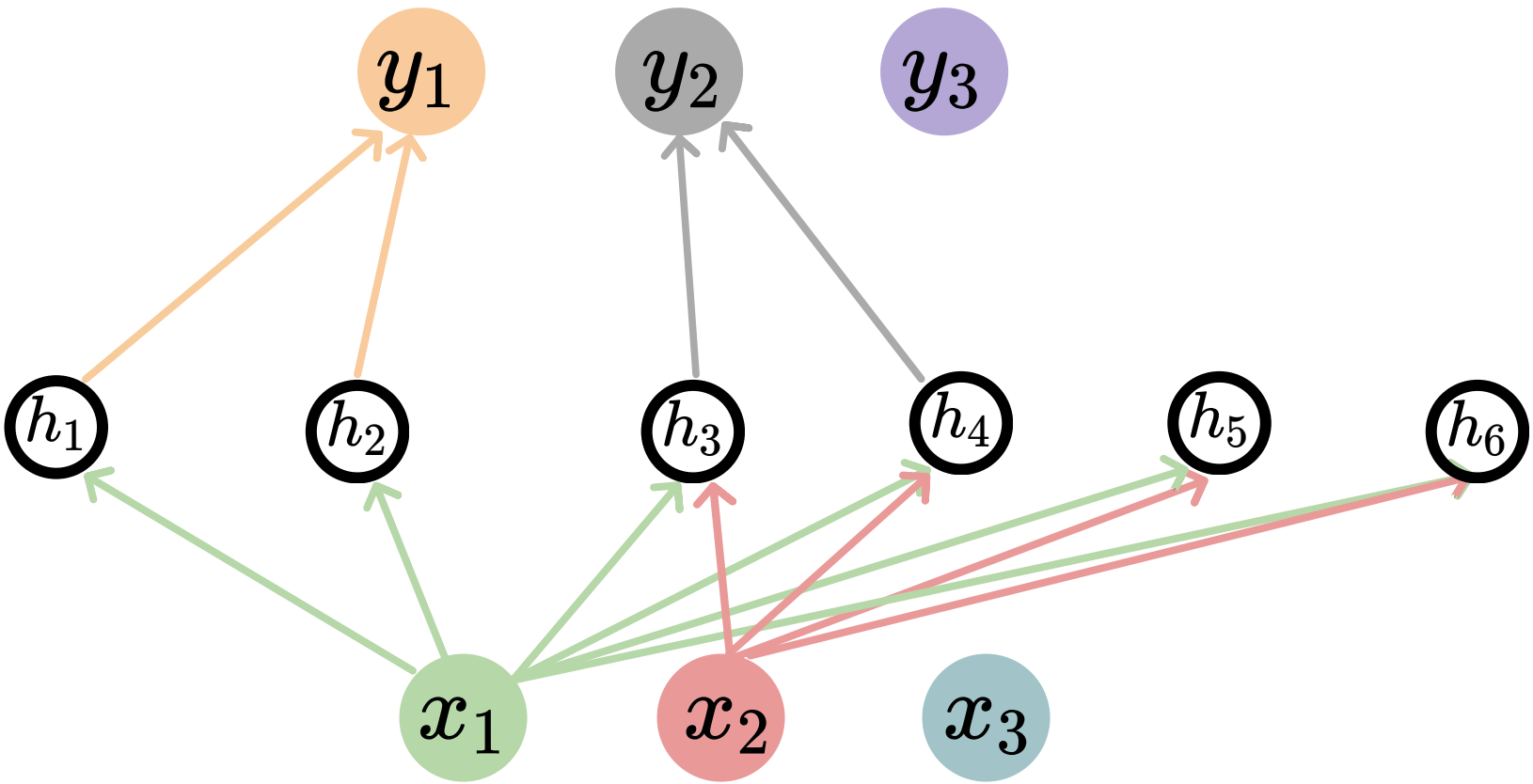


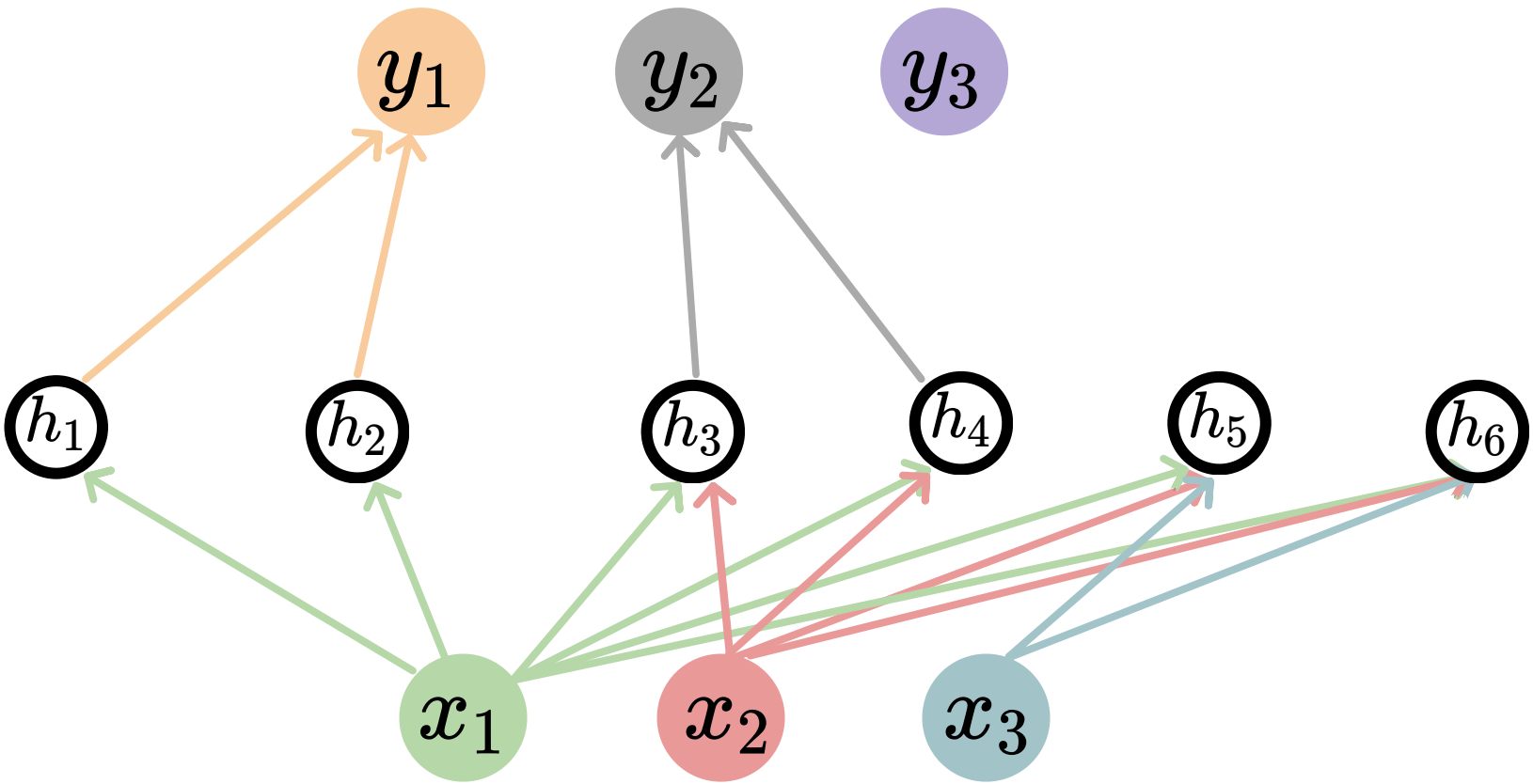
Masked MLP

$$y_i = \mu_i, \alpha_i = f_{\phi_i}(x_{1:i-1})$$



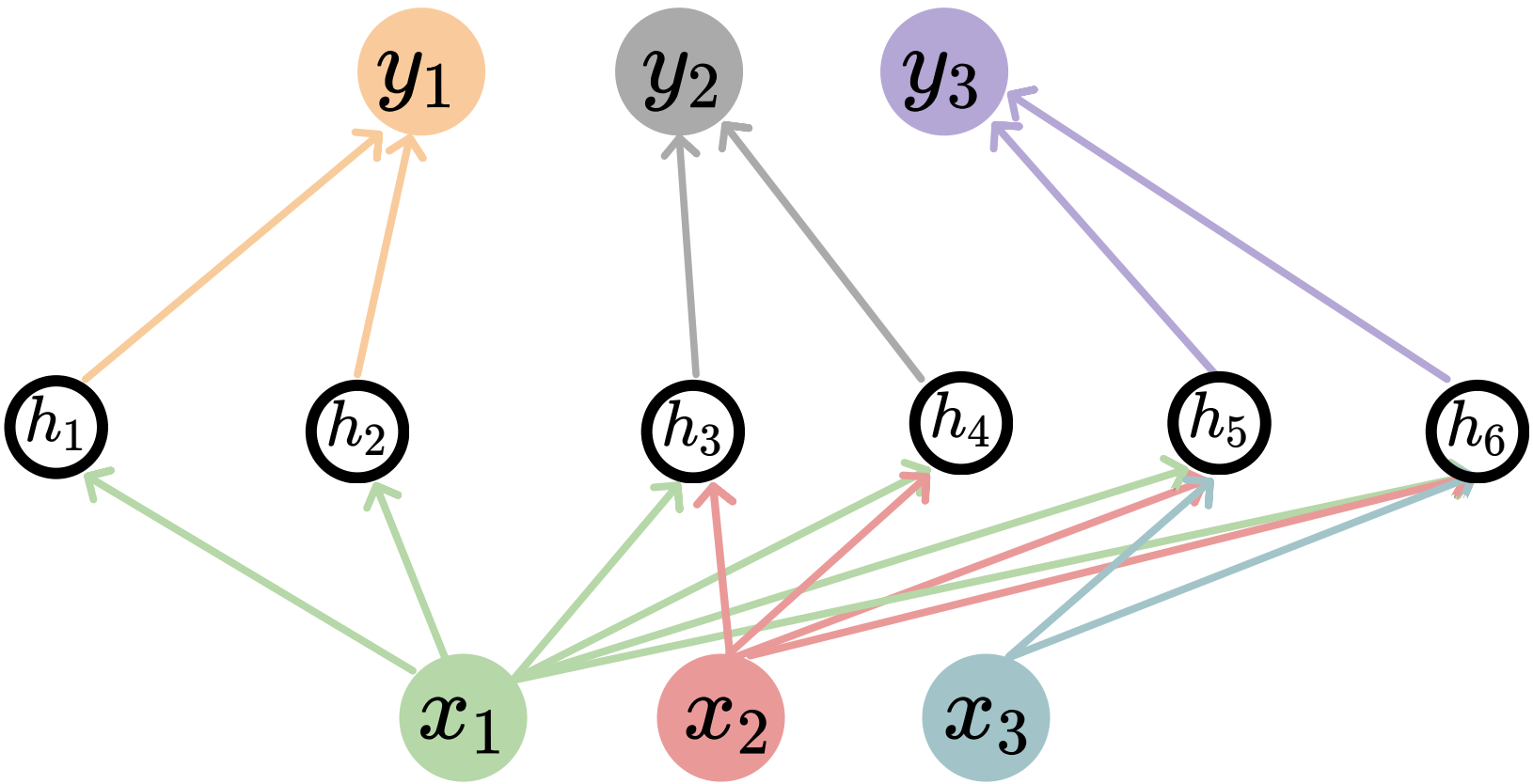
Masked MLP

$$y_i = \mu_i, \alpha_i = f_{\phi_i}(x_{1:i-1})$$



Masked MLP

$$y_i = \mu_i, \alpha_i = f_{\phi_i}(x_{1:i-1})$$



$$\log p(x) = \log p(z_0) - \sum_{k=1}^{K} \log \left| \det J_{f_k}(z_{k-1}) \right|$$

Computational Complexity

$$\mathcal{O}(N^3)$$

$$\log p(x) = \log p(z_0) - \sum_{k=1}^{K} \log \left| \det J_{f_k}(z_{k-1}) \right|$$

Computational Complexity

$$\mathcal{O}(N^3)$$

Autoregressive = Triangular matrix

$$\frac{\partial u_k^{(d)}}{\partial u_{k-1}^{(>d)}} == 0 \implies \begin{pmatrix} \frac{\partial u_k^{(1)}}{\partial u_{k-1}^{(1)}} & 0 & \cdots & 0 \\ \frac{\partial u_k^{(2)}}{\partial u_{k-1}^{(1)}} & \frac{\partial u_k^{(2)}}{\partial u_{k-1}^{(2)}} & \cdots & 0 \\ \vdots & \cdots & \cdots & \vdots \\ \frac{\partial u_k^{(D)}}{\partial u_{k-1}^{(1)}} & \cdots & \cdots & \frac{\partial u_k^{(D)}}{\partial u_{k-1}^{(D)}} \end{pmatrix}$$

$$\log p(x) = \log p(z_0) - \sum_{k=1}^{K} \log \left| \det J_{f_k}(z_{k-1}) \right|$$

Computational Complexity

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$\mathcal{O}(N)$

$$\frac{\partial u_k^{(d)}}{\partial u_{k-1}^{(>d)}} == 0 \implies \begin{pmatrix} \frac{\partial u_k^{(1)}}{\partial u_{k-1}^{(1)}} & 0 & \cdots & 0 \\ \frac{\partial u_k^{(2)}}{\partial u_{k-1}^{(1)}} & \frac{\partial u_k^{(2)}}{\partial u_{k-1}^{(2)}} & \cdots & 0 \\ \vdots & \cdots & \cdots & \vdots \\ \frac{\partial u_k^{(D)}}{\partial u_{k-1}^{(1)}} & \cdots & \cdots & \frac{\partial u_k^{(D)}}{\partial u_{k-1}^{(D)}} \end{pmatrix}$$

Simulation-based Inference

Parameters

θ

Predict

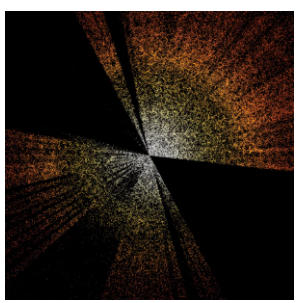
Forward Model

Observable

x

$\Omega_m, w_0, w_a, f_{\rm NL} \cdots$

Dark matter | Dark energy | Inflation



Simulation-based Inference

Parameters

$p(\theta|x)$

Predict

Forward Model

Inverse mapping

Infer

Observable

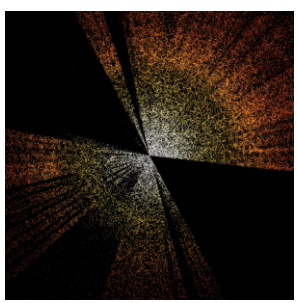
x

$\Omega_m, w_0, w_a, f_{\rm NL} \cdots$

Dark matter

Dark energy

Inflation



Simulation-based Inference

Parameters

$p(\theta|x)$

Normalizing flow

Predict

Forward Model

Inverse mapping

Infer

Observable

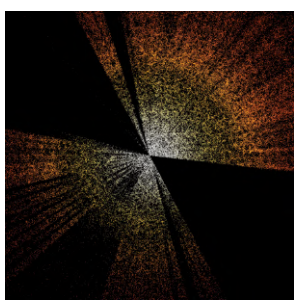
x

$\Omega_m, w_0, w_a, f_{\mathrm{NL}} \cdots$

Dark matter

Dark energy

Inflation



In continuous time

$$\frac{dx_t}{dt} = v_t^{\phi}(x_t)$$

[Image Credit: "Understanding Deep Learning" Simon J.D. Prince]

In continuous time

$$\frac{dx_t}{dt} = v_t^{\phi}(x_t)$$

$$x_1 = x_0 + \int_0^1 v_t^{\phi}(x_t)dt$$

$$x_0 = x_1 + \int_1^0 v_t^{\phi}(x_t)dt$$

[Image Credit: "Understanding Deep Learning" Simon J.D. Prince]

In continuous time

$$\frac{dx_t}{dt} = v_t^{\phi}(x_t)$$

$$x_1 = x_0 + \int_0^1 v_t^{\phi}(x_t)dt$$

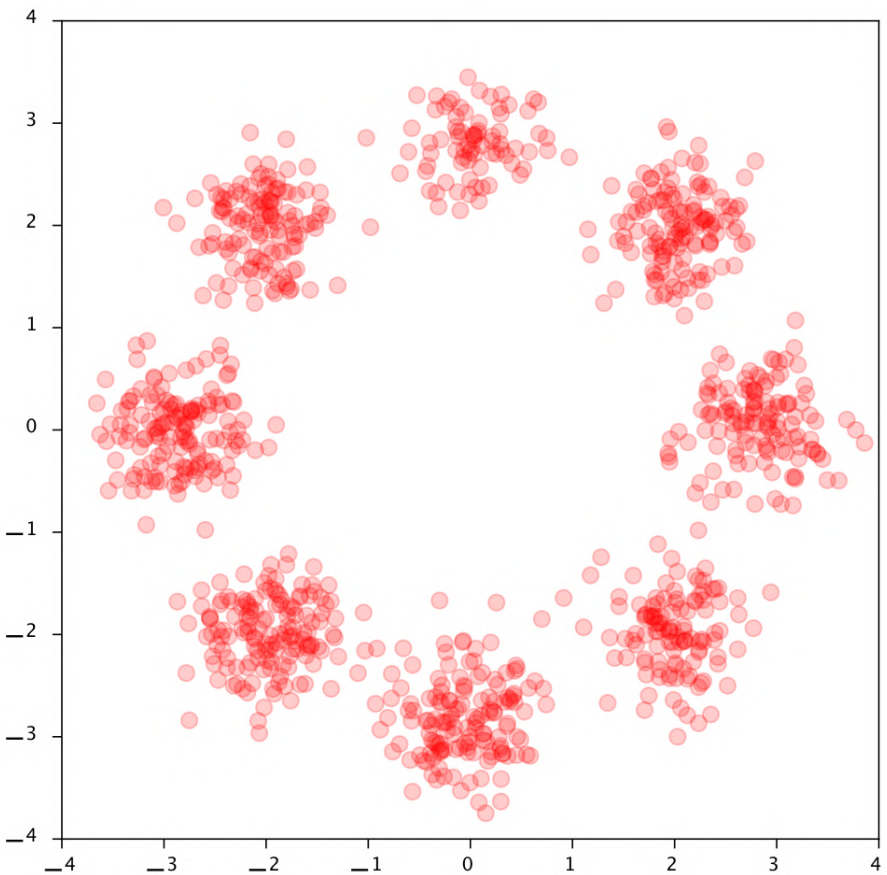
$$x_0 = x_1 + \int_1^0 v_t^{\phi}(x_t)dt$$

$$\frac{dp(x_t)}{dt} = -\nabla\left(v_t^{\phi}(x_t)p(x_t)\right)$$

Continuity Equation

[Image Credit: "Understanding Deep Learning" Simon J.D. Prince]

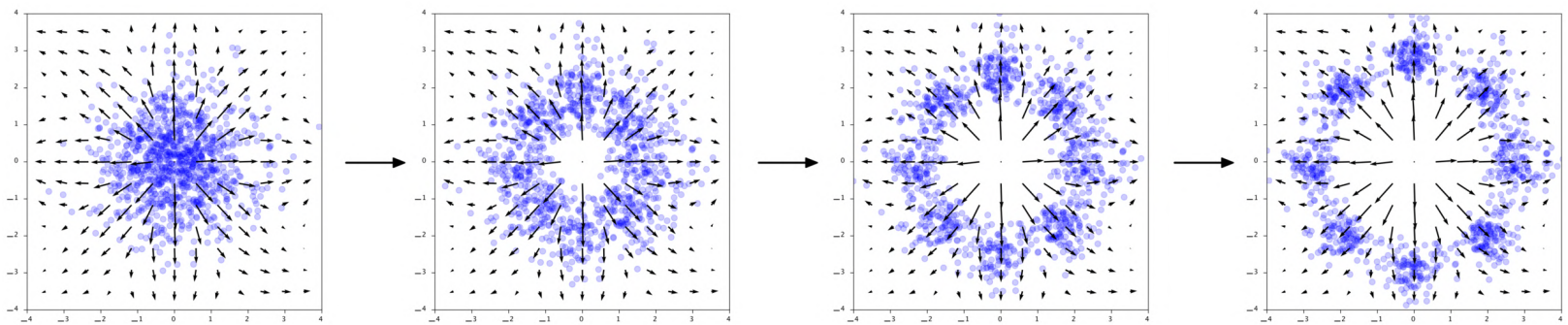
$$x_1 = x_0 + \int_0^1 v_\theta(x(t), t)dt$$



Chen et al. (2018), Grathwohl et al. (2018)

$$x_1 = x_0 + \int_0^1 v_\theta(x(t), t)dt$$

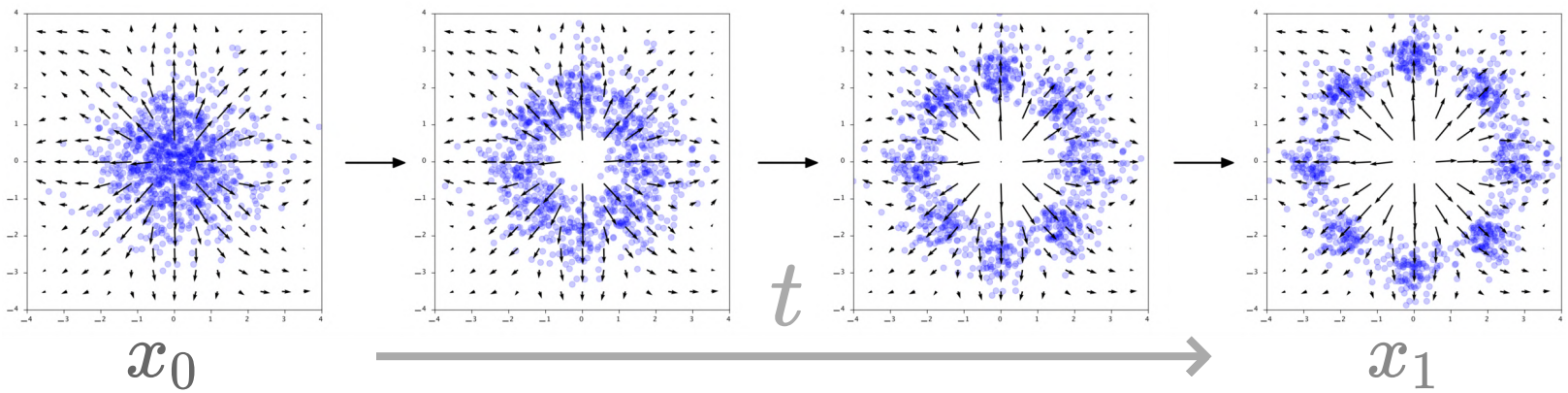
Generate



Chen et al. (2018), Grathwohl et al. (2018)

$$x_1 = x_0 + \int_0^1 v_\theta(x(t), t)dt$$

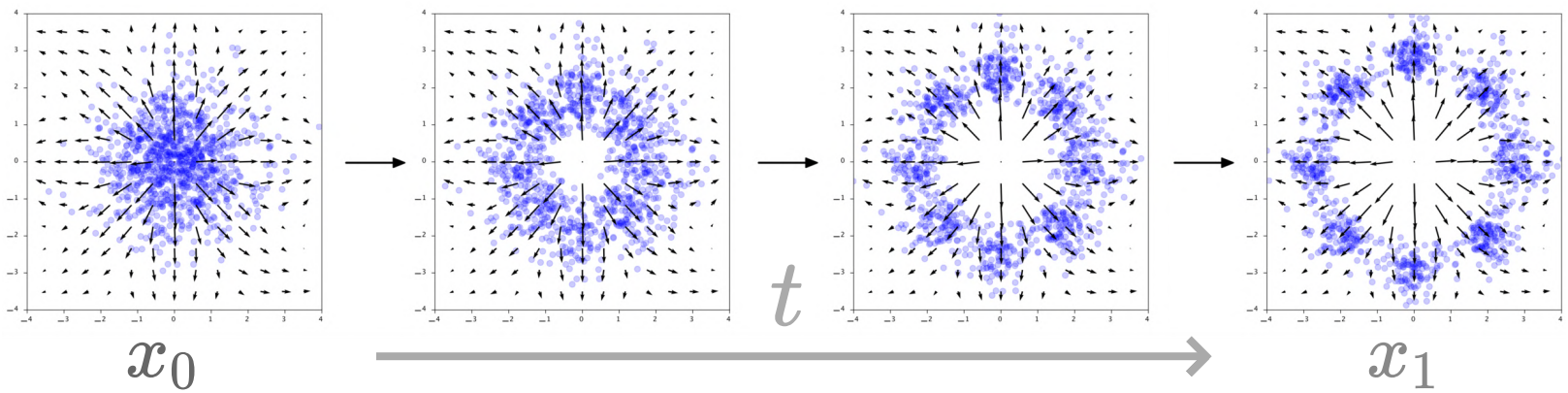
Generate



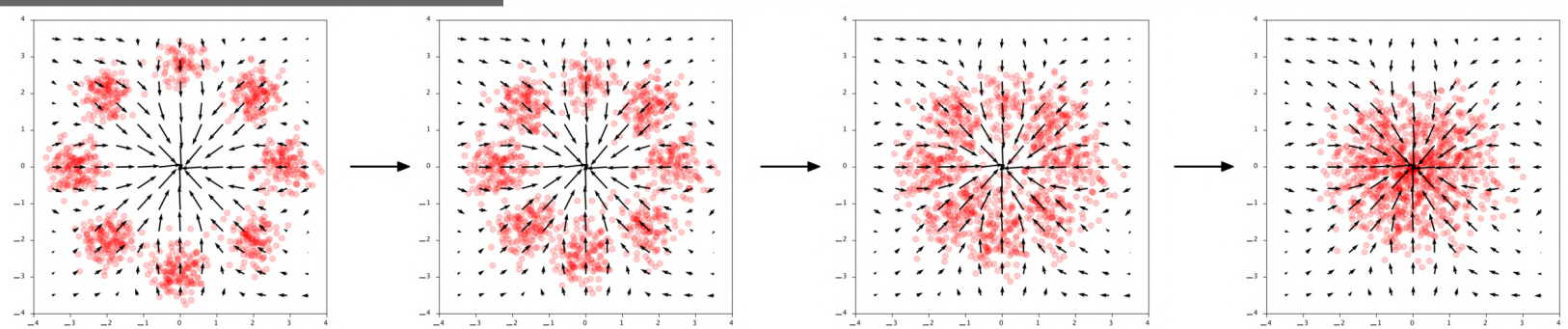
Chen et al. (2018), Grathwohl et al. (2018)

$$x_1 = x_0 + \int_0^1 v_\theta(x(t), t)dt$$

Generate

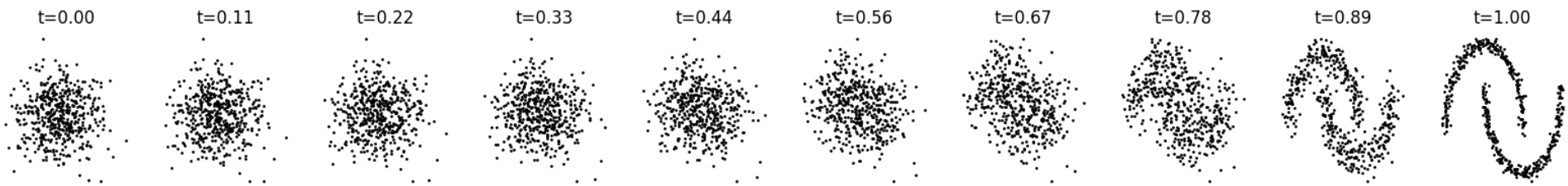


Evaluate Probability



Chen et al. (2018), Grathwohl et al. (2018)

Tutorial 2: Continuous time normalizing flows



x_0

Gaussian

x_1

Two Moons

$$\log p_X(x) = \log p_Z(z) + \int_0^1 \mathrm{Tr} J_v(x(t)) dt$$

$$\log p_X(x) = \log p_Z(z) + \int_0^1 \mathrm{Tr} J_v(x(t))dt$$

Loss requires solving an ODE!

$$\log p_X(x) = \log p_Z(z) + \int_0^1 \mathrm{Tr} J_v(x(t))dt$$

Loss requires solving an ODE!

Diffusion, Flow matching, Interpolants...
All ways to avoid this ***at training time***

Conditional Flow matching

["Flow Matching for Generative Modeling" Lipman et al]

["Stochastic Interpolants: A Unifying framework for Flows and Diffusions" Albergo et al]

Conditional Flow matching

Assume a conditional vector field (known at training time)

$$x_t = (1-t)x_0 + tx_1$$

["Flow Matching for Generative Modeling" Lipman et al]
["Stochastic Interpolants: A Unifying framework for Flows and Diffusions" Albergo et al]

Conditional Flow matching

Assume a conditional vector field (known at training time)

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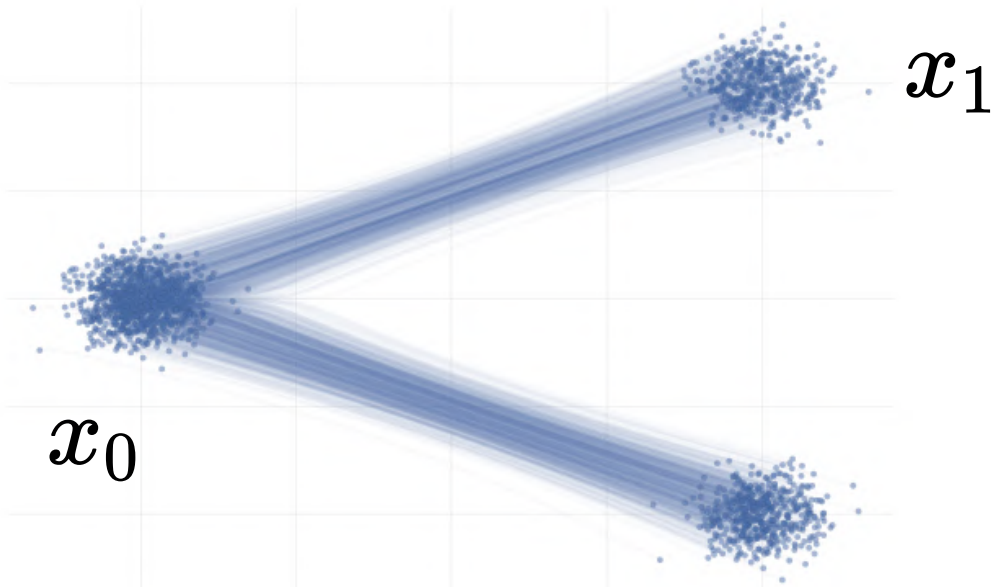

["Flow Matching for Generative Modeling" Lipman et al]
["Stochastic Interpolants: A Unifying framework for Flows and Diffusions" Albergo et al]

Conditional Flow matching

Assume a conditional vector field (known at training time)

$$x_t = (1-t)x_0 + tx_1$$

$$p_t(x) = \int p_t(x|x_1)q(x_1)\,dx_1$$

$$u_t^{\text{target}}(x) = \int u_t(x|x_1)\frac{p_t(x|x_1)p_1(x_1)}{p_t(x)}\,dx_1$$

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Conditional Flow matching

Assume a conditional vector field (known at training time)

$$p_t(x) = \int p_t(x|x_1) q(x_1)\, dx_1$$

$$x_t = (1-t)x_0 + t x_1$$

$$u_t^{\text{target}}(x) = \int u_t(x|x_1) \frac{p_t(x|x_1) p_1(x_1)}{p_t(x)}\, dx_1$$

$$\mathcal{L}_{\text{FM}} = \mathbb{E}_{t\sim U, x\sim p_t}\left[\| u_t^{\phi}(x) - u_t^{\text{target}}(x) \|^2 \right]$$

["Flow Matching for Generative Modeling" Lipman et al]

["Stochastic Interpolants: A Unifying framework for Flows and Diffusions" Albergo et al]

Conditional Flow matching

Assume a conditional vector field (known at training time)

$$x_t = (1-t)x_0 + tx_1$$

Intractable

$$p_t(x) = \int p_t(x|x_1)q(x_1)\,dx_1$$

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$$\mathcal{L}_{\text{FM}} = \mathbb{E}_{t\sim U, x\sim p_t}\left[\|u_t^{\phi}(x) - u_t^{\text{target}}(x)\|^2\right]$$

The loss that we can compute

$$\mathcal{L}_{\text{CFM}} = \mathbb{E}_{t\sim U, x_1\sim p_1, x_t\sim p_t}\left[\|u_t^{\phi}(x_t) - u_t^{\text{target}}(x|x_1)\|^2\right]$$

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Conditional Flow matching

Assume a conditional vector field (known at training time)

$$x_t = (1-t)x_0 + t x_1$$

Intractable

$$p_t(x) = \int p_t(x|x_1) q(x_1)\, dx_1$$

$$u_t^{\text{target}}(x) = \int u_t(x|x_1) \frac{p_t(x|x_1) p_1(x_1)}{p_t(x)}\, dx_1$$

$$\mathcal{L}_{\text{FM}} = \mathbb{E}_{t\sim U, x\sim p_t}\left[\|u_t^{\phi}(x) - u_t^{\text{target}}(x)\|^2\right]$$

The loss that we can compute

$$\mathcal{L}_{\text{CFM}} = \mathbb{E}_{t\sim U, x_1\sim p_1, x_t\sim p_t}\left[\|u_t^{\phi}(x_t) - u_t^{\text{target}}(x|x_1)\|^2\right]$$

The gradients of the losses are the same!

$$\nabla_\phi \mathcal{L}_{\text{CFM}} = \nabla_\phi \mathcal{L}_{\text{FM}}$$

["Flow Matching for Generative Modeling" Lipman et al]

["Stochastic Interpolants: A Unifying framework for Flows and Diffusions" Albergo et al]

Flow Matching

$$\frac{dz_t}{dt} = u_t^{\phi}(z_t)$$

[Image Credit: "Understanding Deep Learning" Simon J.D. Prince]

Flow Matching

$$\frac{dz_t}{dt} = u_t^{\phi}(z_t)$$

$$x = z_0 + \int_0^1 u_t^{\phi}(z_t)dt$$

[Image Credit: "Understanding Deep Learning" Simon J.D. Prince]

Flow Matching

$$\frac{dz_t}{dt} = u_t^{\phi}(z_t)$$

$$x = z_0 + \int_0^1 u_t^{\phi}(z_t)dt$$

$$\frac{dp(z_t)}{dt} = -\nabla\left(u_t^{\phi}(z_t)p(z_t)\right)$$

Continuity equation

[Image Credit: "Understanding Deep Learning" Simon J.D. Prince]

Flow Matching

$$\frac{dz_t}{dt} = u_t^{\phi}(z_t)$$

✅ *Sample*

$$x = z_0 + \int_0^1 u_t^{\phi}(z_t)dt$$

✅ *Evaluate probabilities*

$$\frac{dp(z_t)}{dt} = -\nabla\left(u_t^{\phi}(z_t)p(z_t)\right)$$

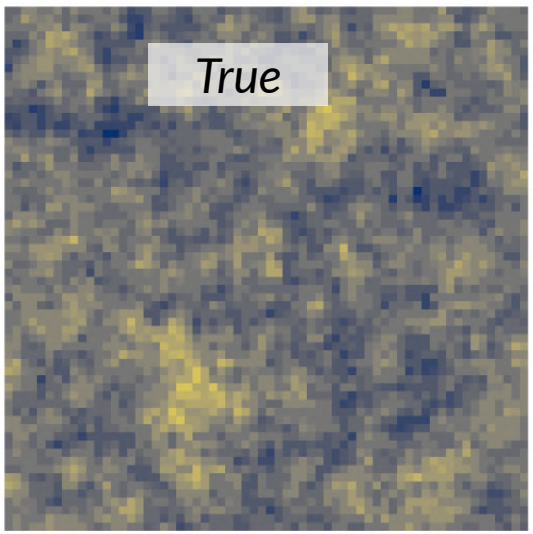
Continuity equation

[Image Credit: "Understanding Deep Learning" Simon J.D. Prince]

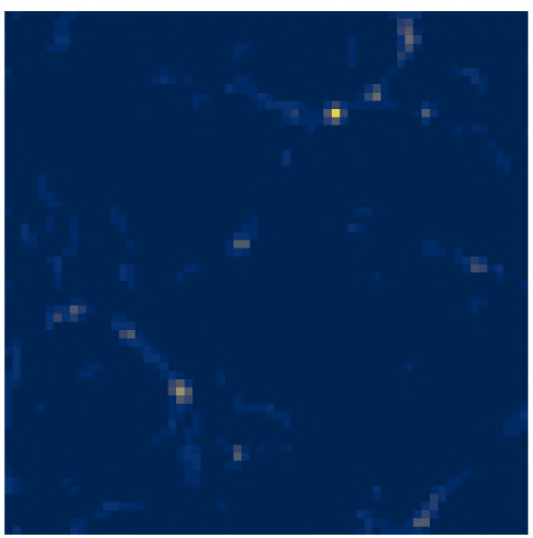
Stochastic Interpolants

$$p(\delta_{\rm ICs}, \theta | \delta_{\rm Obs})$$

$\delta_{\rm ICs}$



$\delta_{\rm Obs}$



"Joint cosmological parameter inference and initial condition reconstruction with Stochastic Interpolants"

Cuesta-Lazaro, Bayer, Albergo et al

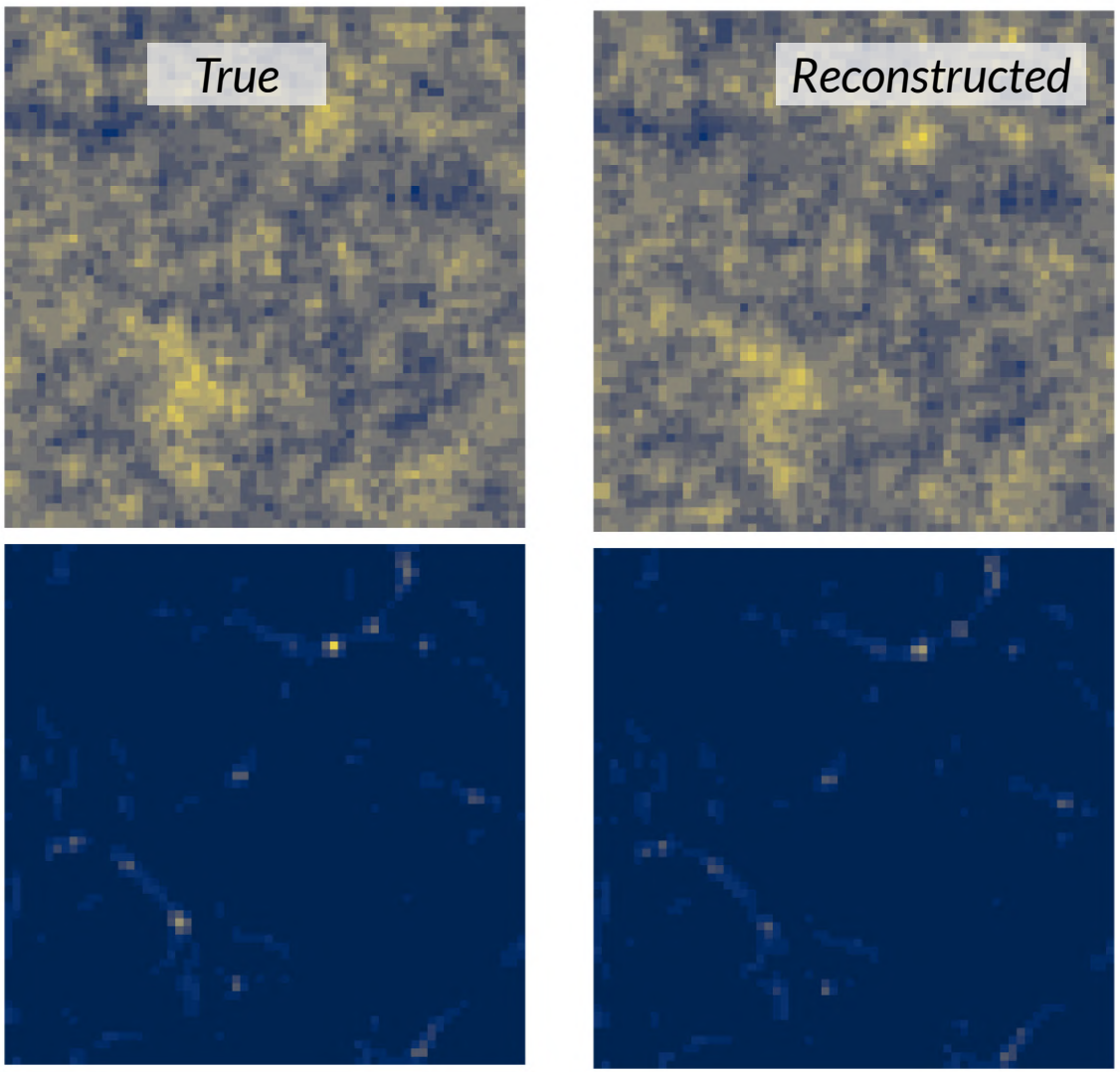
NeurIPs ML4PS 2024 Spotlight talk

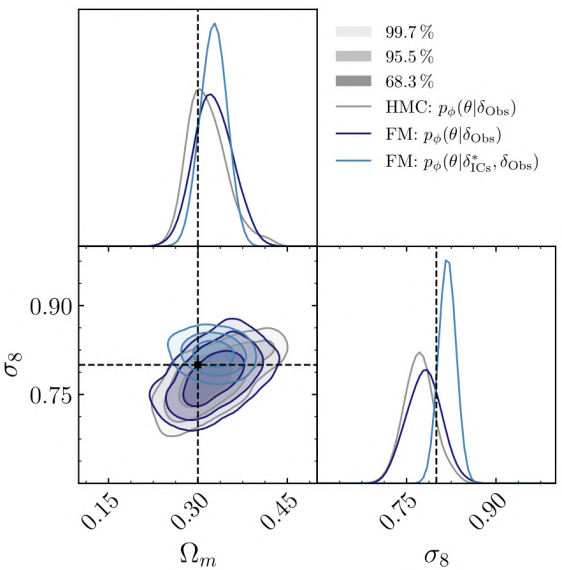
Stochastic Interpolants

$$p(\delta_{\mathrm{ICs}}, \theta | \delta_{\mathrm{Obs}})$$

δ_{ICs}

δ_{Obs}





"Joint cosmological parameter inference and initial condition reconstruction with Stochastic Interpolants"

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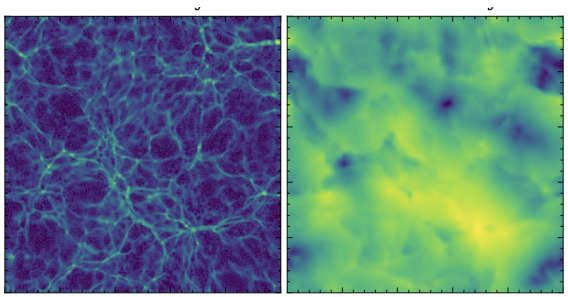
Hydro Simulations at scale

Particle Mesh for Gravity



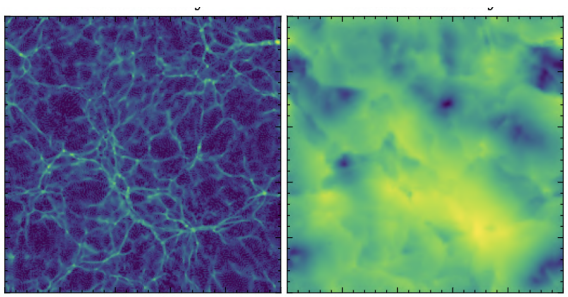
CAMELS Volumes

$25h^{-1}\mathrm{Mpc}$

["BaryonBridge: Interpolants models for fast hydrodynamical simulations" Horowitz, Cuesta-Lazaro, Yehia ML4Astro workshop 2025]

Hydro Simulations at scale

Particle Mesh for Gravity



CAMELS Volumes

$25h^{-1}\mathrm{Mpc}$

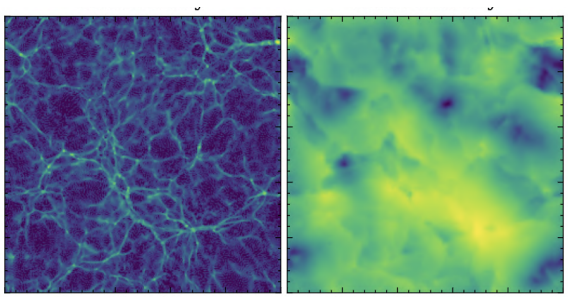
$+\mathcal{C}, \mathcal{A}$

1000 boxes with varying
cosmology and ***feedback*** models

["BaryonBridge: Interpolants models for fast hydrodynamical simulations" Horowitz, Cuesta-Lazaro, Yehia ML4Astro workshop 2025]

Hydro Simulations at scale

Particle Mesh for Gravity



CAMELS Volumes

$25h^{-1}\mathrm{Mpc}$

$$p(\mathrm{Baryons}|\mathrm{DM}, \mathcal{C}, \mathcal{A})$$

$$\longrightarrow$$

$$+\mathcal{C}, \mathcal{A}$$

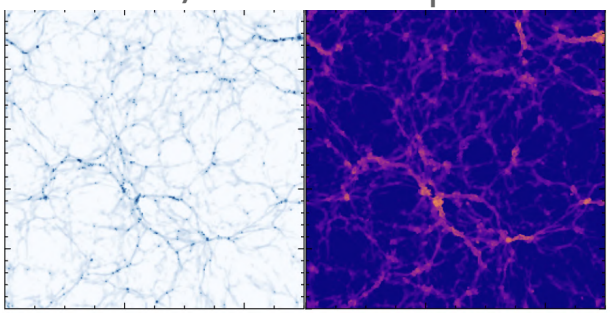
1000 boxes with varying
cosmology and ***feedback*** models

["BaryonBridge: Interpolants models for fast hydrodynamical simulations" Horowitz, Cuesta-Lazaro, Yehia ML4Astro workshop 2025]

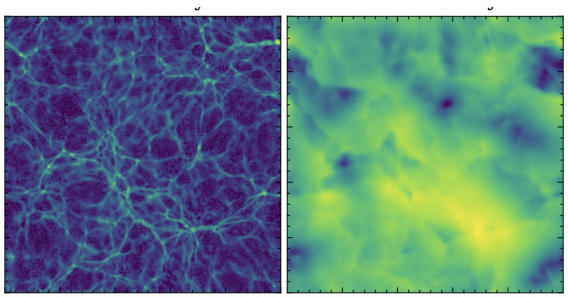
Hydro Simulations at scale

Gas Properties

Density Temperature



Particle Mesh for Gravity



CAMELS Volumes

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$$+\mathcal{C}, \mathcal{A}$$

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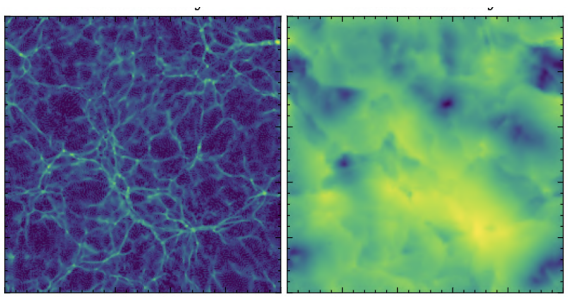
Hydro Simulations at scale

Particle Mesh for Gravity



CAMELS Volumes

$25h^{-1}\mathrm{Mpc}$

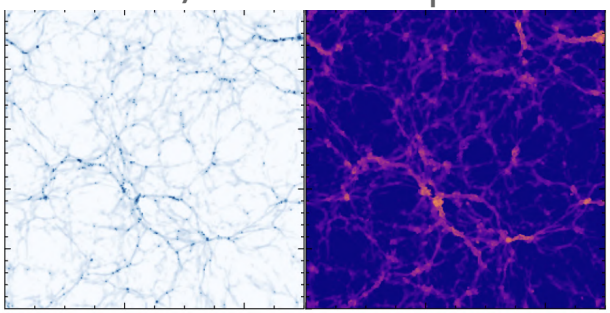
$$p(\mathrm{Baryons}|\mathrm{DM}, \mathcal{C}, \mathcal{A})$$

$$+\mathcal{C}, \mathcal{A}$$

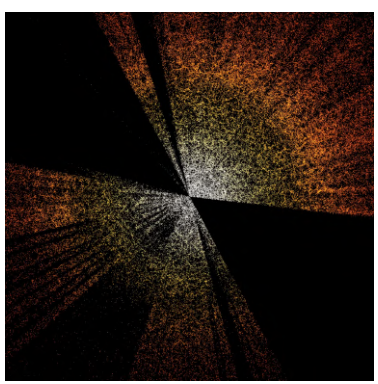
1000 boxes with varying
cosmology and ***feedback*** models

Gas Properties

Density Temperature



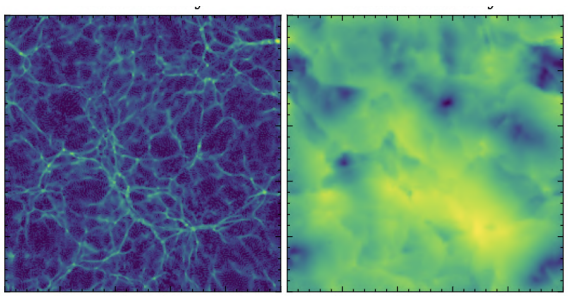
Galaxy Distribution



["BaryonBridge: Interpolants models for fast hydrodynamical simulations" Horowitz, Cuesta-Lazaro, Yehia ML4Astro workshop 2025]

Hydro Simulations at scale

Particle Mesh for Gravity



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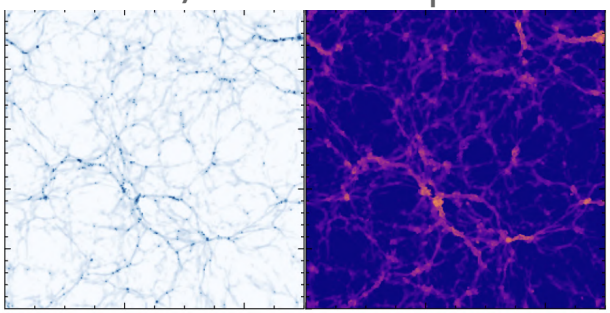

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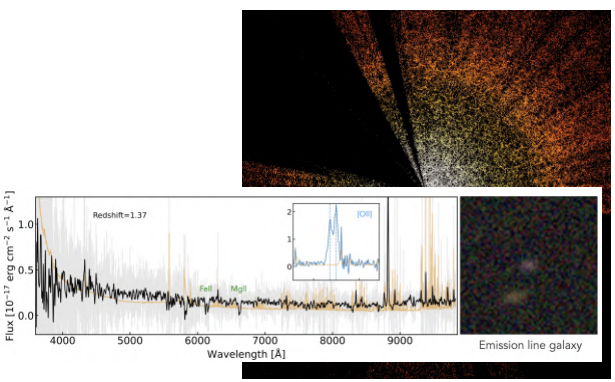

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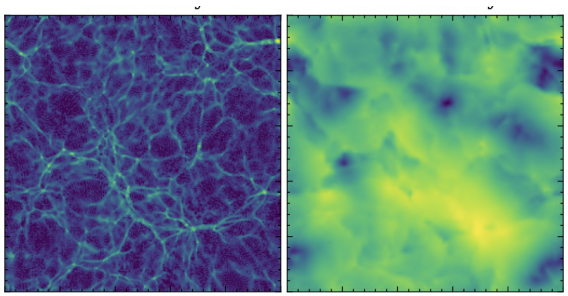
Hydro Simulations at scale

Particle Mesh for Gravity



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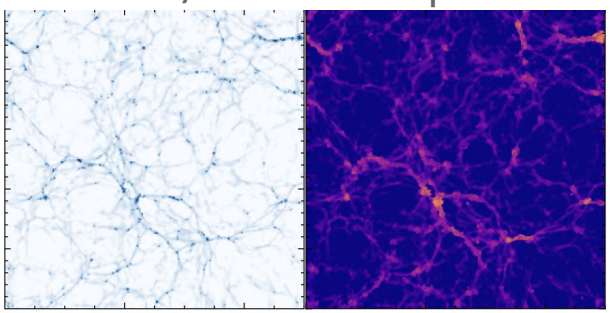
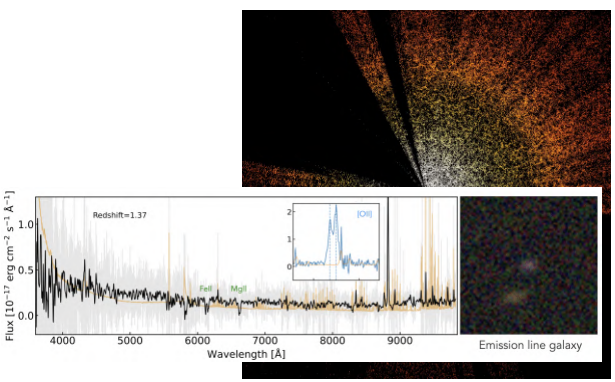


Galaxy Distribution



Current model optimised for Lyman Alpha forest

7 GPU minutes for a 50 Mpc simulation

130 million CPU core hours for TNG50

["BaryonBridge: Interpolants models for fast hydrodynamical simulations" Horowitz, Cuesta-Lazaro, Yehia ML4Astro workshop 2025]

Find straighter paths with OT

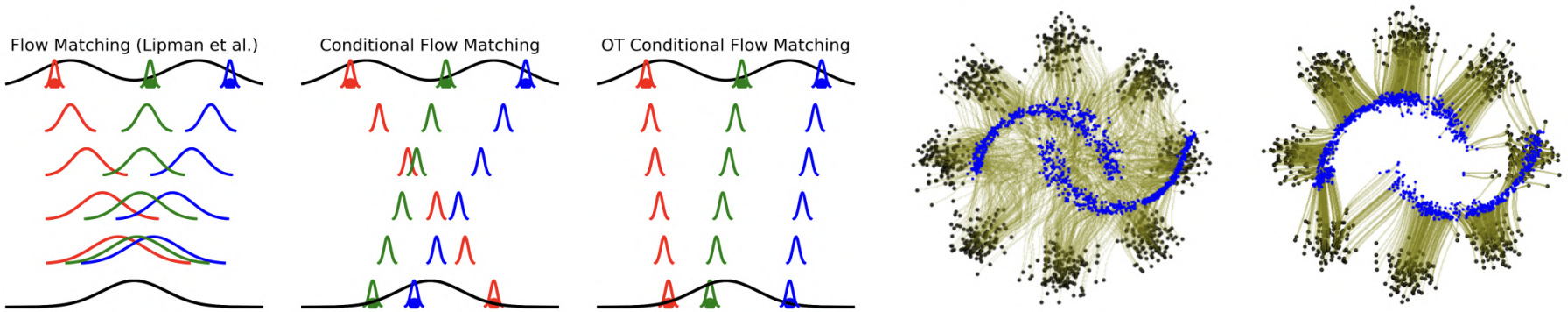
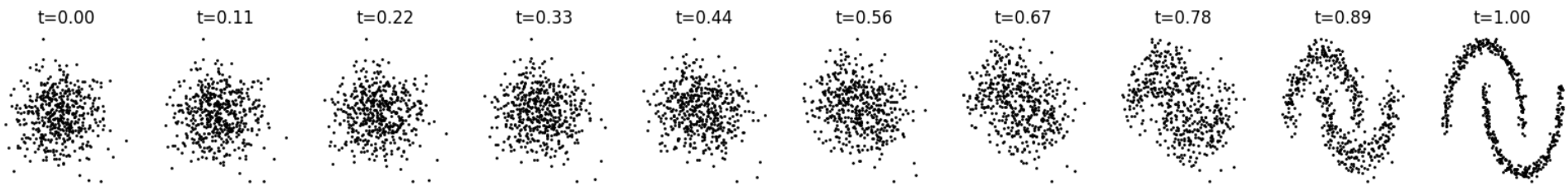


Figure 1: **Left:** Conditional flows from FM (Lipman et al., 2023), I-CFM (§3.2.2), and OT-CFM (§3.2.3). **Right:** Learned flows (green) from moons (blue) to 8gaussians (black) using I-CFM (centre-right) and OT-CFM (far right).

["Improving and generalizing flow-based generative models with minibatch optimal transport" Tong et al]

Tutorial 3: Flow Matching from scratch



x_0

Gaussian

x_1

Two Moons

Diffusion Models

Diffusion Models

Forward diffusion: Add Gaussian noise (fixed)

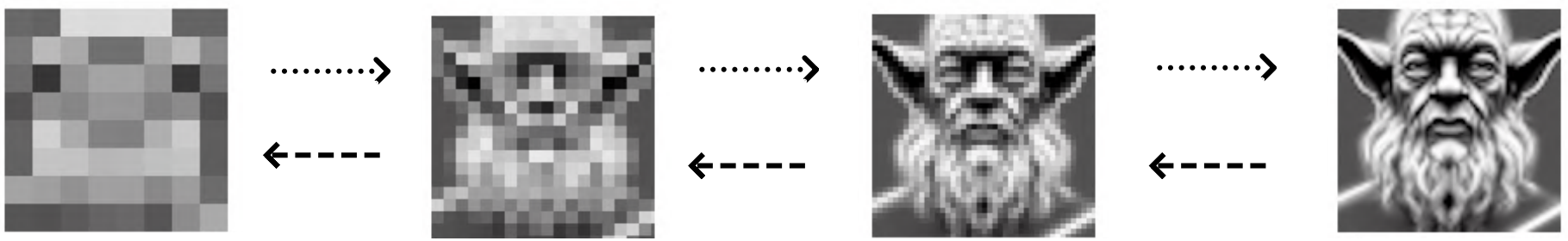
Diffusion Models

Fixed base distribution:

Gaussian

Forward diffusion: Add Gaussian noise (fixed)

Diffusion Models



Fixed base distribution: Gaussian

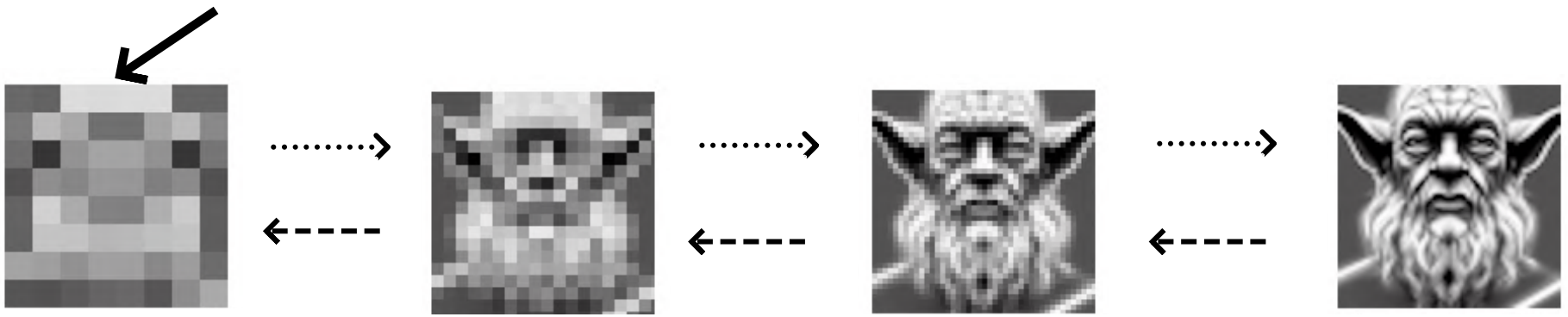
Forward diffusion: Add Gaussian noise (fixed)

Reverse diffusion: Denoise previous step

Diffusion Models

Prompt

A person half Yoda half Gandalf



Fixed base distribution: Gaussian

Forward diffusion: Add Gaussian noise (fixed)

Reverse diffusion: Denoise previous step

Diffusion Models

Prompt

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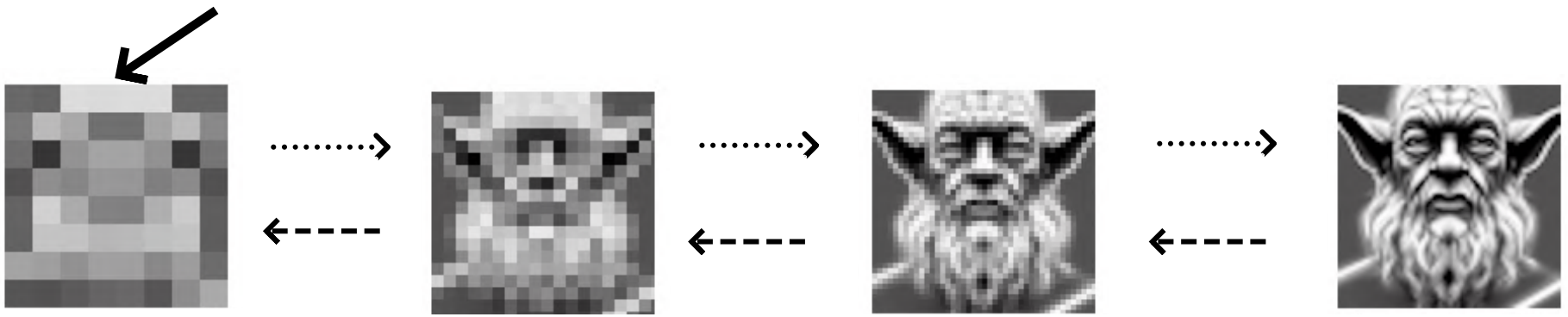


Fixed base distribution: Gaussian

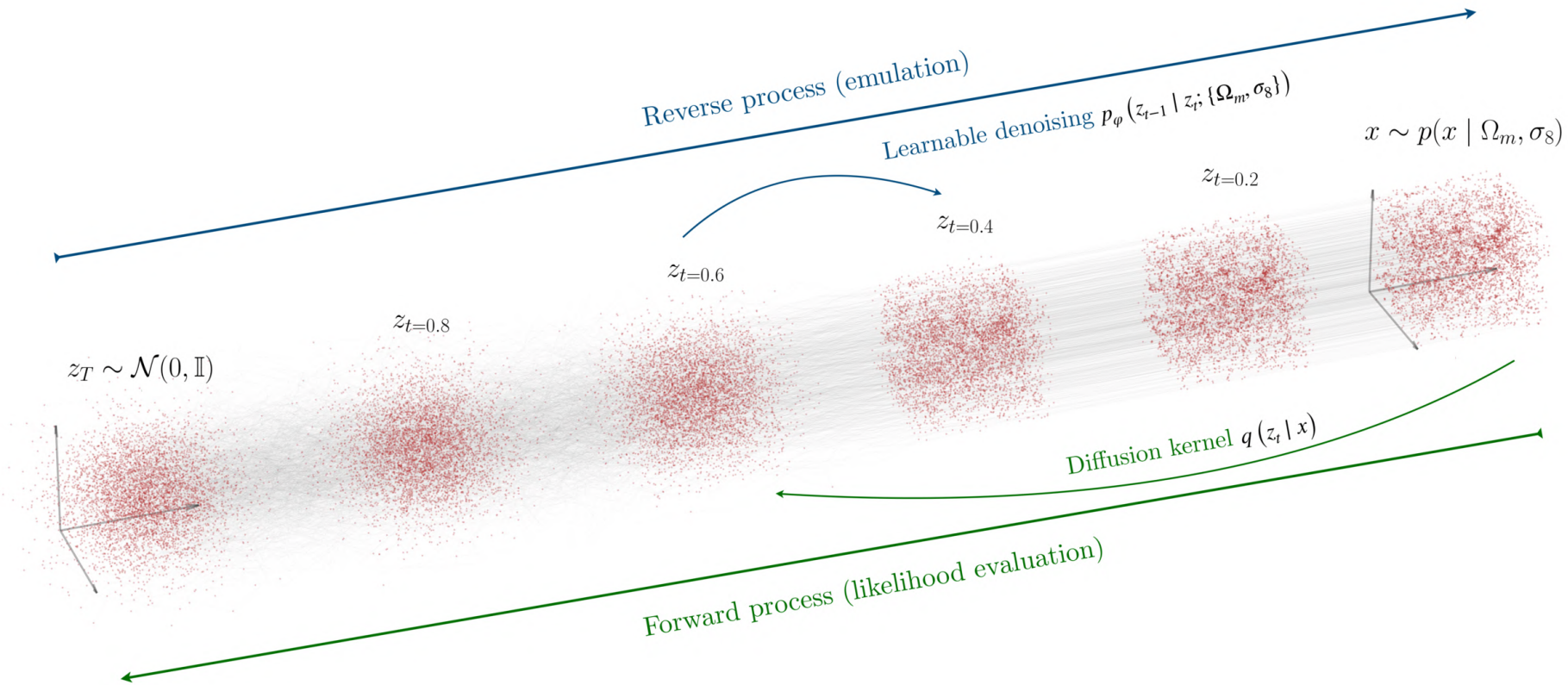
Denoising = Regression

⟵ Forward diffusion: Add Gaussian noise (fixed)

⟶ Reverse diffusion: Denoise previous step

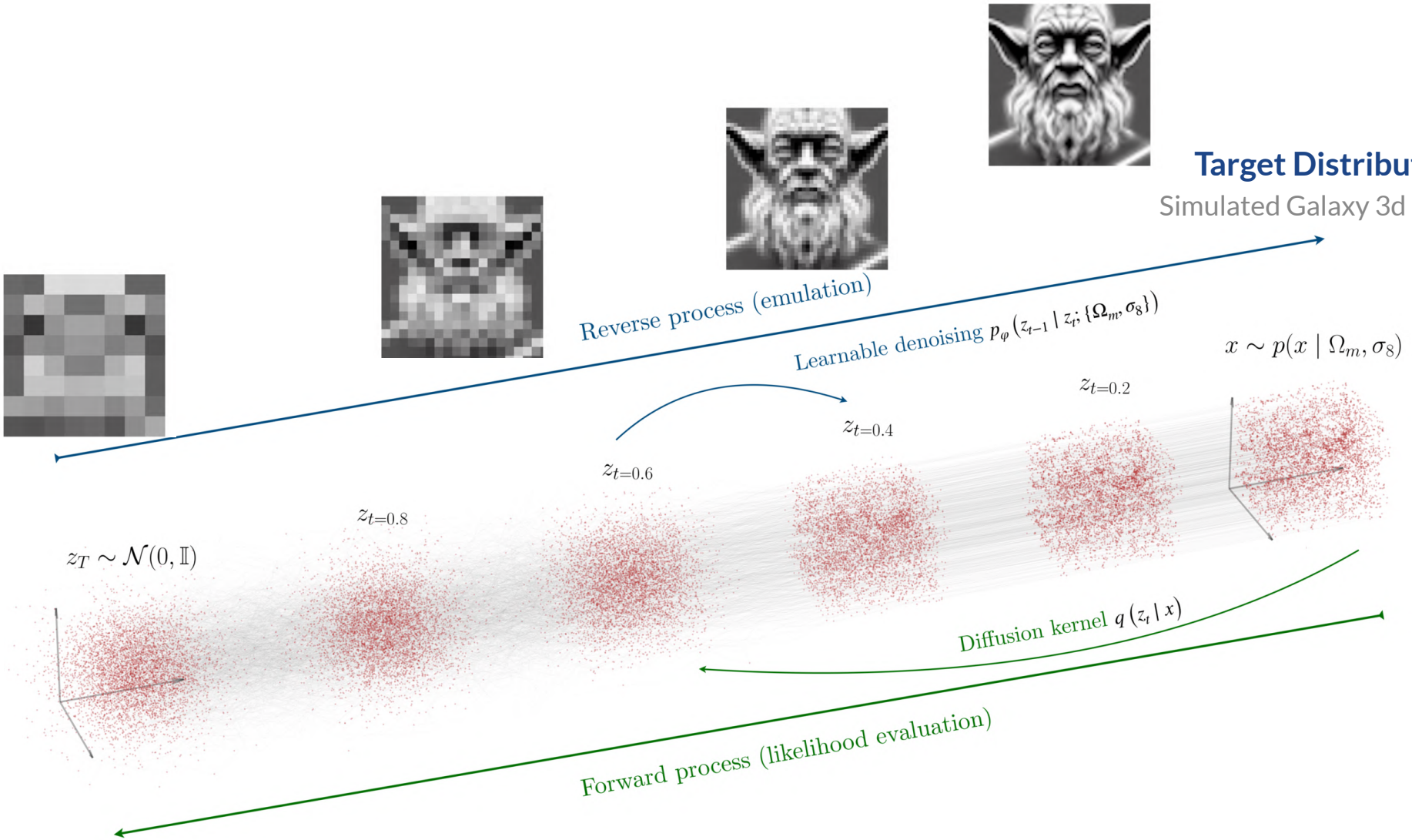
Target Distributio

Simulated Galaxy 3d Ma



Base Distribution

["A point cloud approach to generative modeling for galaxy surveys at the field level"
Cuesta-Lazaro and Mishra-Sharma
International Conference on Machine Learning ICML AI4Astro 2023, Spotlight talk, arXiv:2311.17141]



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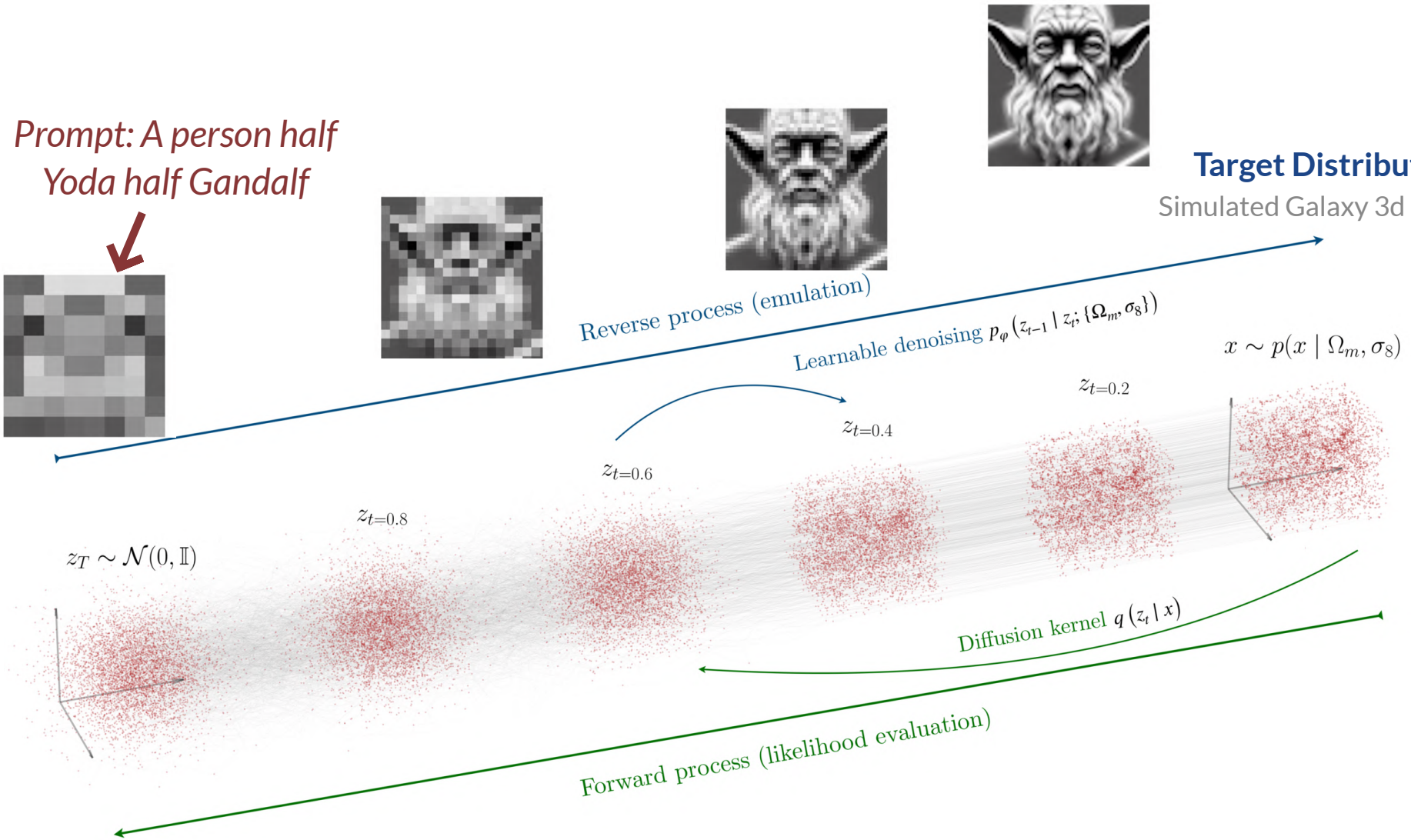

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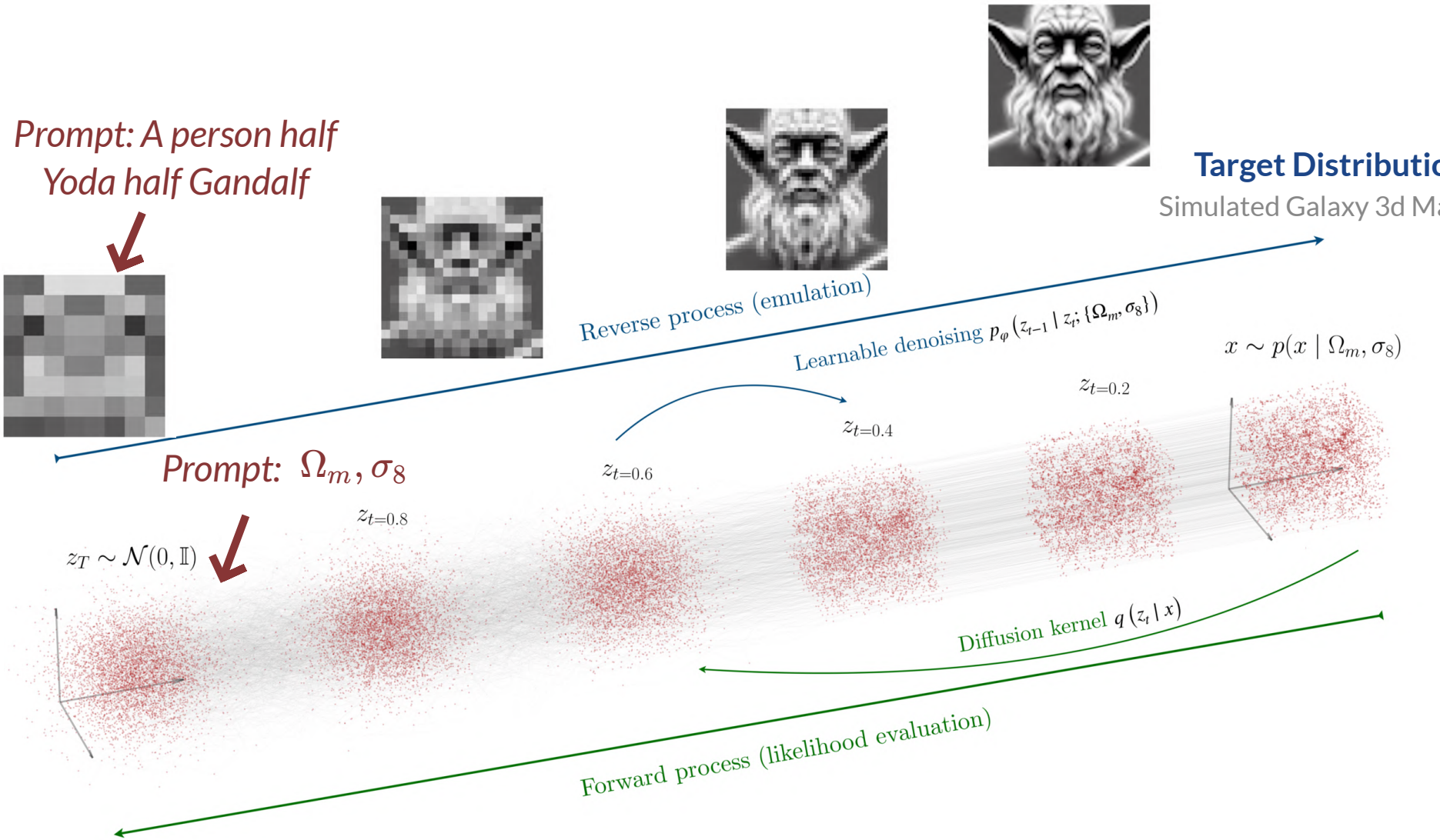

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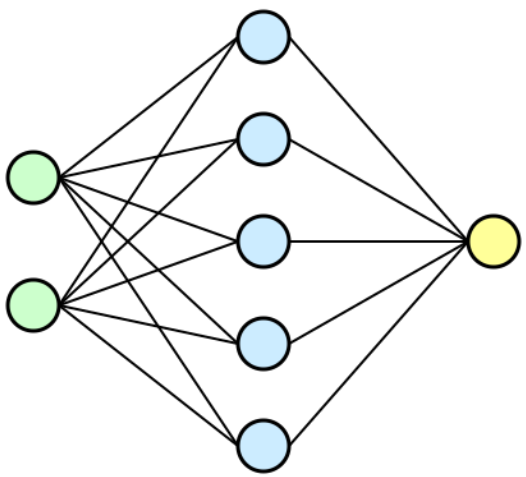
How good is my generative model?

$\mathrm{R} \sim p(\theta|x)$

$\mathrm{F} \sim \hat{p}(\theta|x)$



Real or Fake?

["A Practical Guide to Sample-based Statistical Distances for Evaluating Generative Models in Science" Bischoff et al 2024 arXiv:2403.12636]

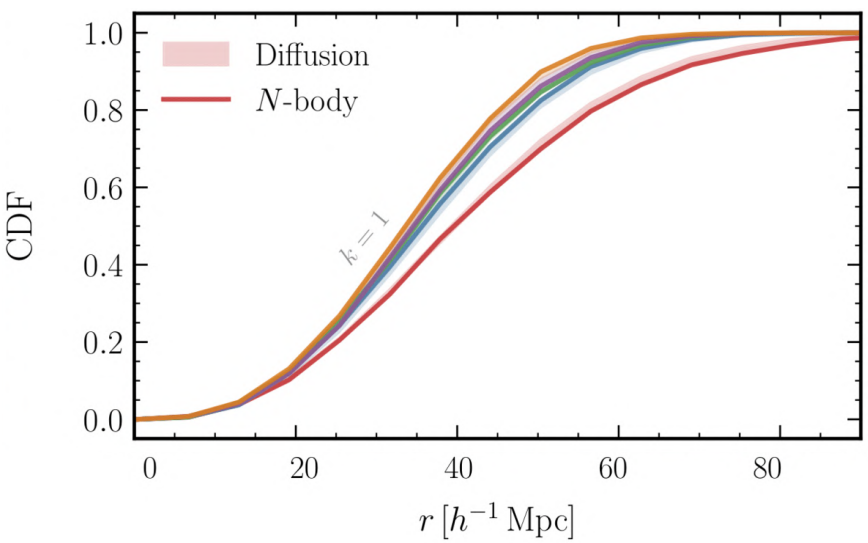
Reproducing summary statistics

Varying cosmological parameters

$\Omega_m = 0.10 \quad \sigma_8 = 0.92$ $\Omega_m = 0.18 \quad \sigma_8 = 0.68$ $\Omega_m = 0.27 \quad \sigma_8 = 0.92$

$\Omega_m = 0.35 \quad \sigma_8 = 0.62$ $\Omega_m = 0.44 \quad \sigma_8 = 0.95$

k Nearest neighbours



Pair separation

Reproducing summary statistics

Varying cosmological parameters

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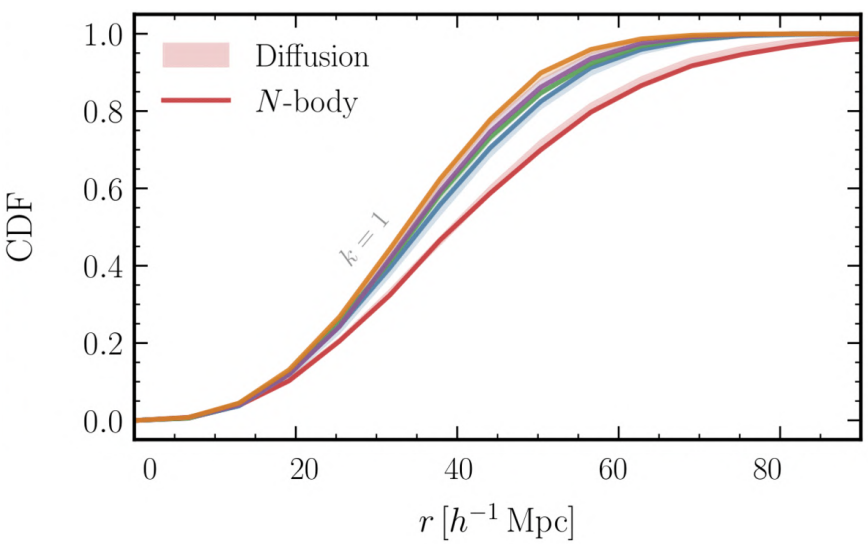
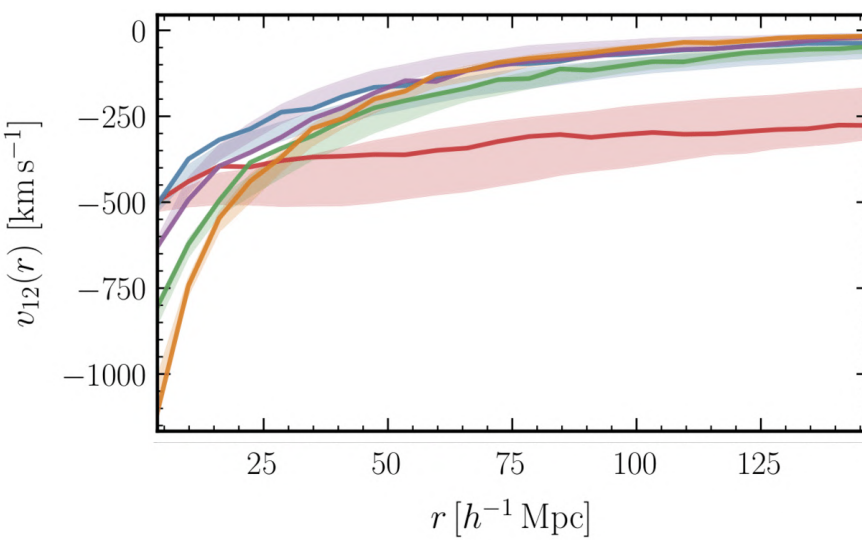


Pair separation

Mean relative velocity



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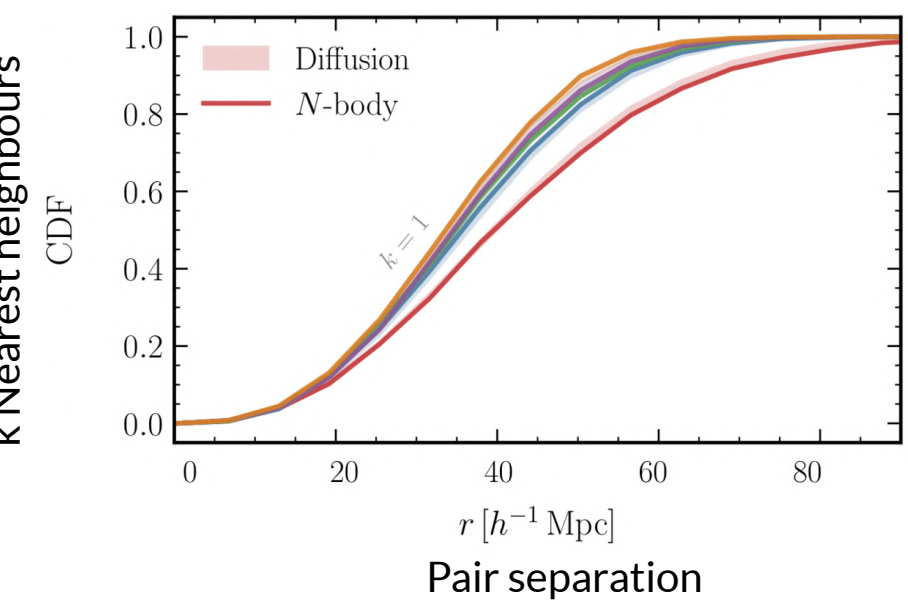
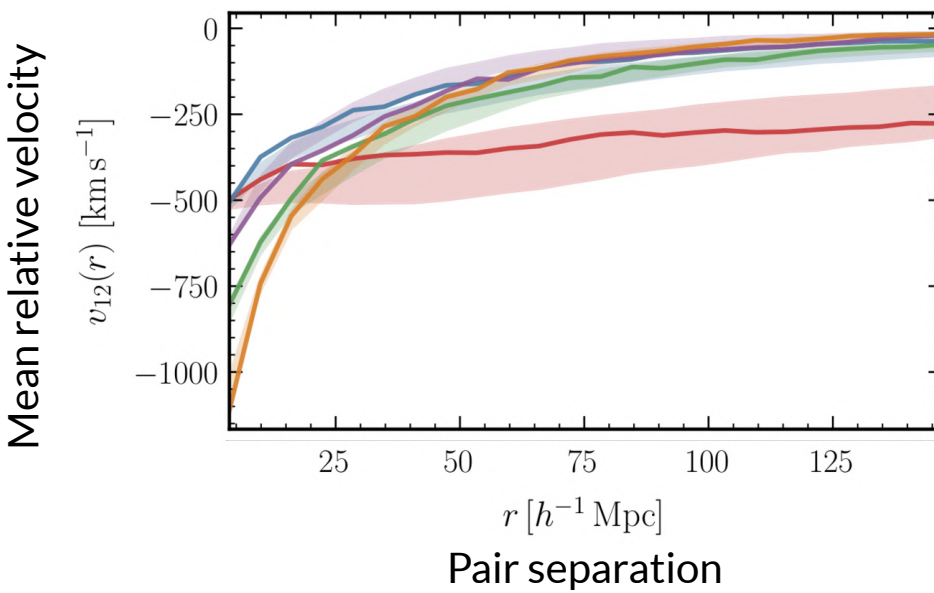


Pair separation

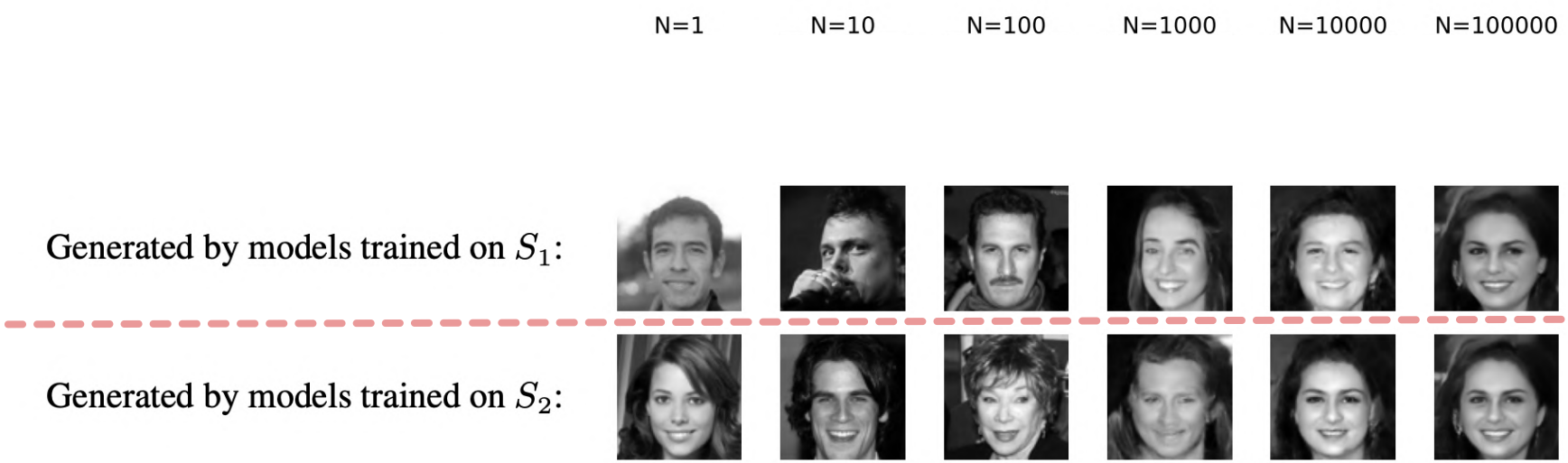


Pair separation

Physics as a testing ground: Well-understood summary statistics enable rigorous validation of generative models

Has my model learned the underlying density?

Split training set into non-overlapping S_1, S_2



["Generalization in diffusion models arises from geometry-adaptive harmonic representations" Kadkhodaie et al (2024)]

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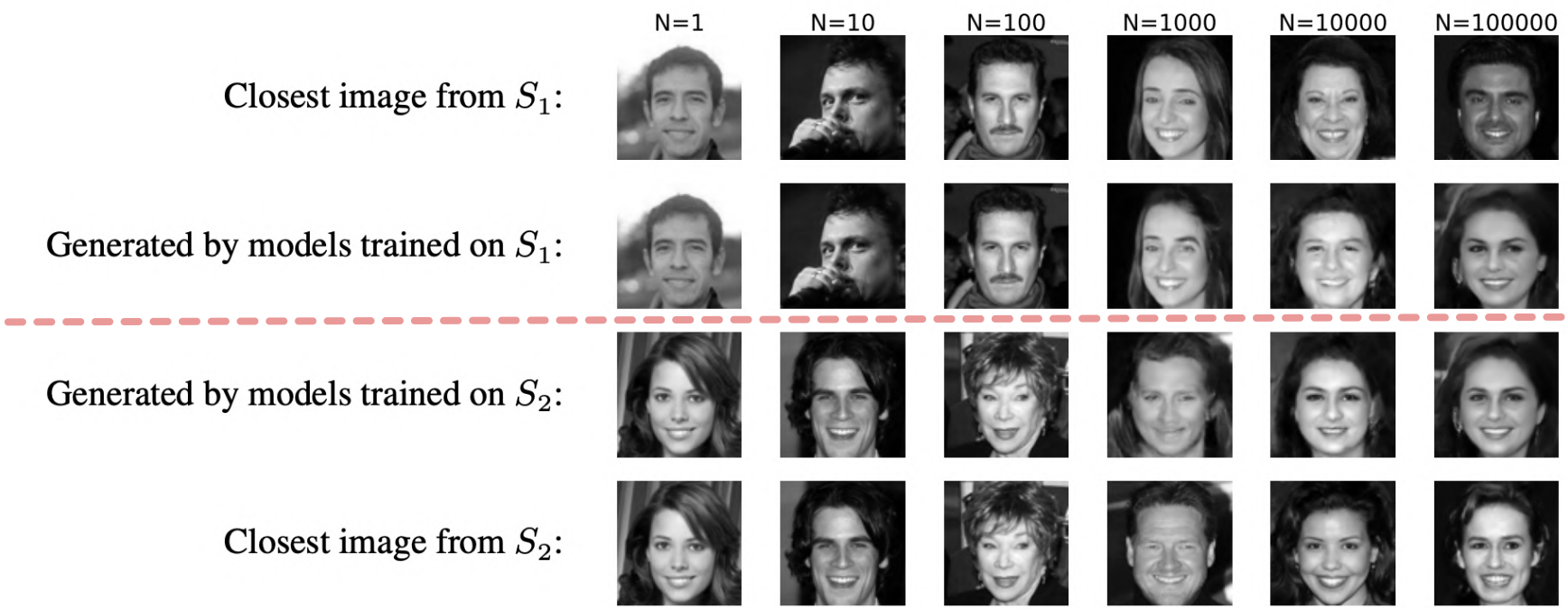

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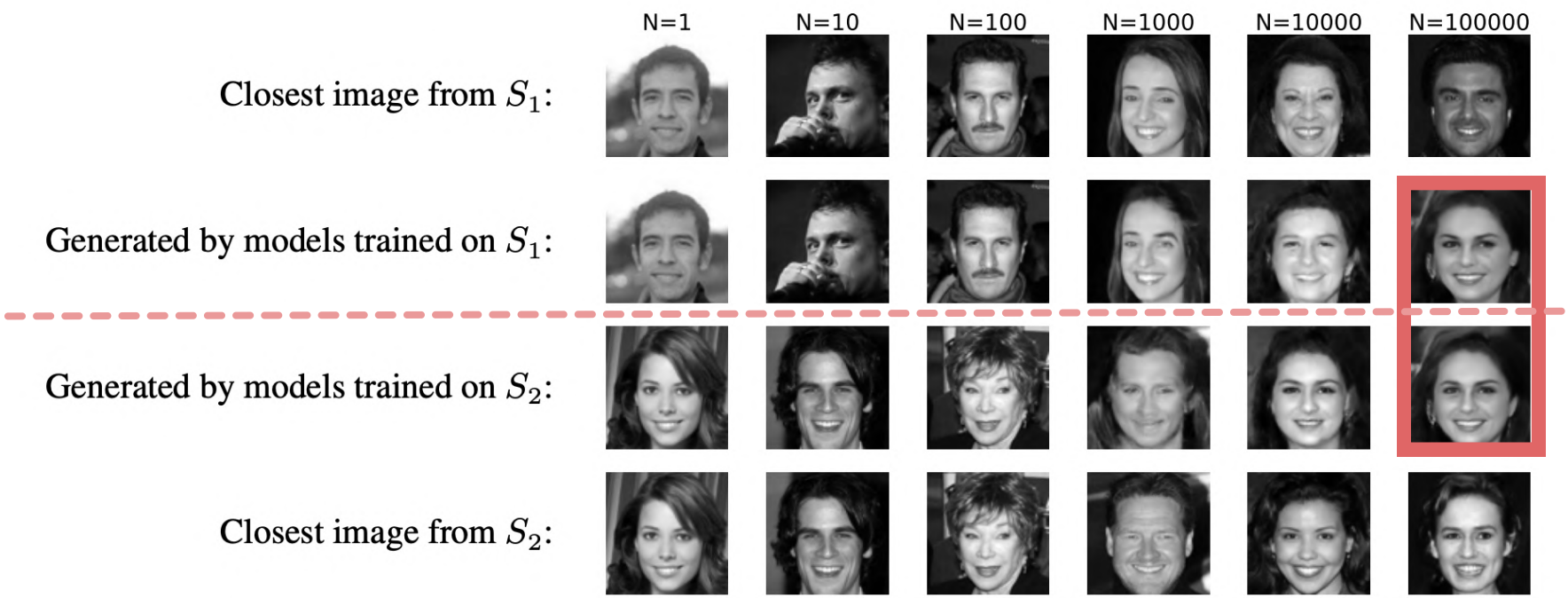

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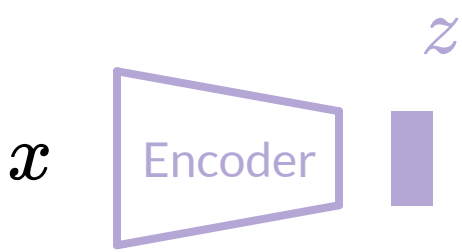
Generate = Understand?

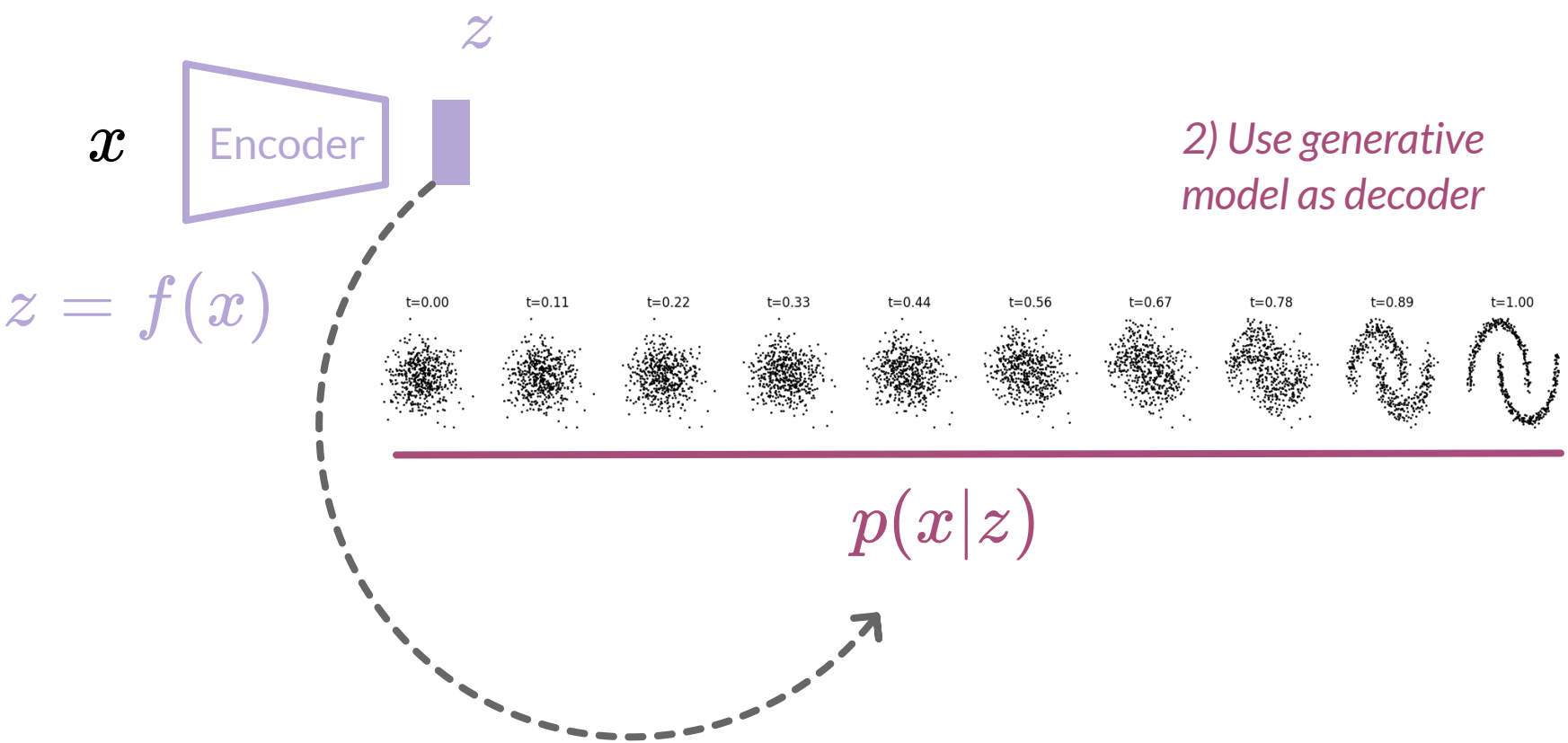
1) Compress into low dimensional latent



$$z = f(x)$$

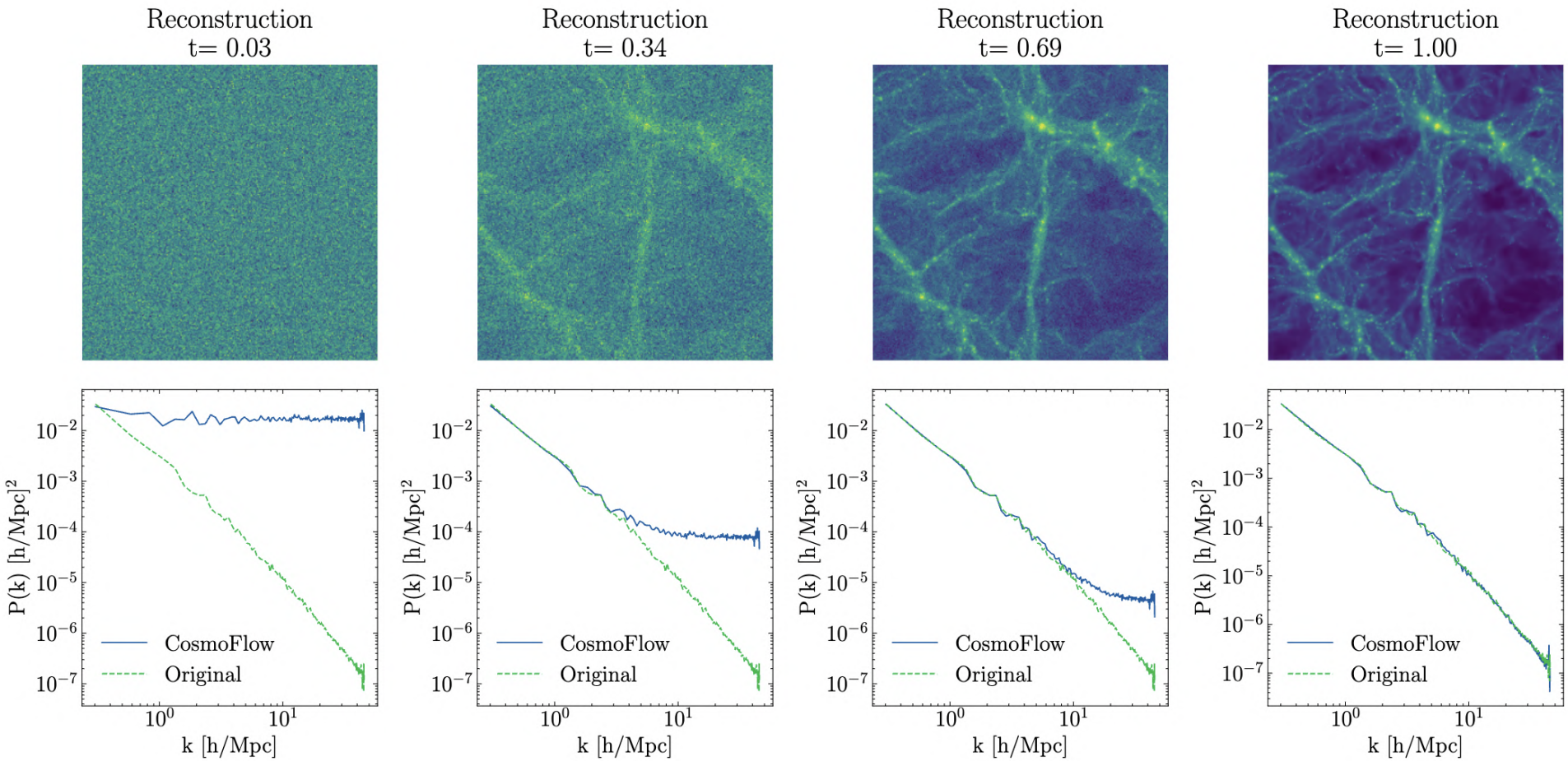
Generate = Understand?

1) Compress into low dimensional latent



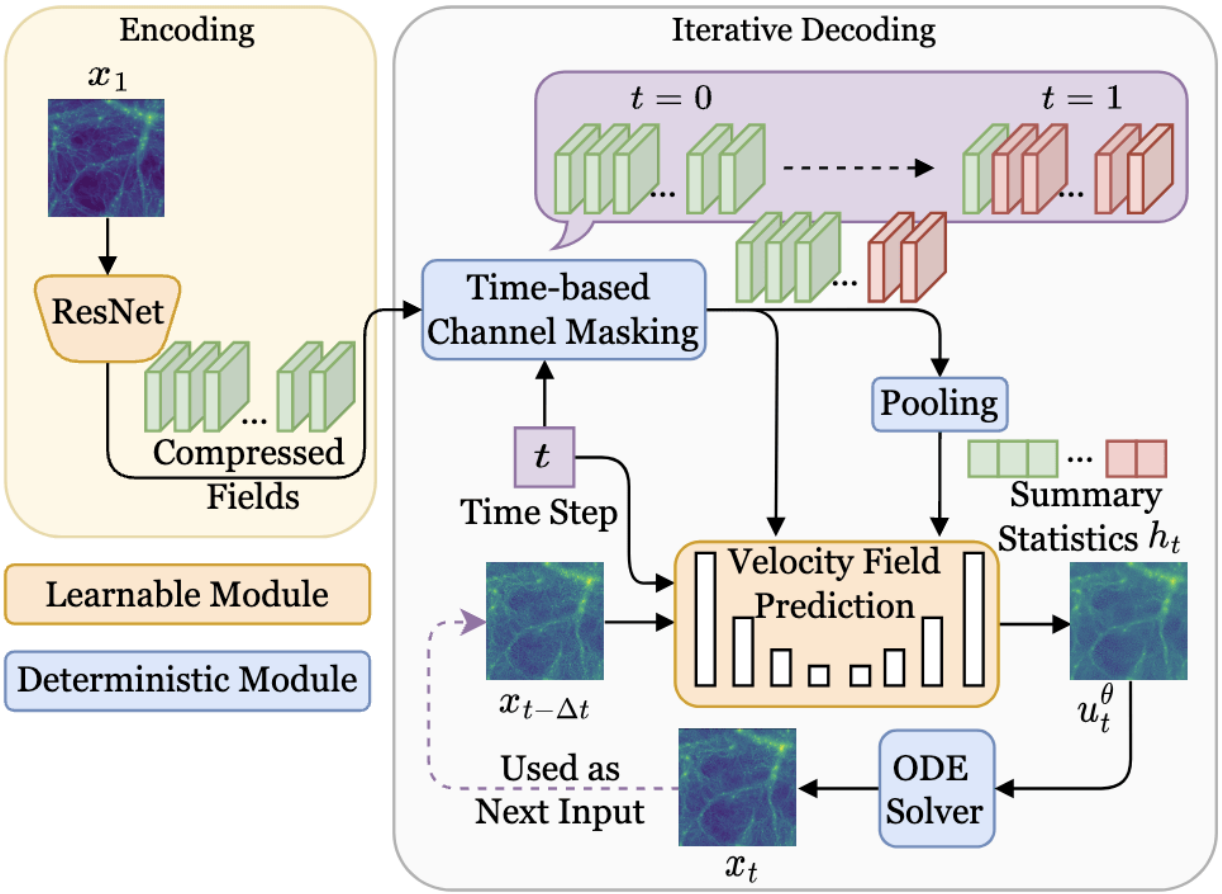
2) Use generative model as decoder

Autoregressive in Frequency



["CosmoFlow: Scale-Aware Representation Learning for Cosmology with Flow Matching" Kannan, Qiu, Cuesta-Lazaro, Jeong (in prep)]

Generate = Understand?



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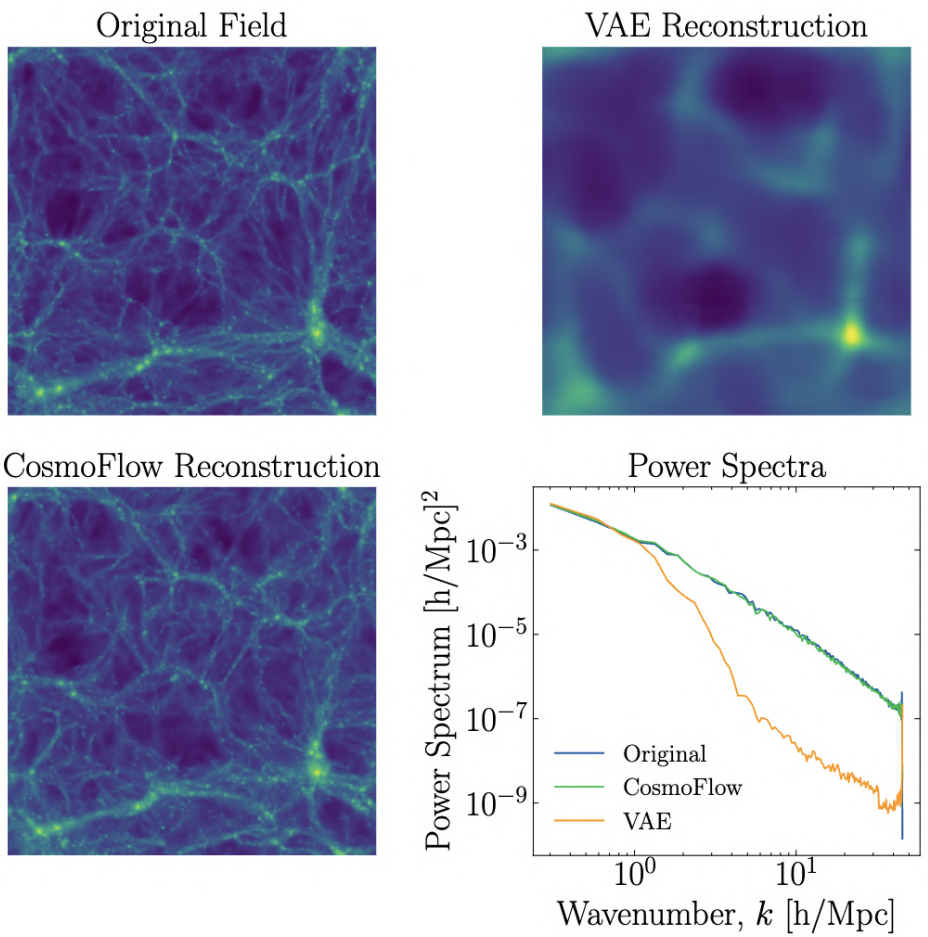

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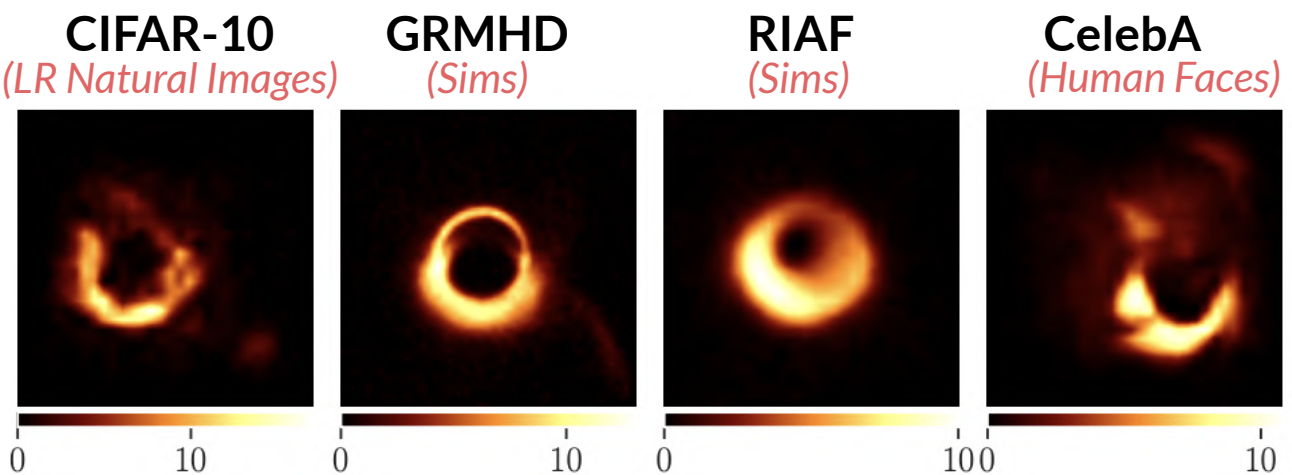
Generative Priors: Plug and Play

$$\log p(x|y) = \log p(y|x) + \log p(x) + \text{constant}$$

Prior

EHT posterior samples with different priors



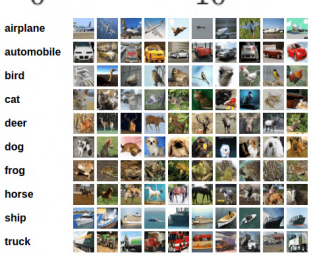
["Event-horizon-scale Imaging of M87* under Different Assumptions via Deep Generative Image Priors" Feng et al]

Generative Priors: Plug and Play

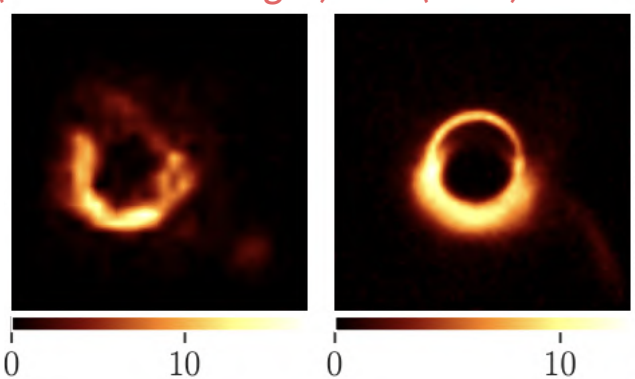
$$\log p(x|y) = \log p(y|x) + \underbrace{\log p(x)}_{\text{Prior}} + \text{constant}$$

EHT posterior samples with different priors

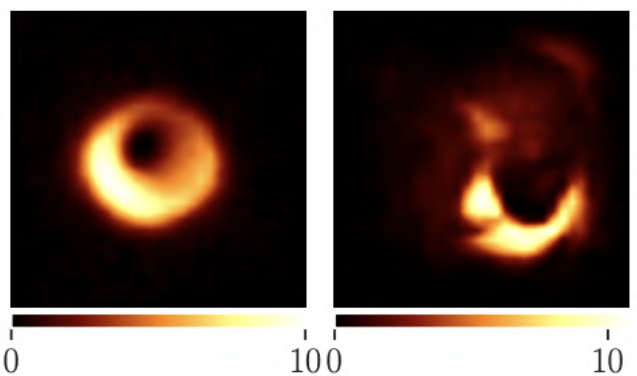
CIFAR-10 *(LR Natural Images)*



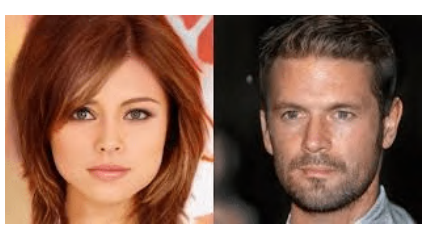
GRMHD *(Sims)*



RIAF *(Sims)*



CelebA *(Human Faces)*



["Event-horizon-scale Imaging of M87* under Different Assumptions via Deep Generative Image Priors" Feng et al]

Generative priors: learn directly?

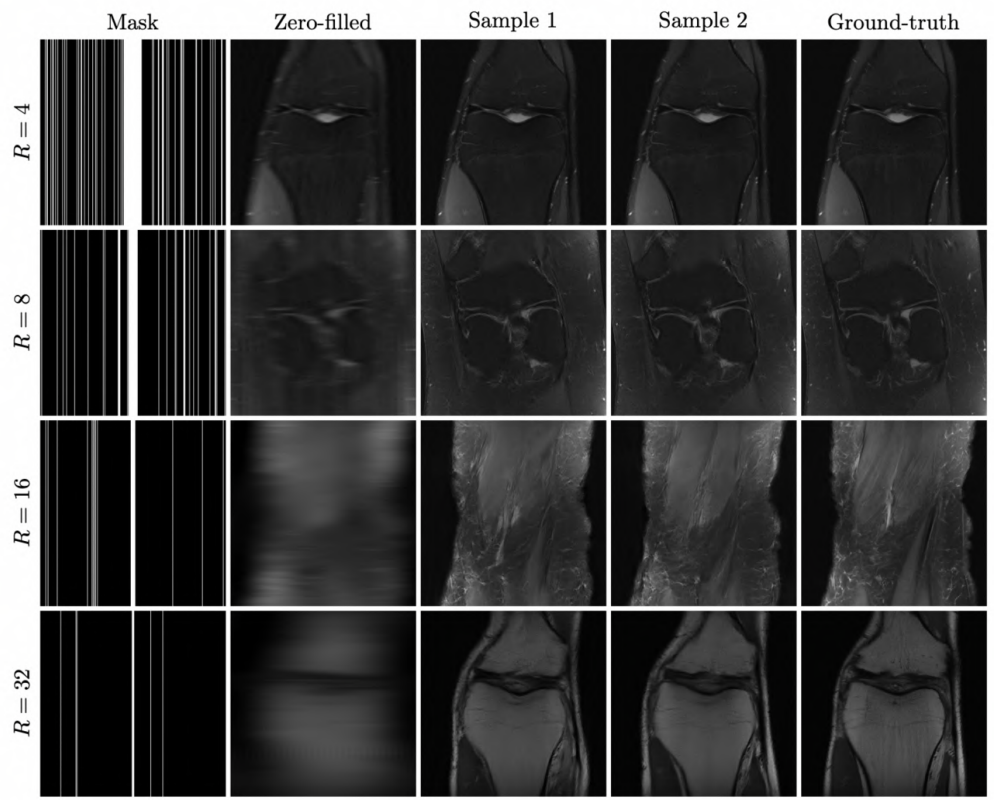


Figure 6. Examples of posterior samples for accelerated MRI using a diffusion prior trained from k-space observations only. Posterior samples are detailed and present plausible variations, while remaining consistent with the observation. We provide the zero-filled inverse, where missing frequencies are set to zero, as baseline.

["Learning Diffusion Priors from Observations by Expectation Maximization"

Rozet et al]

Bridging two distributions

How is the bridge constrained?

Normalizing flows: Reverse = Forward inverse

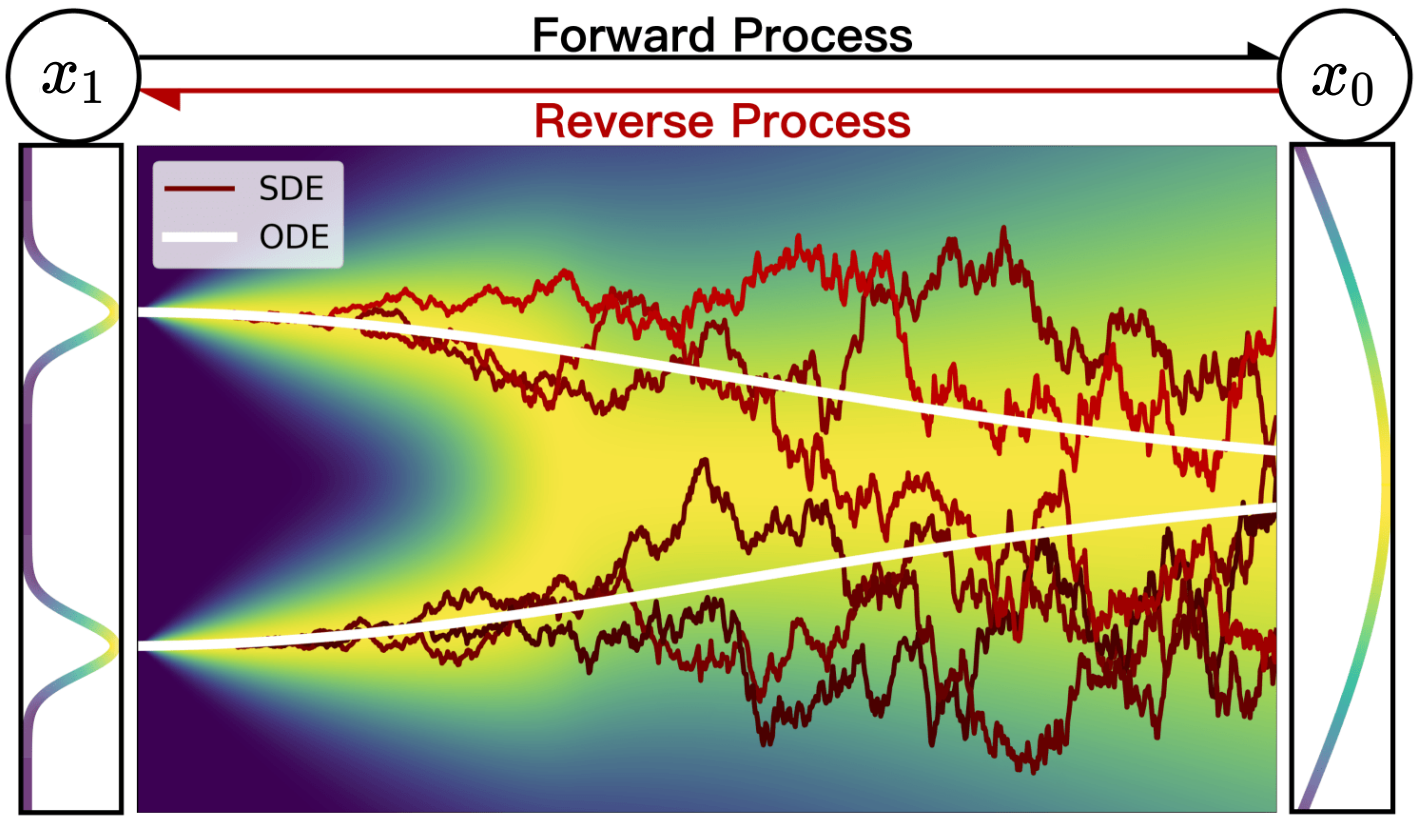
Diffusion: Forward = Gaussian noising

Flow Matching: Forward = Interpolant

is p(x0) restricted?

Diffusion: p(x0) is Gaussian

Normalising flows: p(x0) can be evaluated



Data

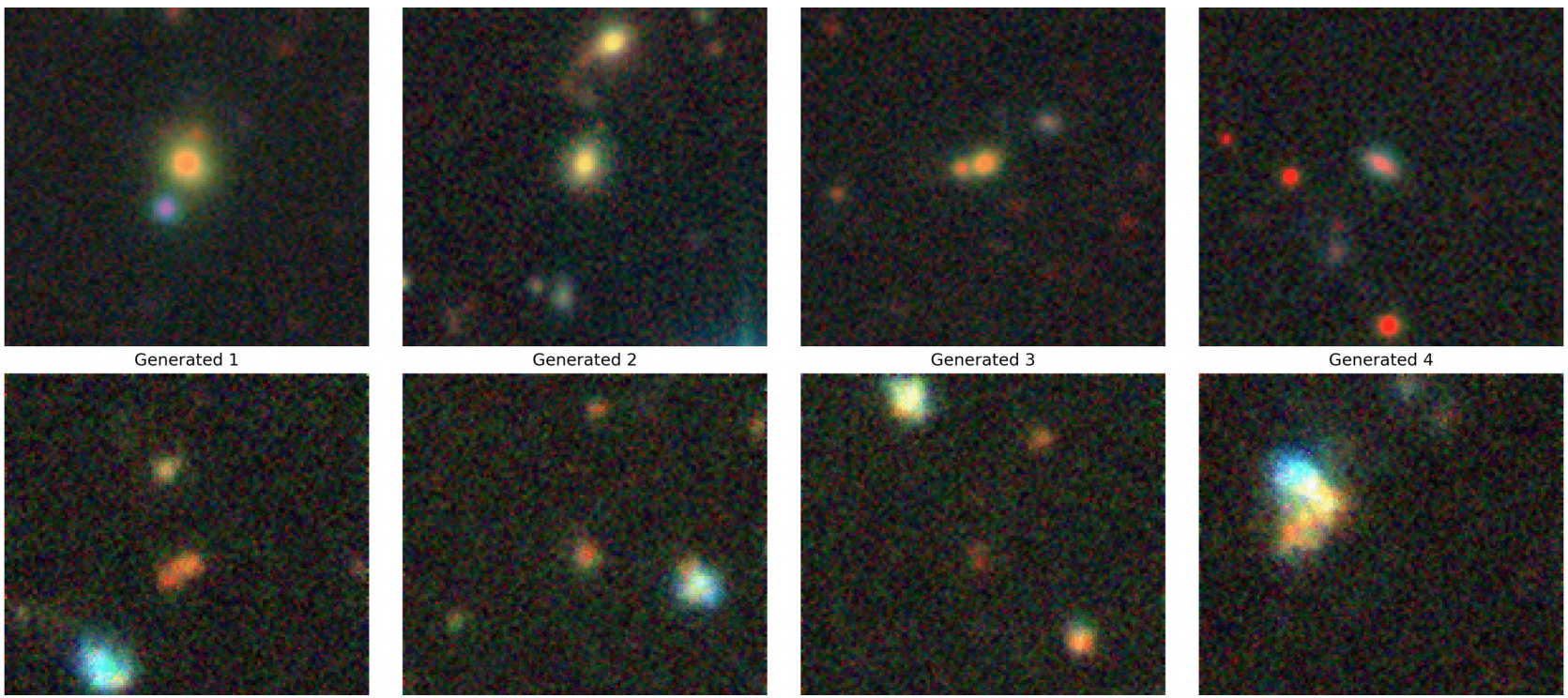
Base

(Exact likelihood evaluation)

Is bridge stochastic (SDE) or deterministic (ODE)?

Diffusion: Stochastic (SDE) *Normalising flows: Deterministic (ODE)*

Tutorial 4: Generating Galaxy Images



References

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- **Books** by Kevin P. Murphy
  - *Machine learning, a probabilistic perspective*
  - *Probabilistic Machine Learning: advanced topics*
- **ML4Astro workshop** *https://ml4astro.github.io/icml2023/*
- **ProbAI summer school** *https://github.com/probabilisticai/probai-2023*
- **IAIFI Summer school**
  - *https://github.com/iaifi/summer-school-2023*
  - Tutorials *https://github.com/florpi/summer_school_generative*
- **Blogposts**
  - *https://lilianweng.github.io/posts/2018-10-13-flow-models/*
  - *https://sander.ai/2023/07/20/perspectives.html*
  - https://mlg.eng.cam.ac.uk/blog/2024/01/20/flow-matching.html