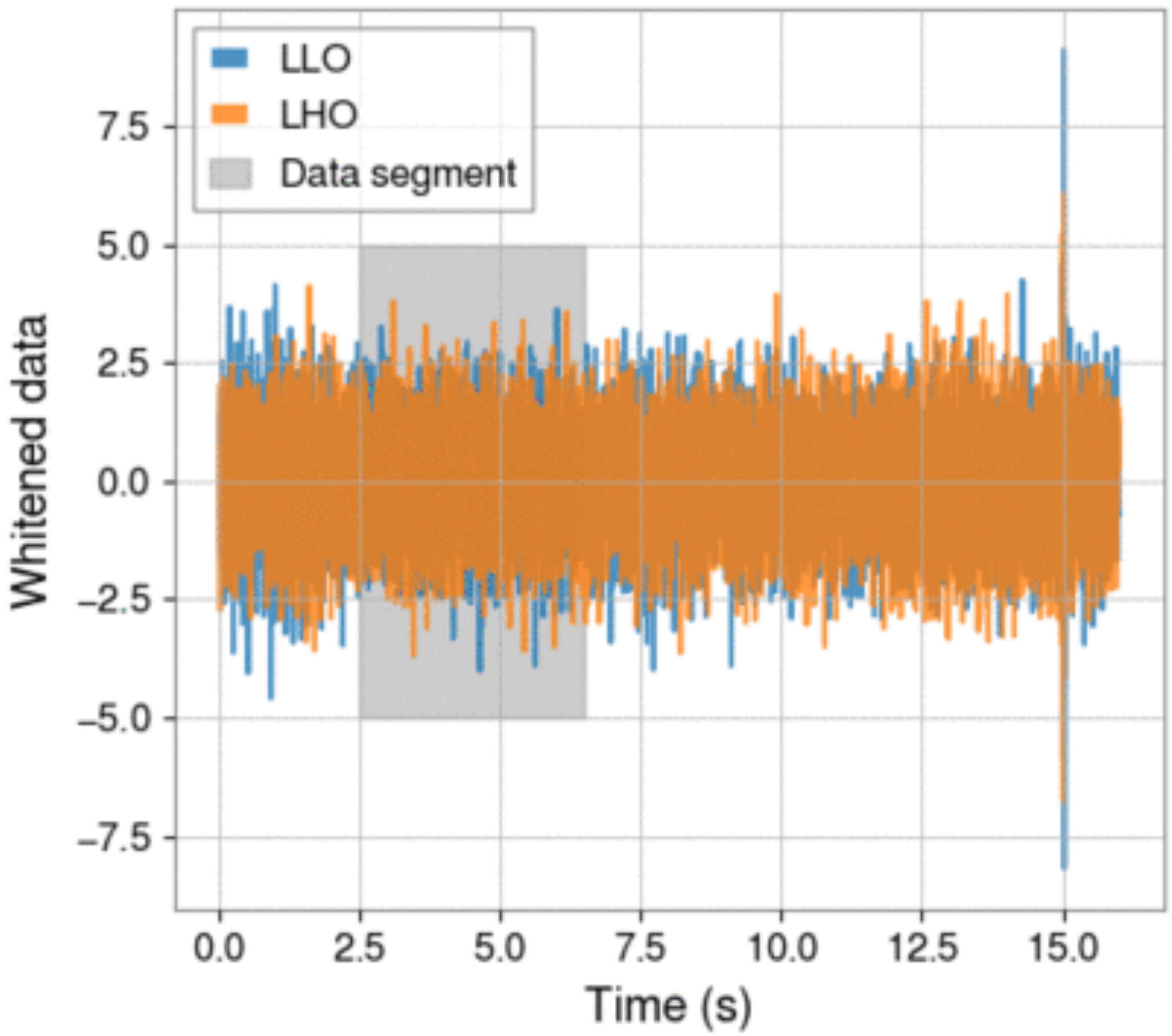
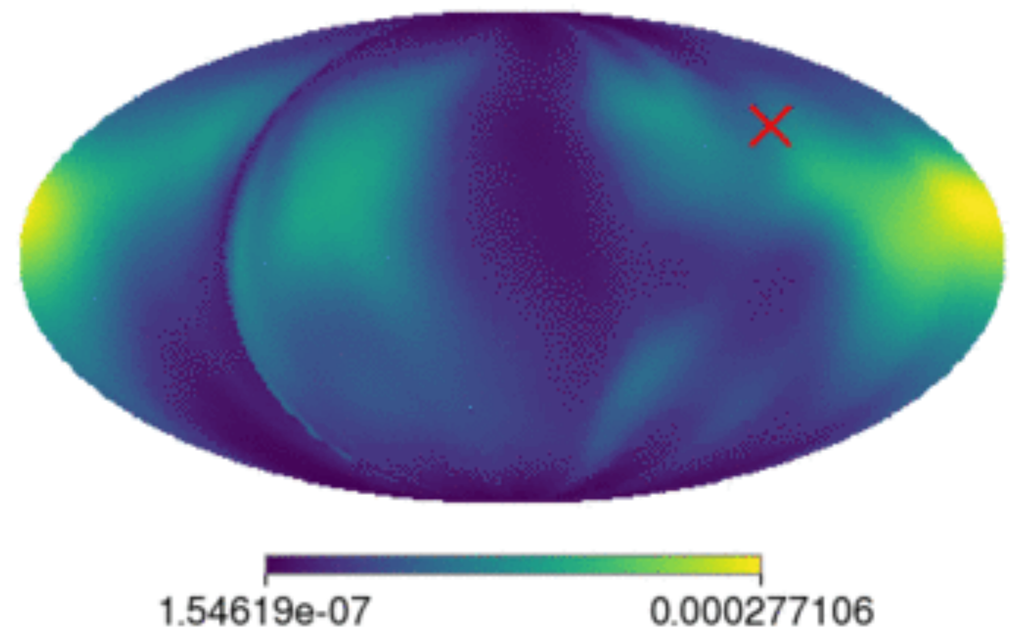


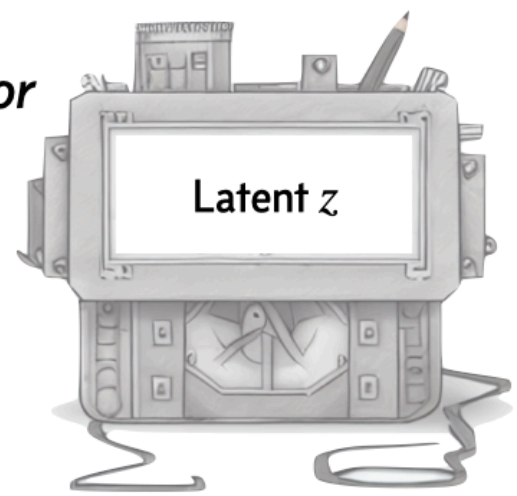


Lecture 23: Simulation Based Inference

Simulation Based Inference

Simulation-based inference (SBI)

Parameters θ → *Simulator* → Observations x



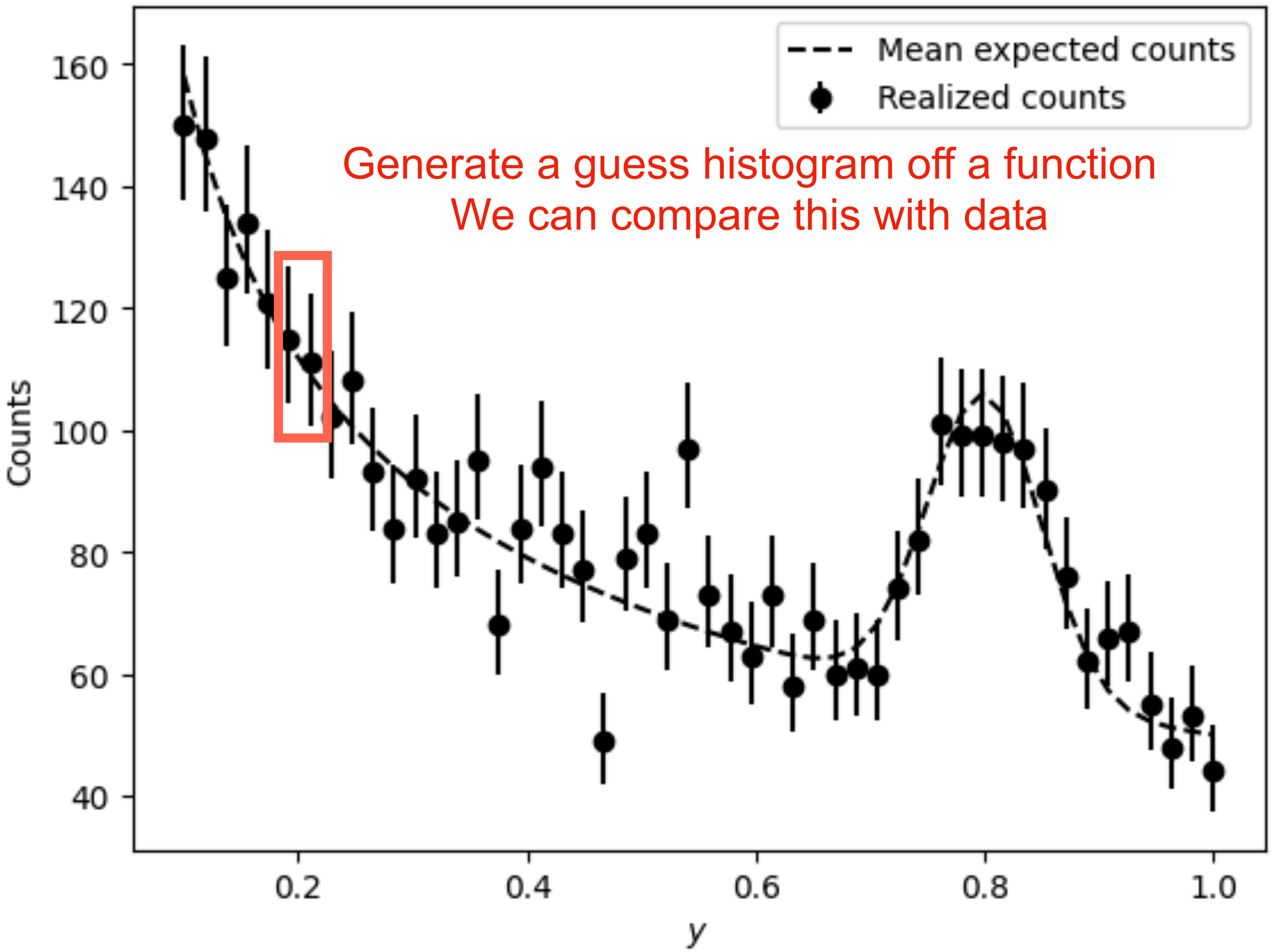
Prediction:

- Mechanistic forward model
- We can generate samples from a simulator $x \sim p(x \mid \theta)$

Inference:

- Likelihood $p(x \mid \theta) = \int \mathrm{d}z\, p(x, z \mid \theta)$ is intractable
- *Inference is challenging*

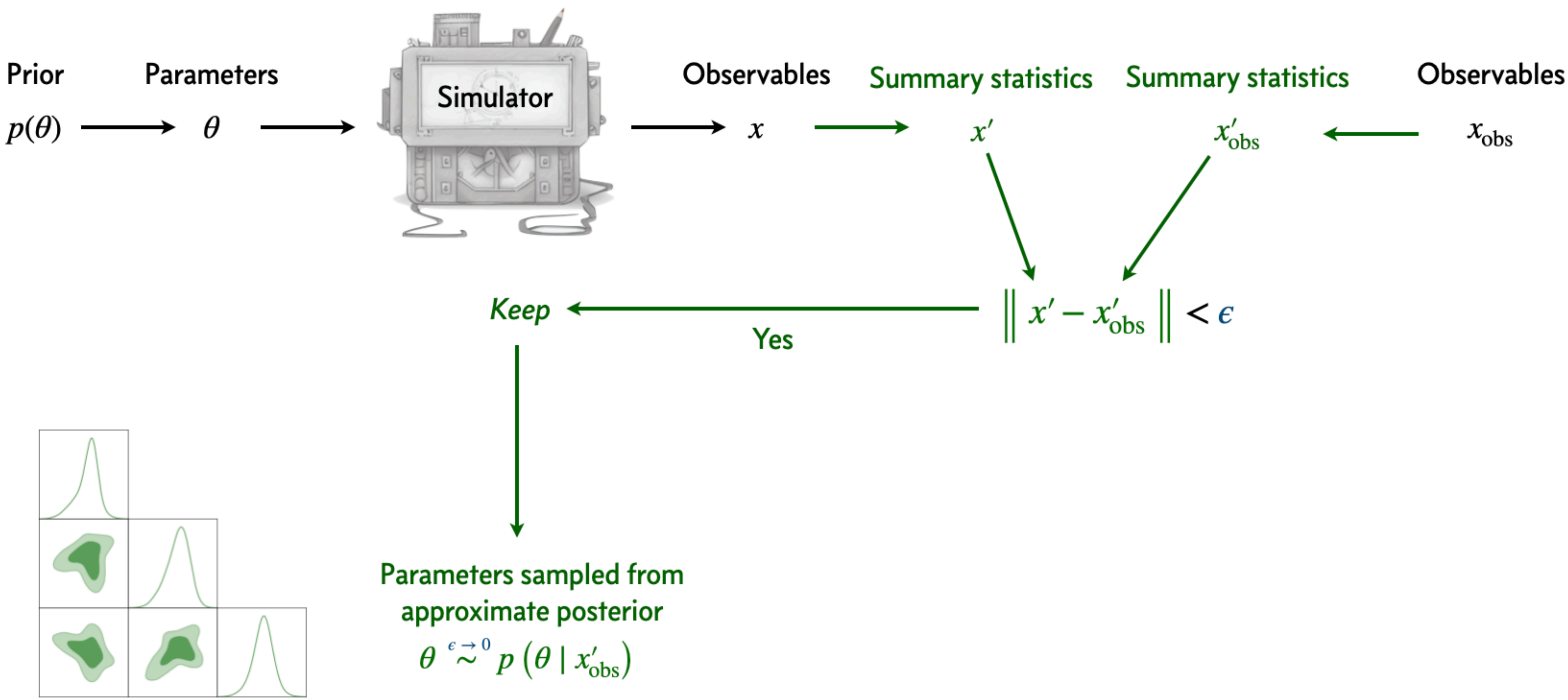
Poisson Fluctuation



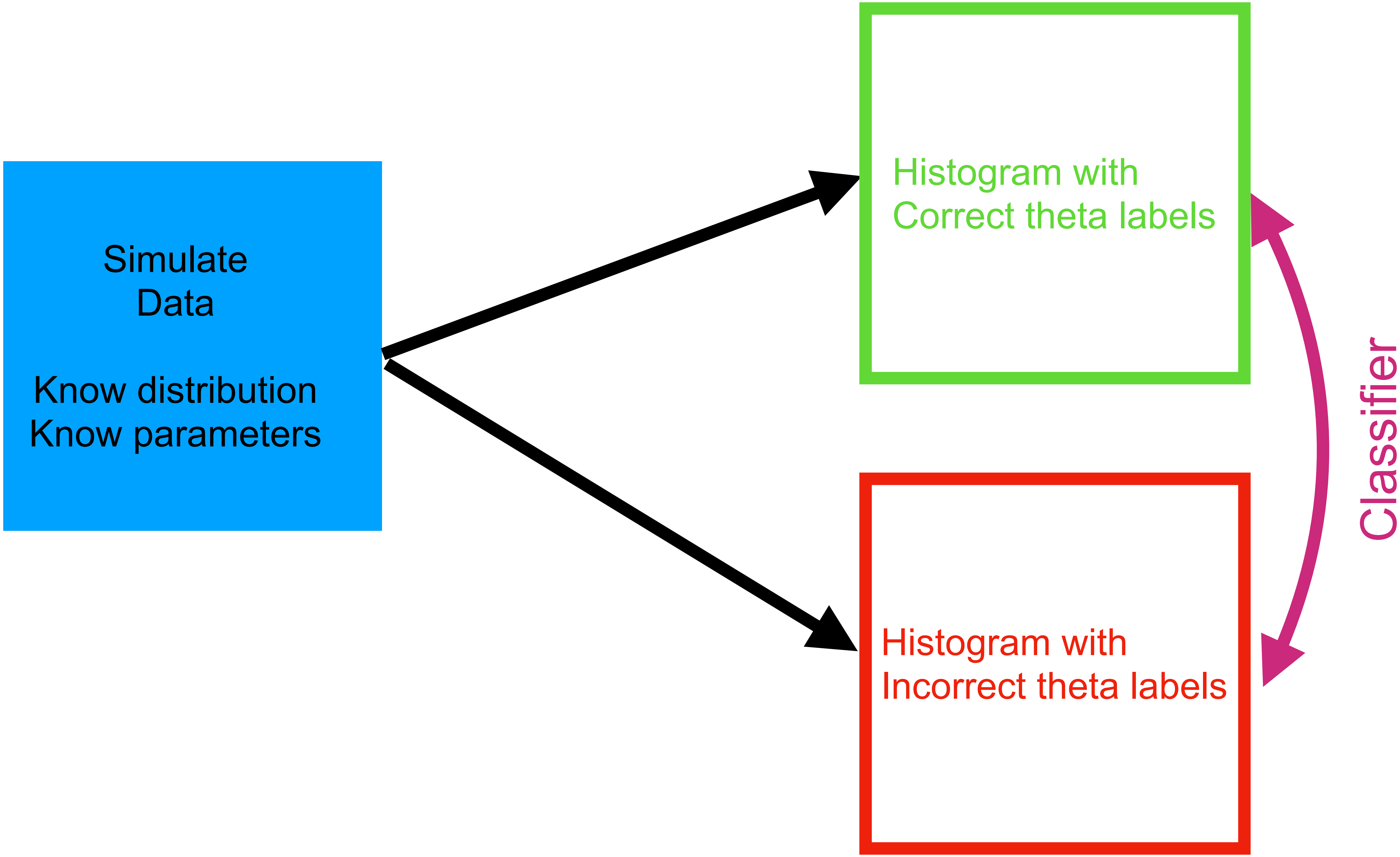
Poisson flucutate a func

"Traditional" SBI: *Approximate Bayesian Computation*

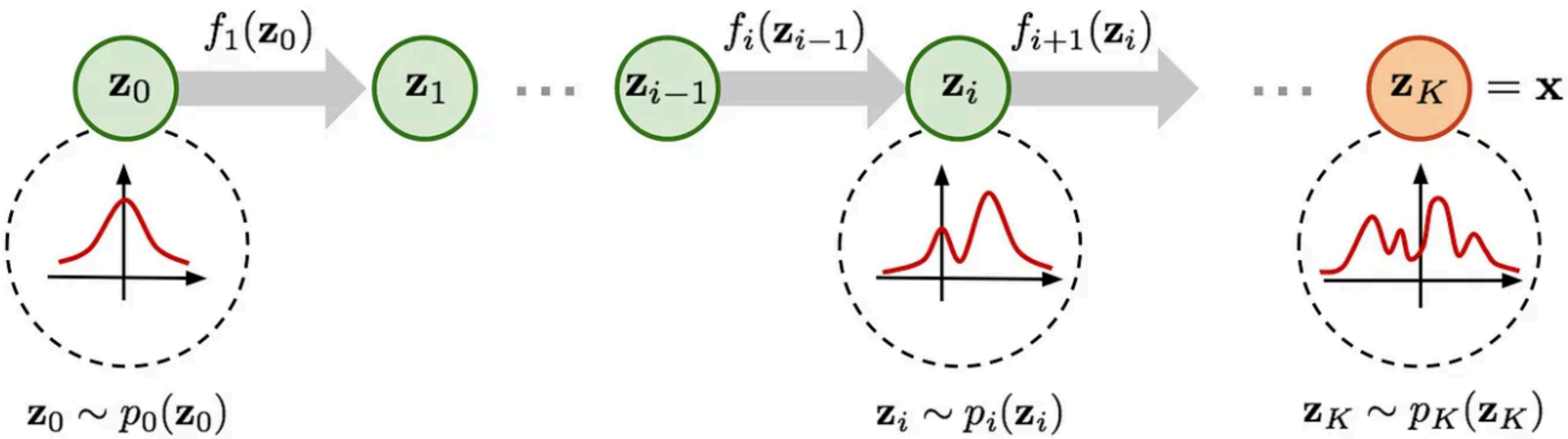
[Rubin 1984]



Importance Sampling



Normalizing Flow



$$z \sim p_\theta(z) = N(z; 0, 1)$$

$$x = f_\theta(z) = f_K \circ \ldots f_2 \circ f_1(z)$$

$$\textit{each } f_i \textit{ is invertible}$$

How Does it Work?

$$f : Z \rightarrow X,\ f\, is\, invertible$$
$$p_\theta(z)\, defined\, over\, z \epsilon Z$$
$$p_\theta(x) \neq p_\theta(f_\theta^{-1}(x)))$$

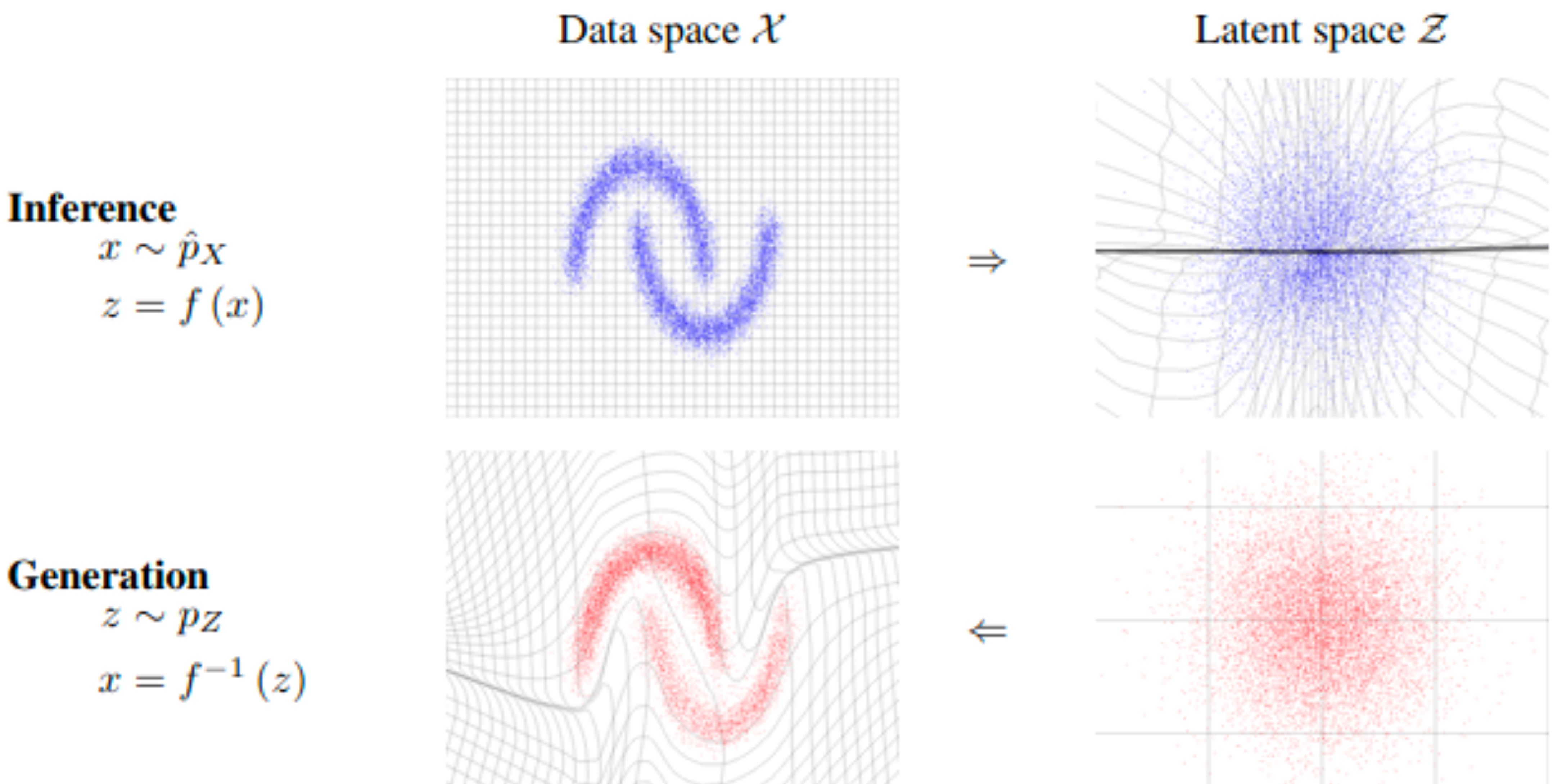
Change of variable formula:

$$p_\theta(x) = p_\theta(f_\theta^{-1}(x))) \left| det(\frac{\partial f^{-1}(x))}{\partial x}) \right|$$
$$p_\theta(x) = p_\theta(z)) \left| det(\frac{\partial z}{\partial x}) \right|$$

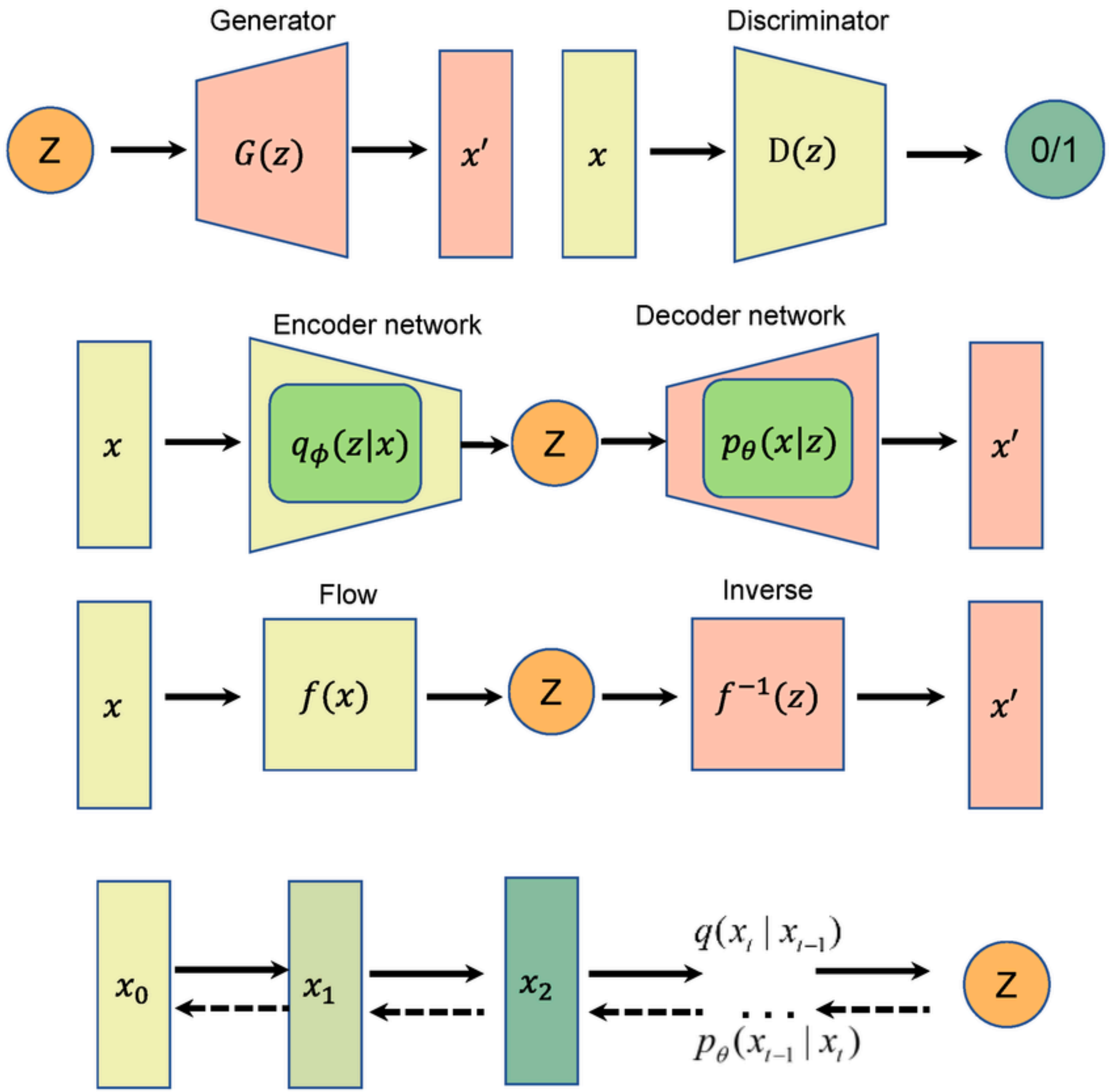
$$\log\left(p_\theta(x)\right) = \log\left(p_\theta(z)\right) + \sum_{i=1}^{K} \log \left| det(\frac{\partial f_i^{-1}}{\partial z_i}) \right|$$

exact likelihood evalutation

Exmple

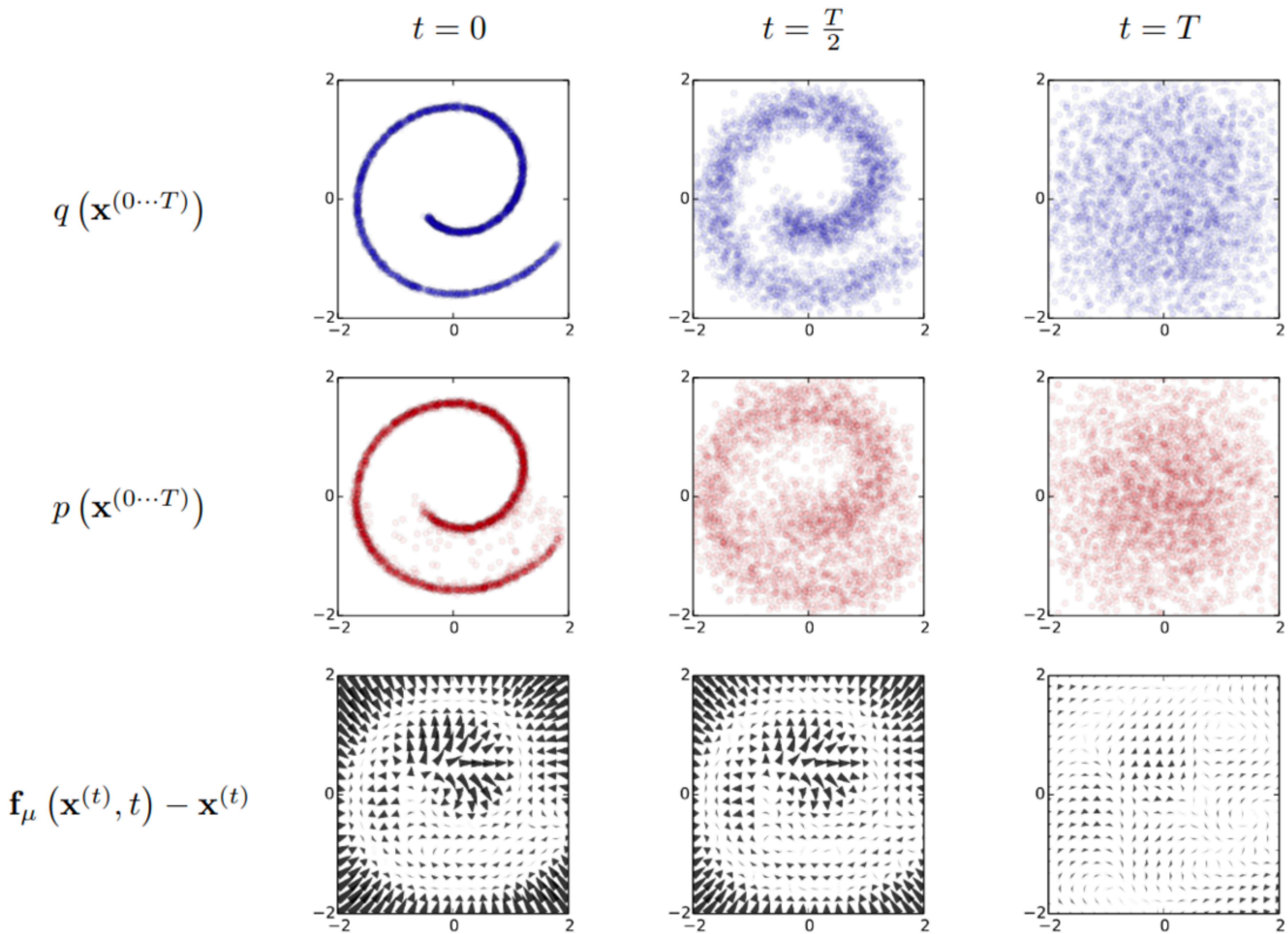

Data space $\mathcal{X}$
Latent space $\mathcal{Z}$
Inference
$x \sim \hat{p}_X$
$z = f(x)$
$\Rightarrow$
Generation
$z \sim p_Z$
$x = f^{-1}(z)$
$\Leftarrow$

Diffusion



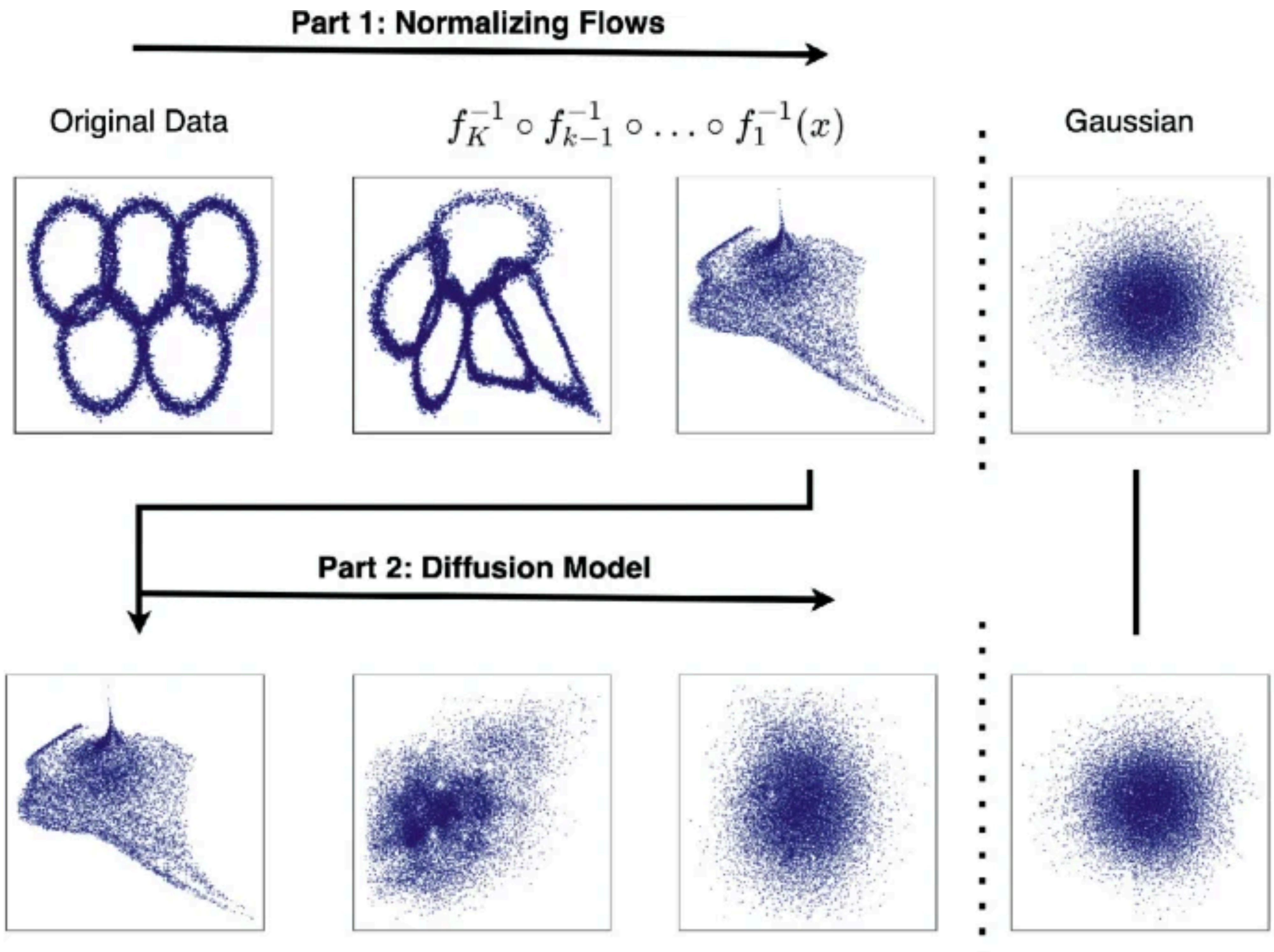
Generator
Discriminator
Z
$G(z)$
x'
x
$D(z)$
0/1
Encoder network
Decoder network
x
$q_\phi(z|x)$
Z
$p_\theta(x|z)$
x'
Flow
Inverse
x
$f(x)$
Z
$f^{-1}(z)$
x'
x_0
x_1
x_2
$q(x_t | x_{t-1})$
...
$p_\theta(x_{t-1} | x_t)$
Z

Exmple



$t = 0$
$t = \frac{T}{2}$
$t = T$
$q\left(\mathbf{x}^{(0\cdots T)}\right)$
$p\left(\mathbf{x}^{(0\cdots T)}\right)$
$\mathbf{f}_{\mu}\left(\mathbf{x}^{(t)}, t\right) - \mathbf{x}^{(t)}$
2
0
−2
−2
0
2

Combo



Part 1: Normalizing Flows
Original Data
$f_K^{-1} \circ f_{k-1}^{-1} \circ \ldots \circ f_1^{-1}(x)$
Gaussian
Part 2: Diffusion Model

Importance Sampling