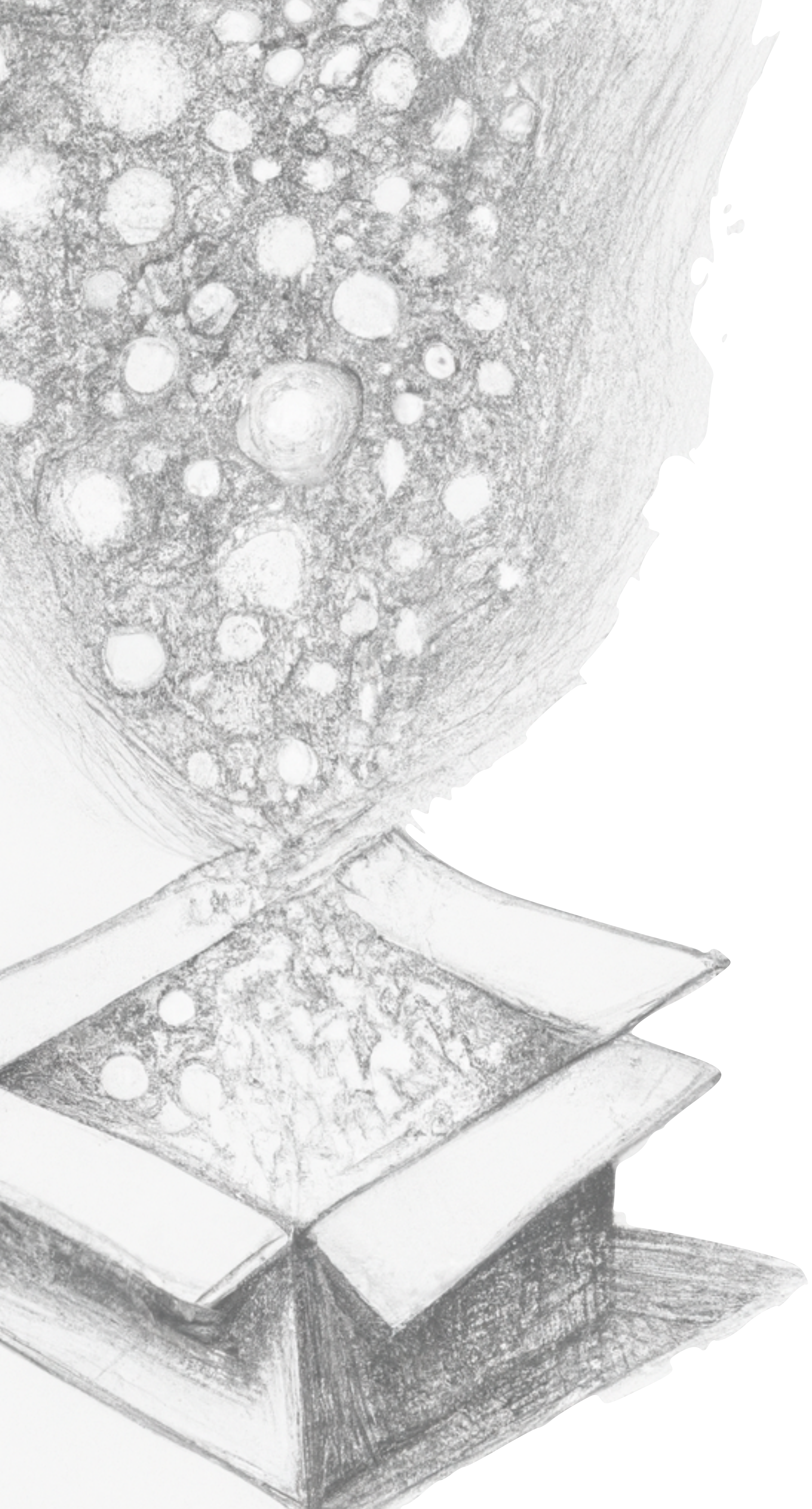


An introduction to generative modeling

with applications in physics

smsharma.io/iaifi-summer-school-2023

Siddharth Mishra-Sharma

(smsharma.io/@kdqg1)

NSF AI Institute for Artificial Intelligence and Fundamental Interactions (IAIFI)

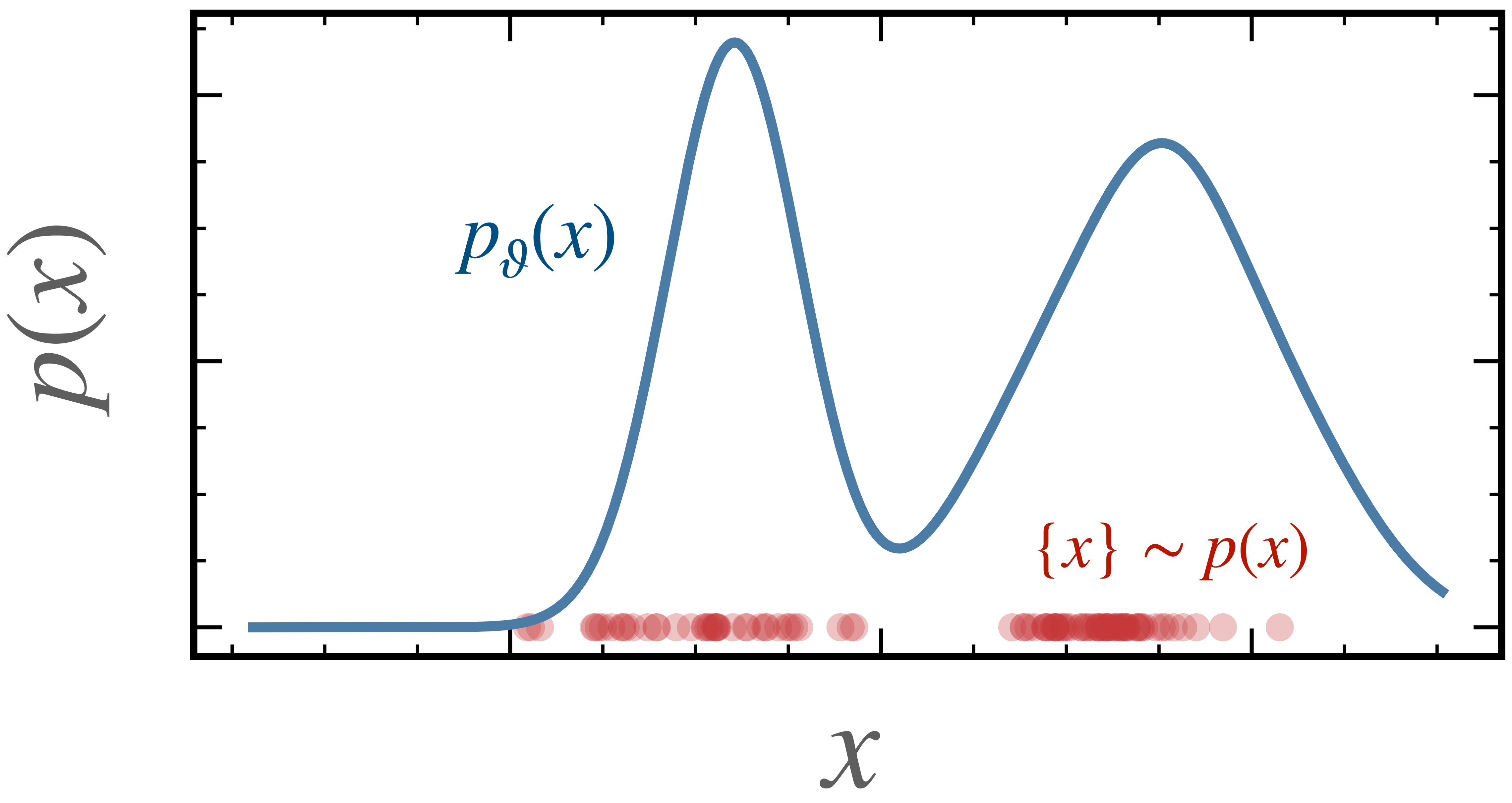
IAIFI Summer School

August 8, 2023

Generative models

Generative models are simulators of the data

Goal: learn a probability distribution $p_\vartheta(x)$ that is as close as possible to the true underlying data distribution $p(x)$



1. Sampling

$$x \sim p_\vartheta(x)$$

2. Density estimation

$$\log p_\vartheta(x)$$

Evolution of deep generative models

Variational autoencoders
(from Kingma et al 2013)

Diffusion models
(*Midjourney* 2023)

The landscape of deep generative models

[Karsten Kreis; CVPR 2022 Tutorial]

Diffusion models

Energy-based models

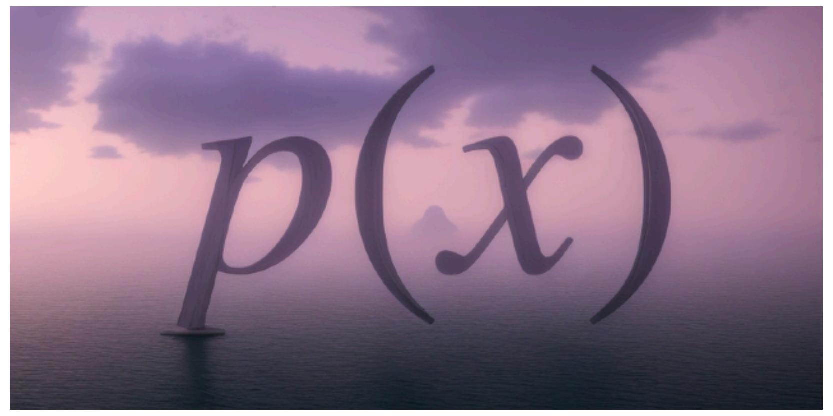
Variational autoencoders

Normalizing flows

Autoregressive models

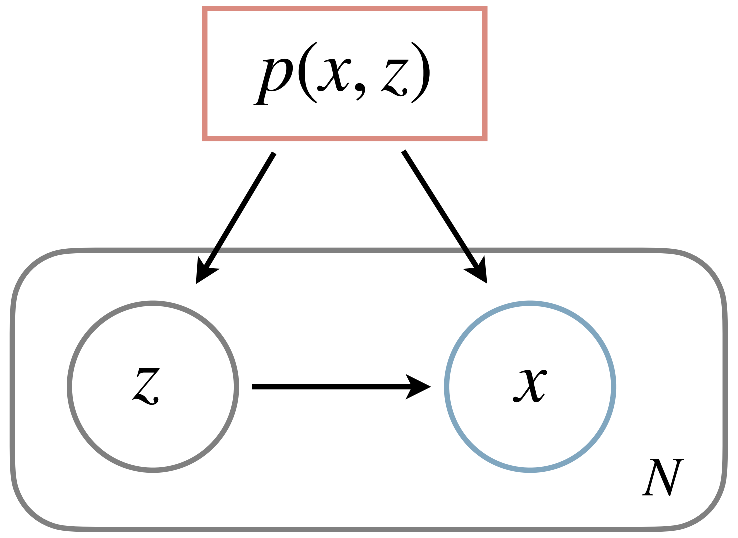
Generative adversarial networks

Outline



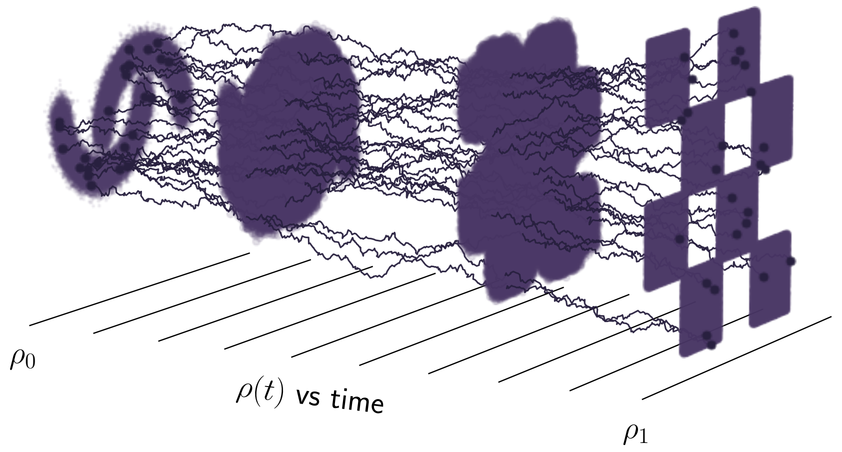
Why (deep) generative modeling?

What is it, and what can it do for you?



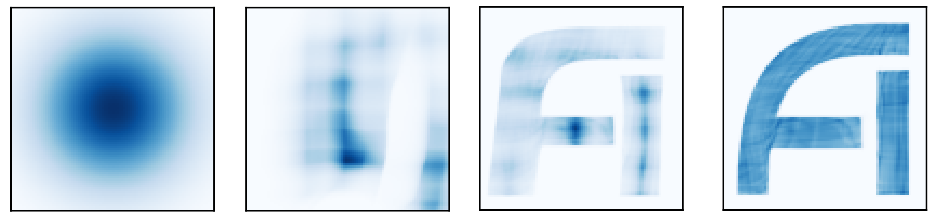
Variational auto encoders

Latent-variable modeling, and compression is all you need



Diffusion models

Models based on iterative refinement



Normalizing flows

Invertible transformations

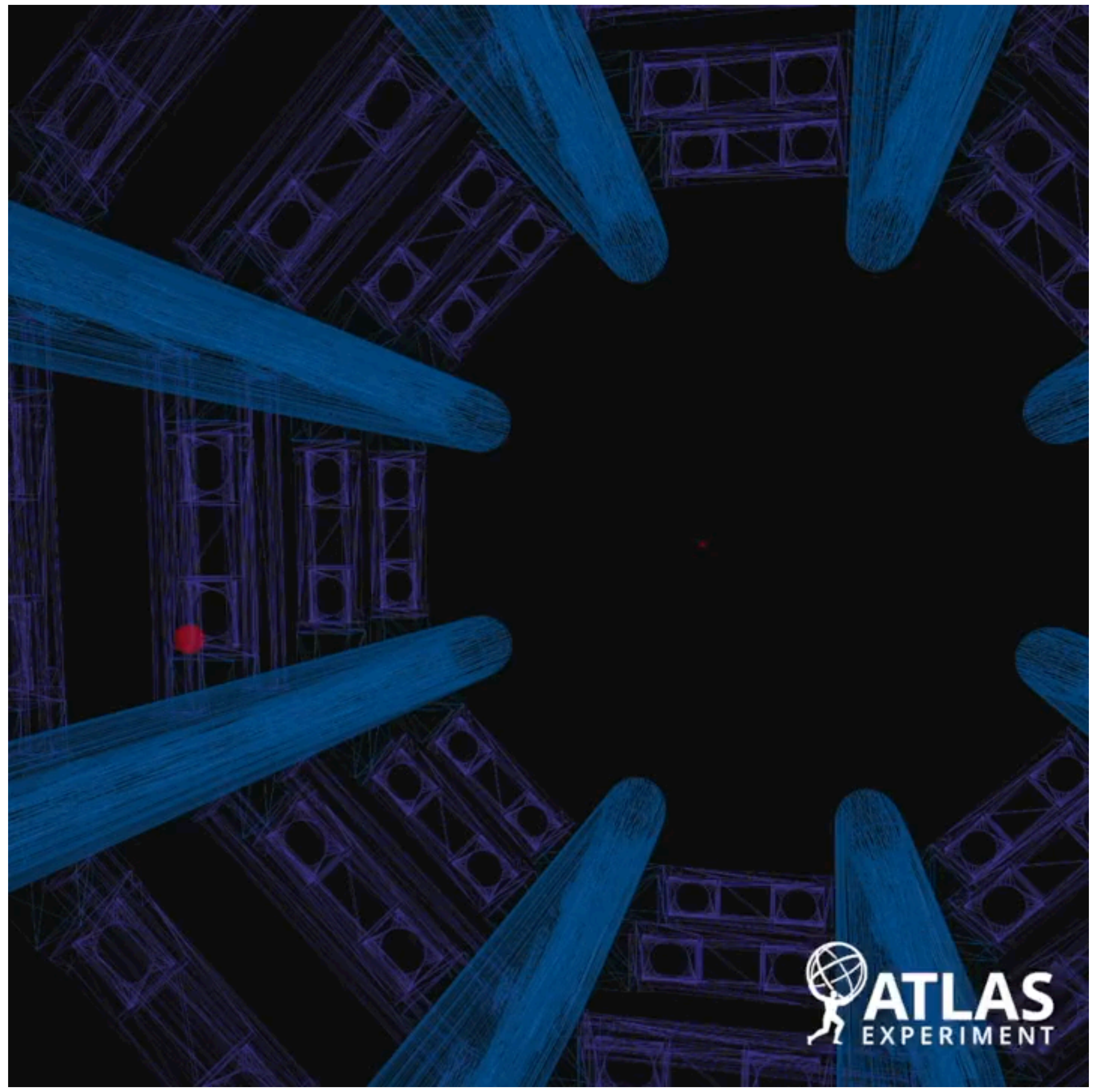
Simulators

$$x \sim p(x)$$

Simulators are ubiquitous: *they prescribe a way to sample from the data distribution*

Collider data

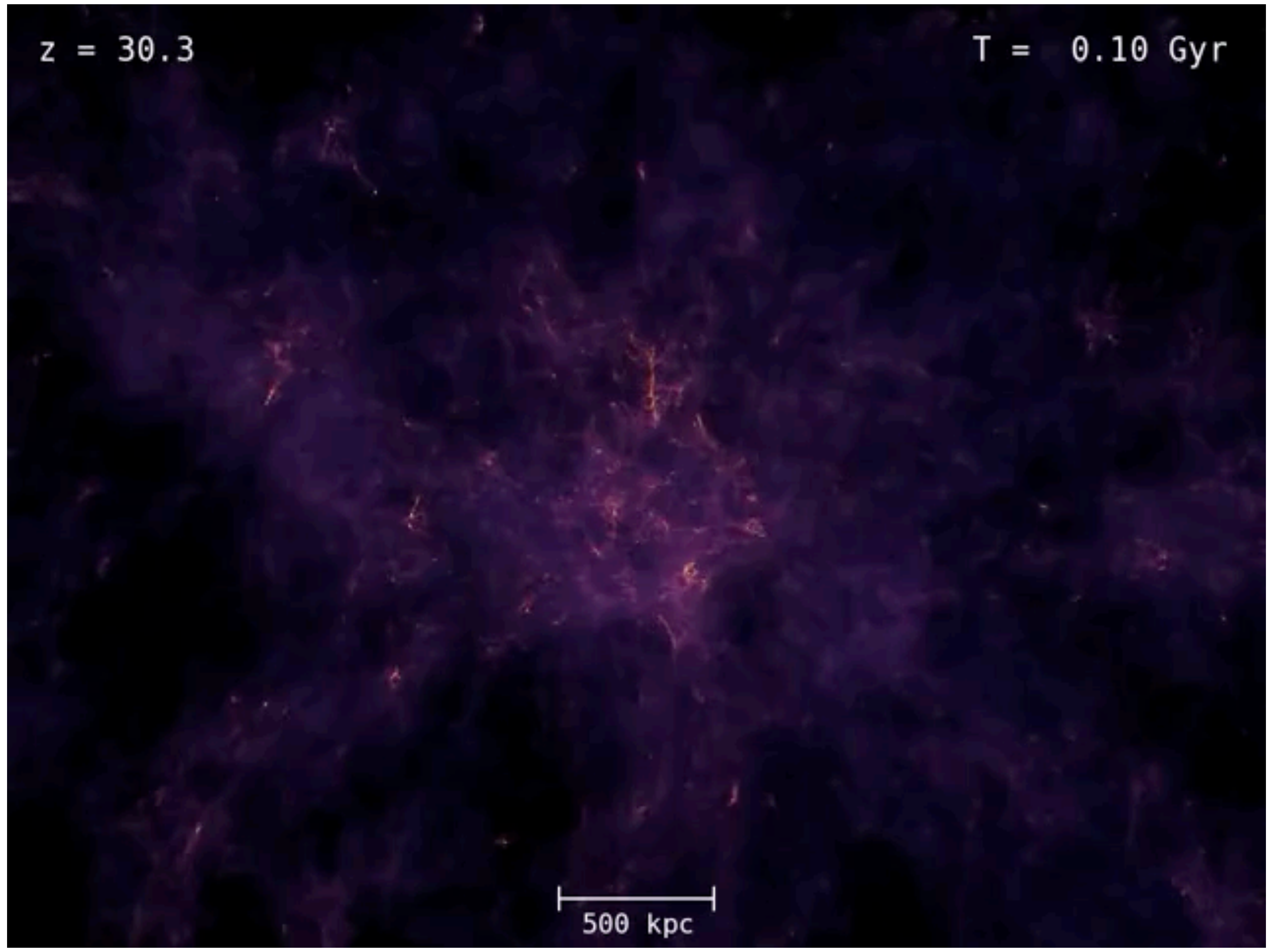
particles $\sim p$(particles)



[C. Cesarotti with ATLAS]

Cosmology data

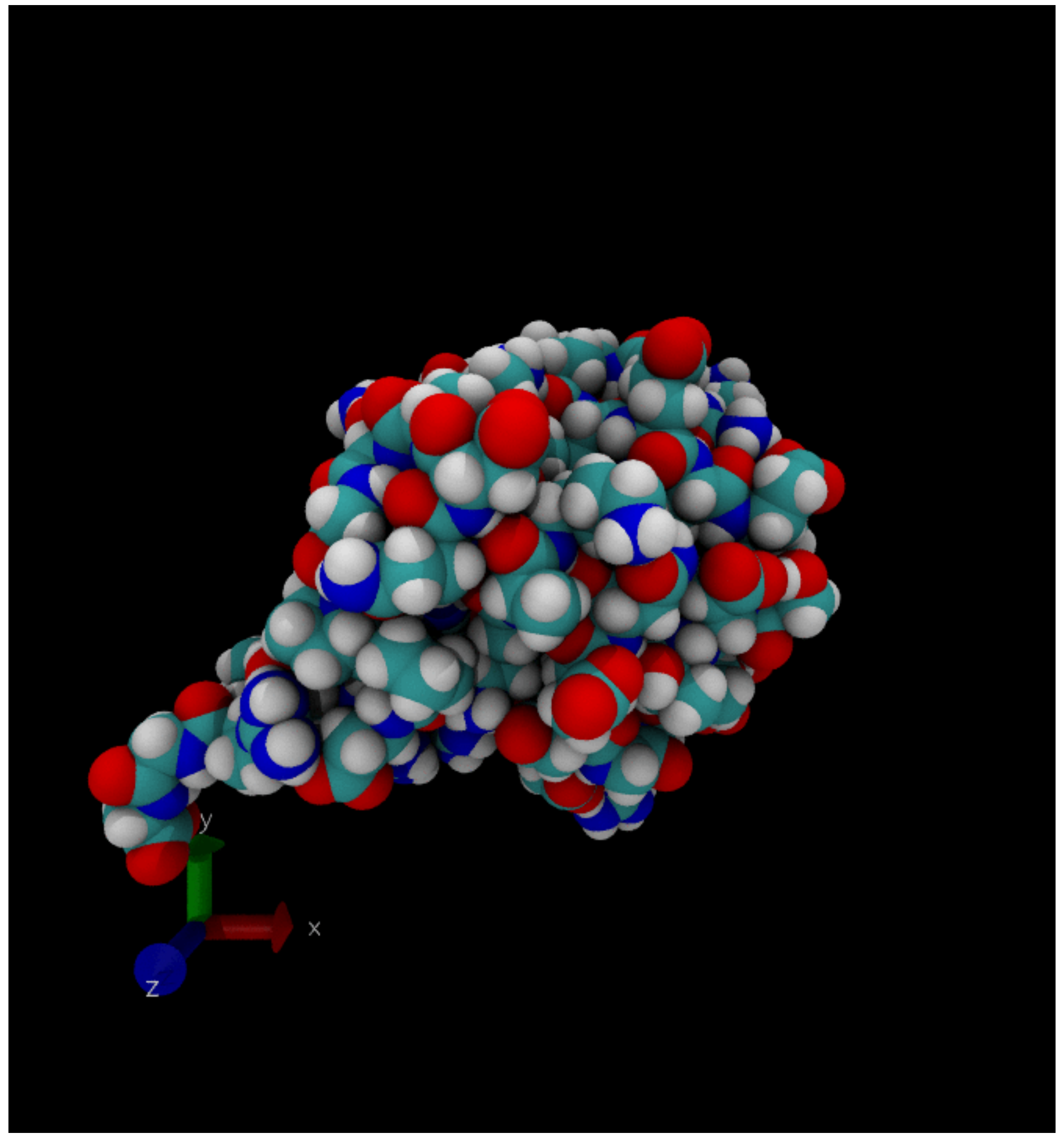
particles $\sim p$(particles)



[Aquarius simulation]

Molecular dynamics

configurations $\sim p$(configurations)



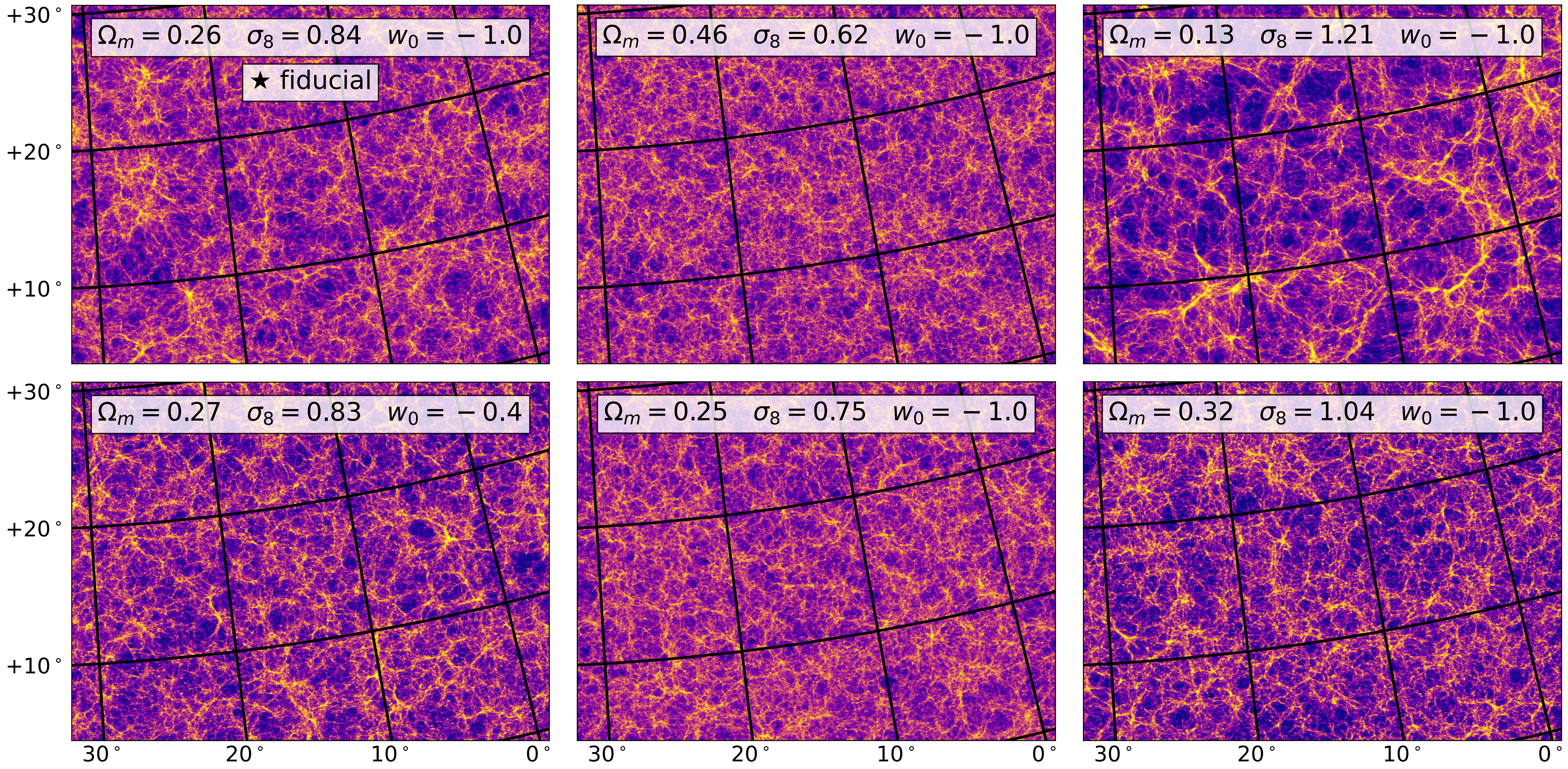
[E. Cances et al]

Conditional simulators

Conditional simulations *sample from the likelihood* $p(x \mid \theta)$

Cosmology data

$$\text{map} \sim p(\text{map} \mid \{\Omega_m, \sigma_8, w_0\})$$



[Kacprzak et al 2022]

$$x \sim p(x; \mathscr{M})$$

Model

or

$$x \sim p(x \mid \theta)$$

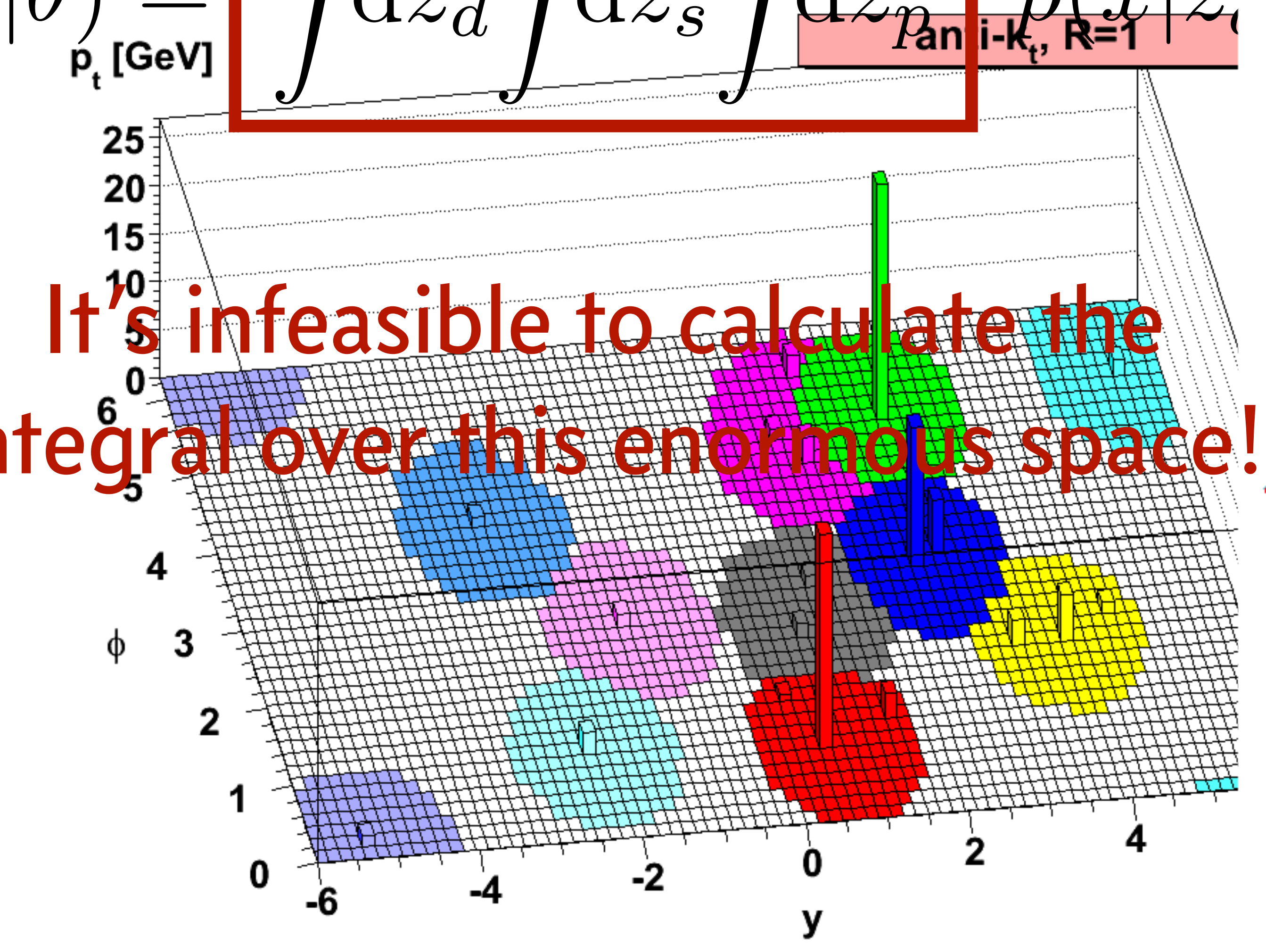
Model parameters

Are simulators all you need?

Latent variables

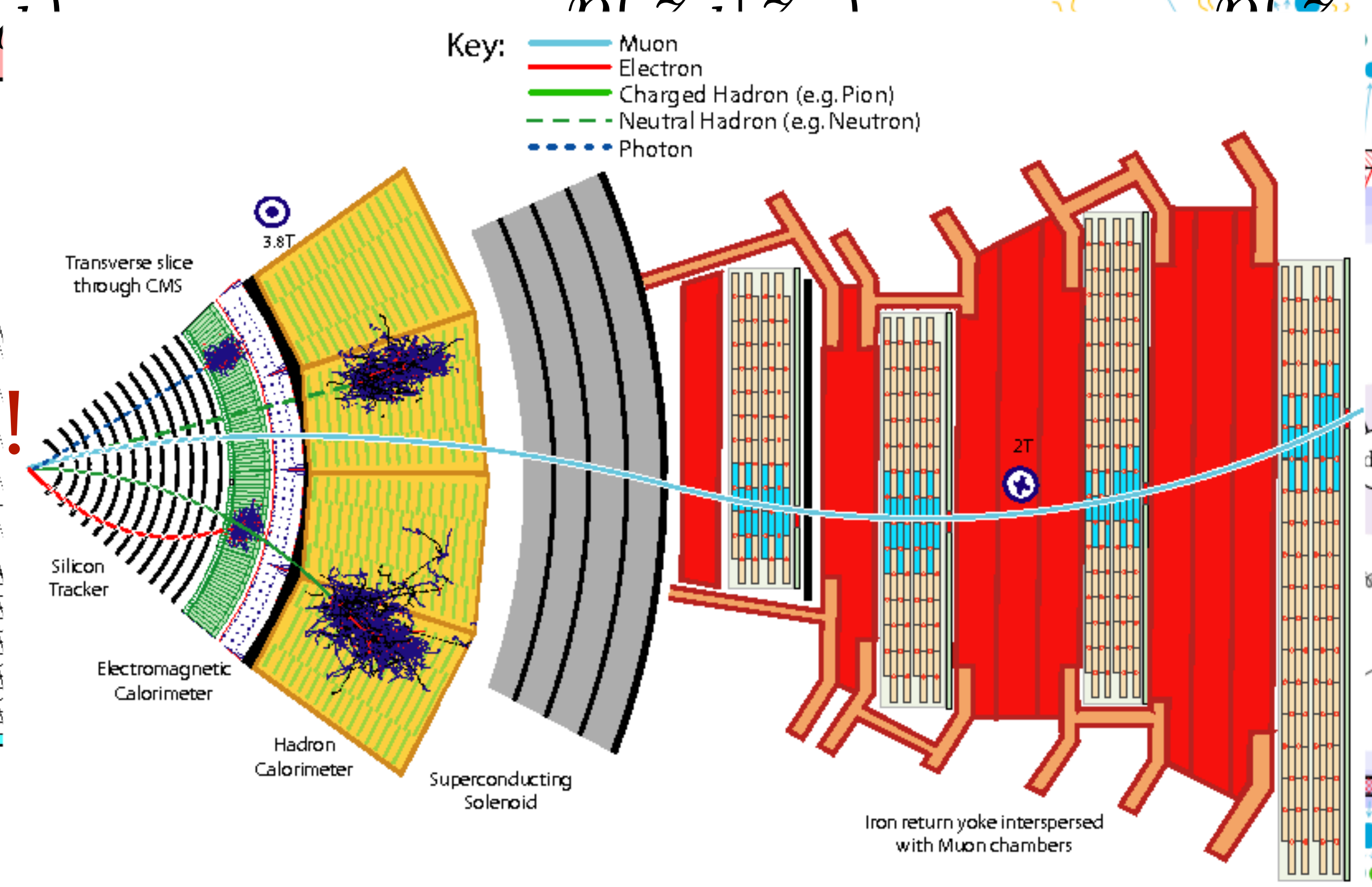
Observables	Detector interactions	Shower splittings	Parton-level momenta	Theory parameters
x ←	z_d ←	z_s ←	z_p ←	θ

$$p(x|\theta) = \boxed{\int \mathrm{d}z_d \int \mathrm{d}z_s \int \mathrm{d}z_p}\; p(x|z_d) \quad p(z_d|z_s) \quad p(z_s|z_p) \quad p(z_p|\theta)$$

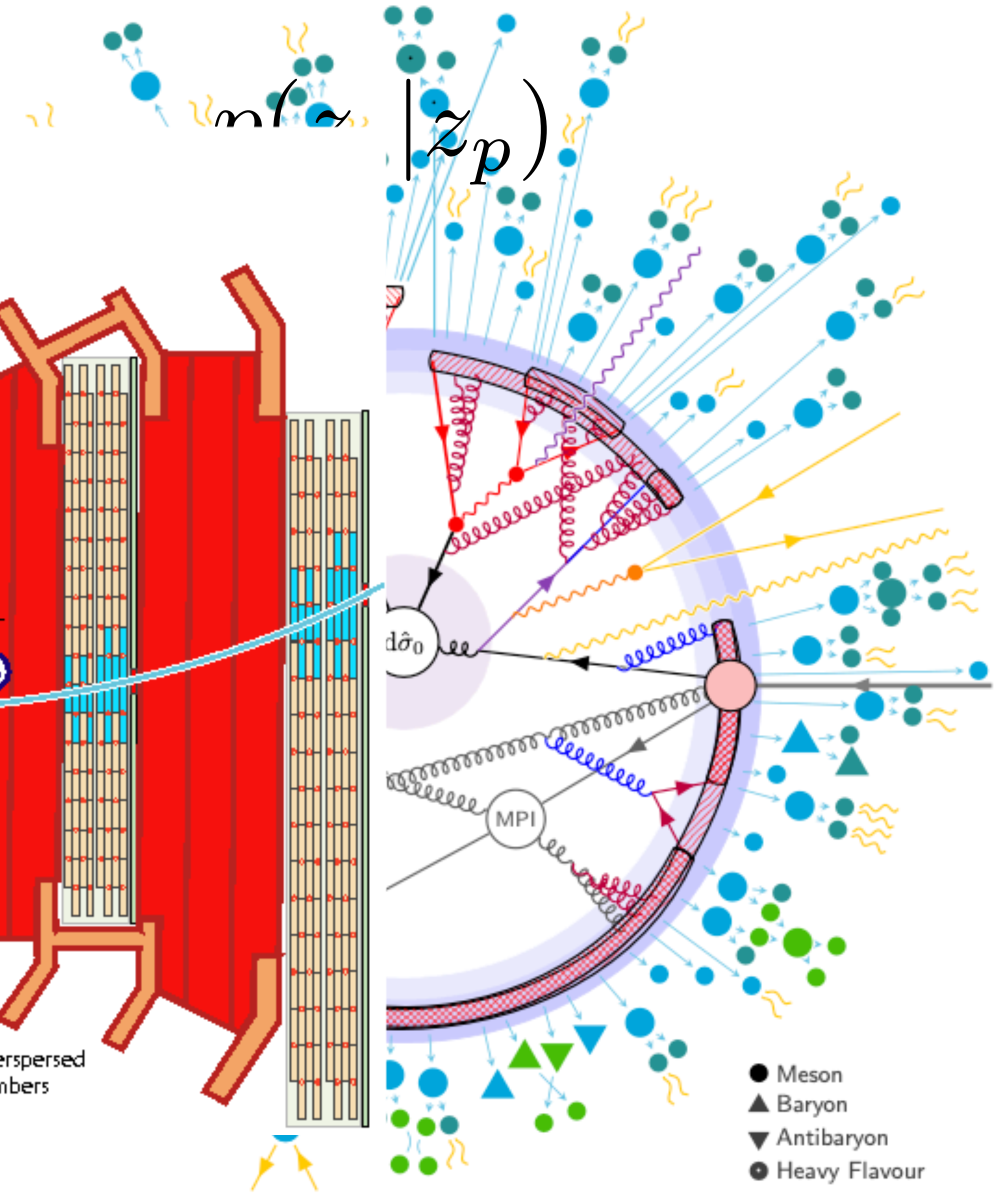


It's infeasible to calculate the integral over this enormous space!

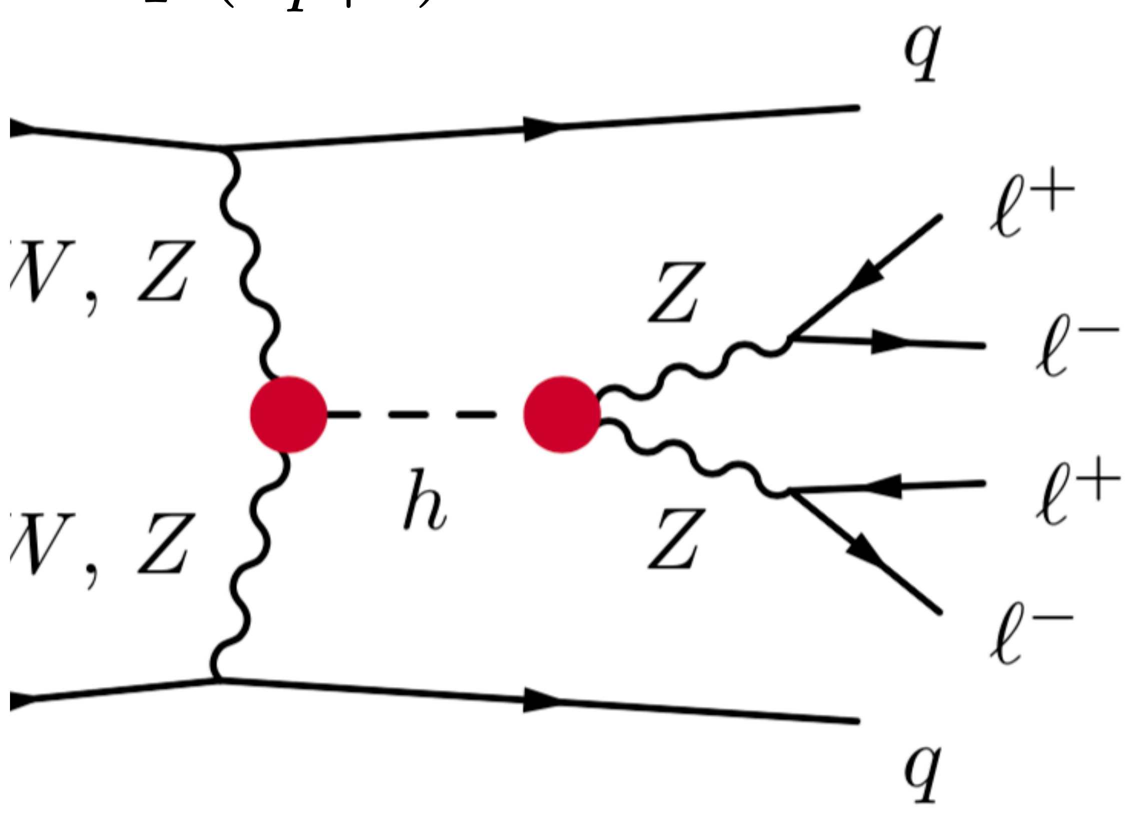
[M. Cacciari, G. Salam, G. Soyez 0802.1189]



[CMS]



[Pythia]



Prediction (simulation)

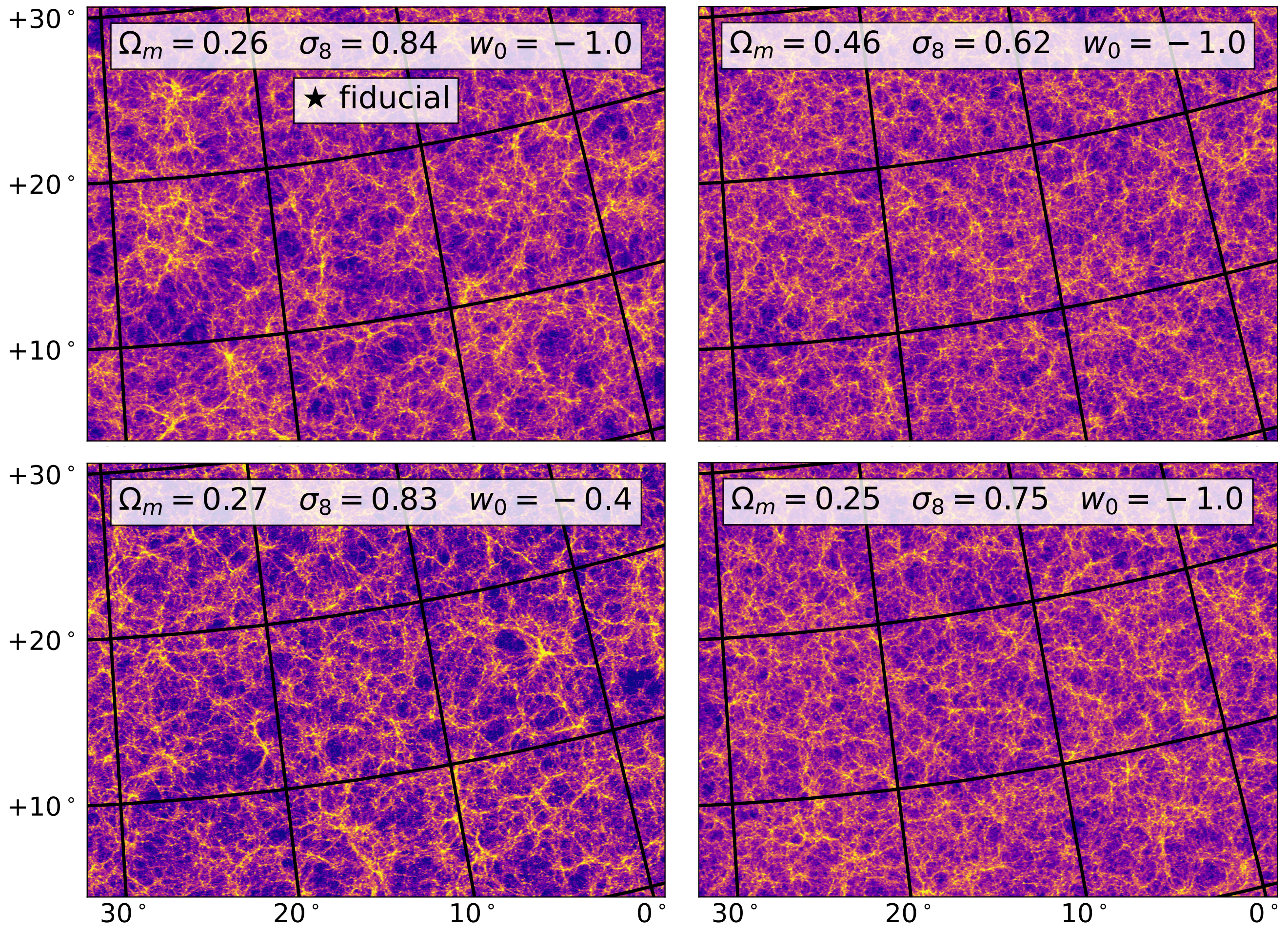
Inference

What could we do with $p(x)$?

Produce samples

for downstream applications: a fast simulator/emulator

$$x \sim p(x \mid \theta)$$

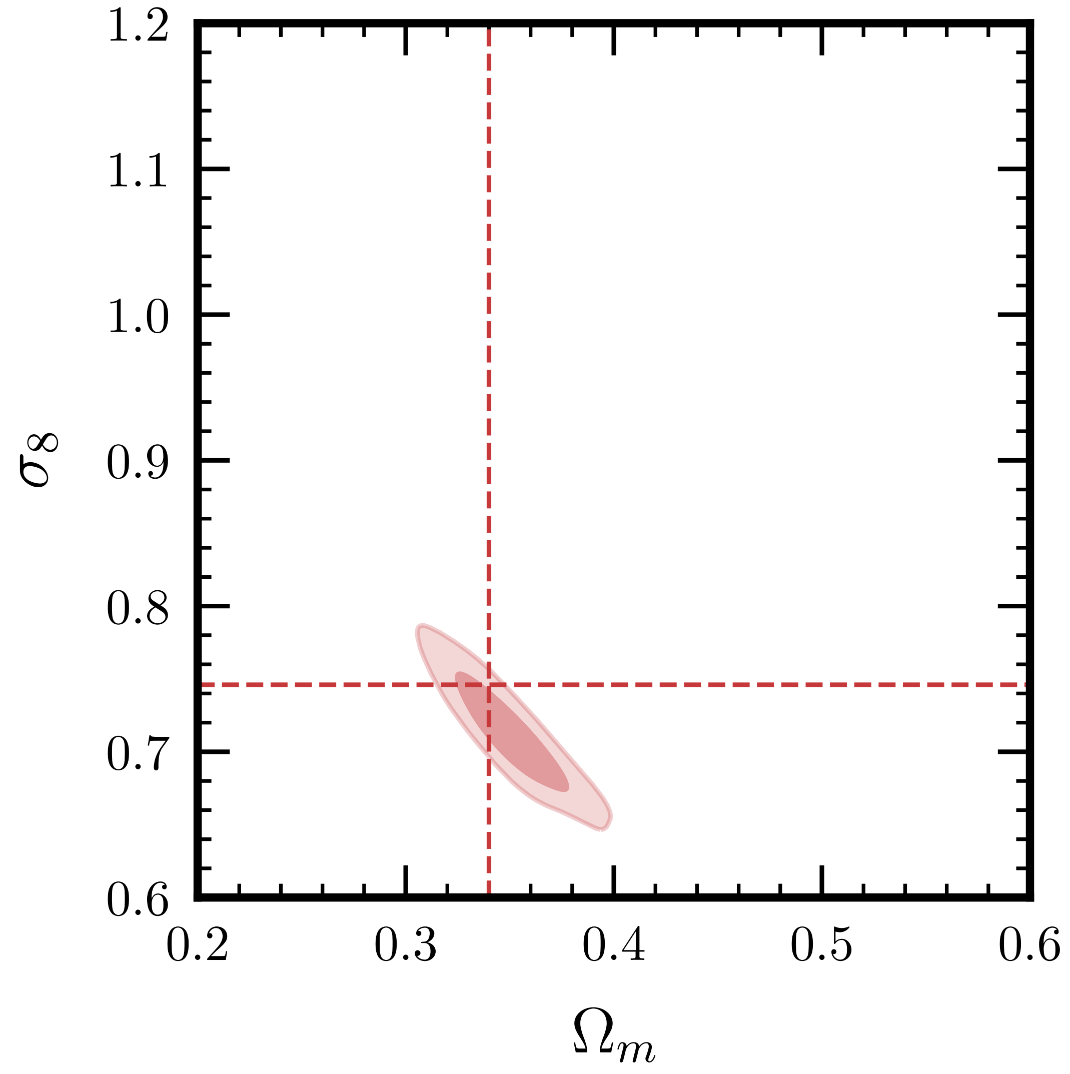


[Kacprzak et al 2022]

Evaluate likelihood

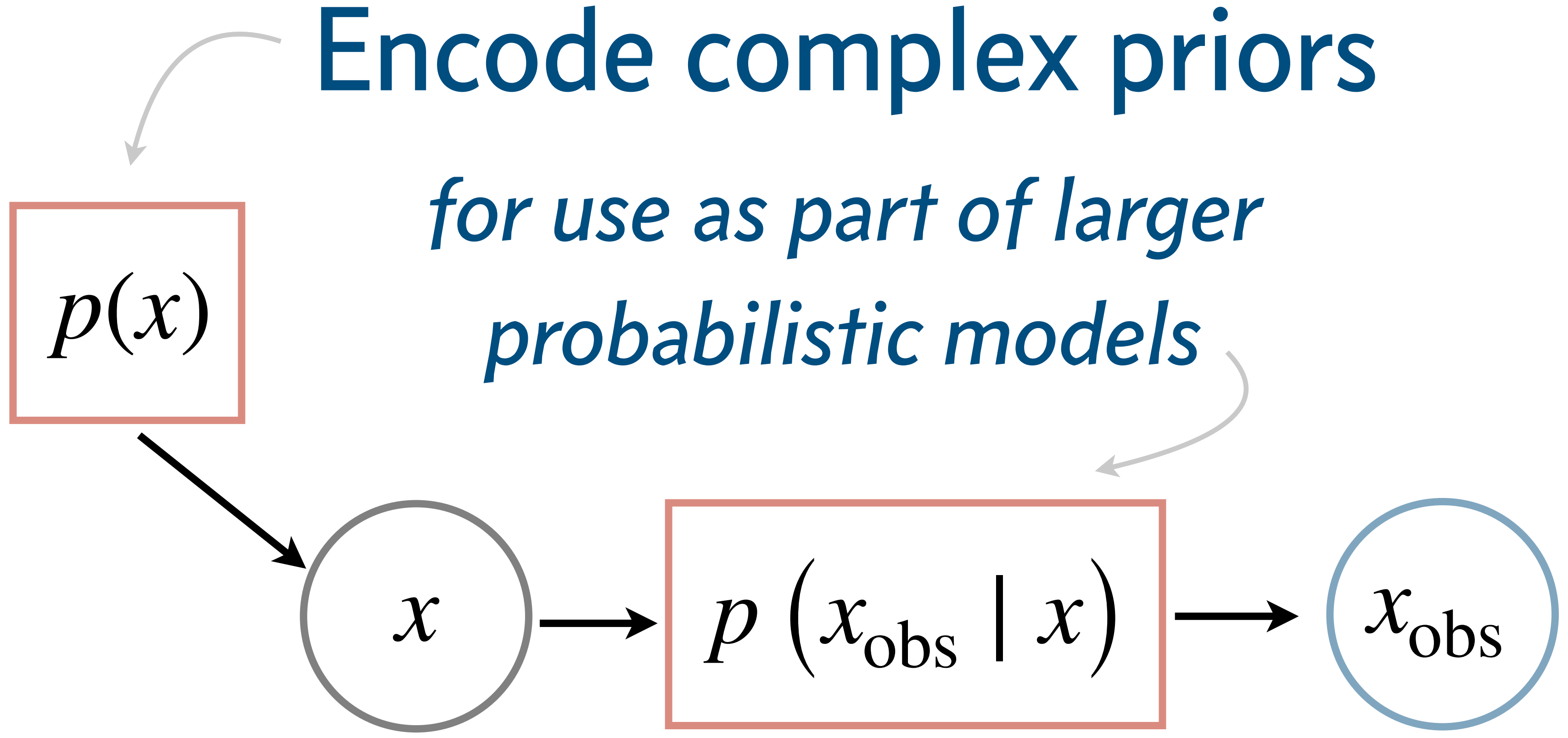
for model selection, parameter inference, outlier detection, …

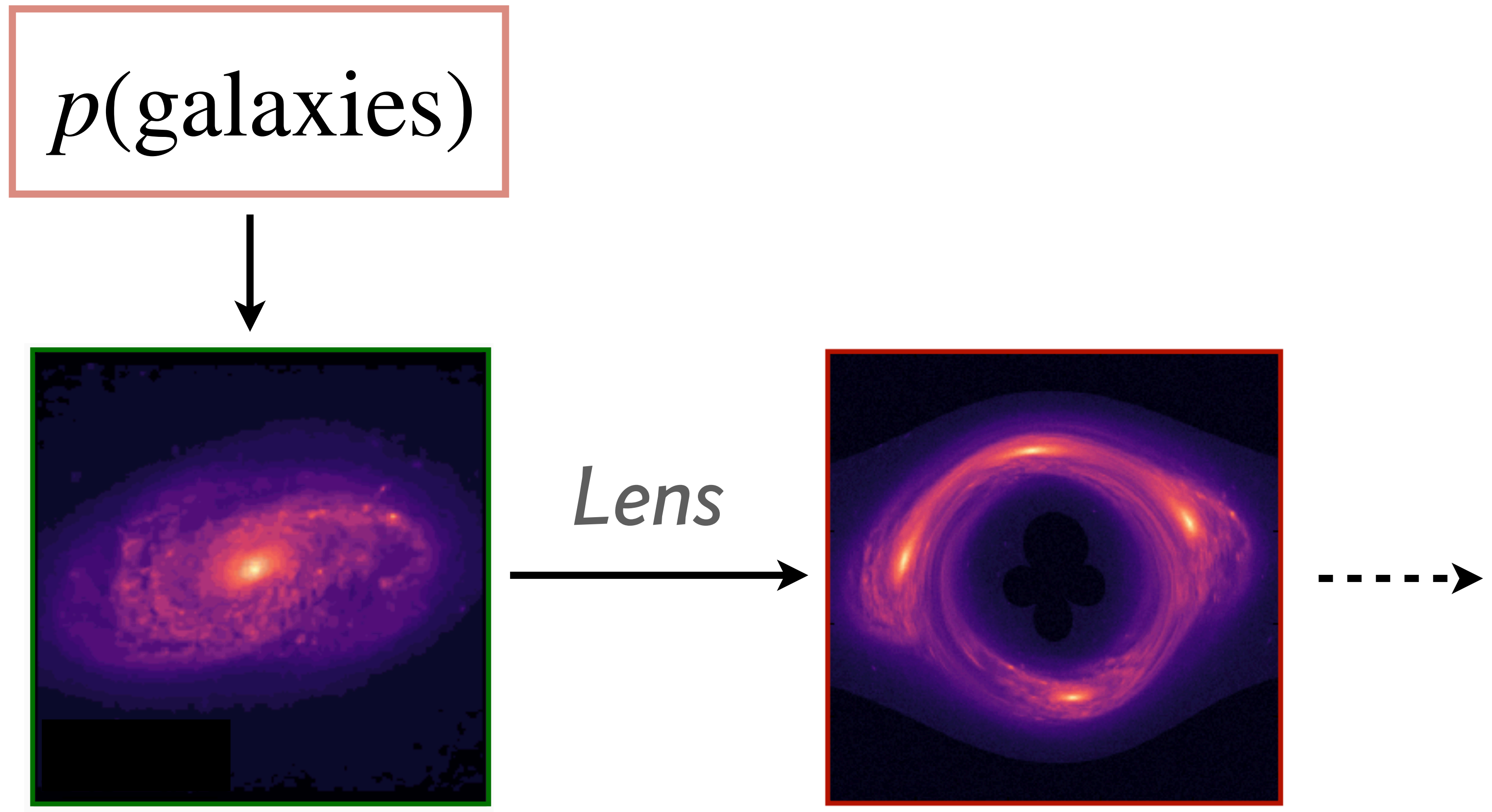
$$p(\theta \mid x) = \frac{p(x \mid \theta) \cdot p(\theta)}{p(x)}$$



Encode complex priors

for use as part of larger probabilistic models

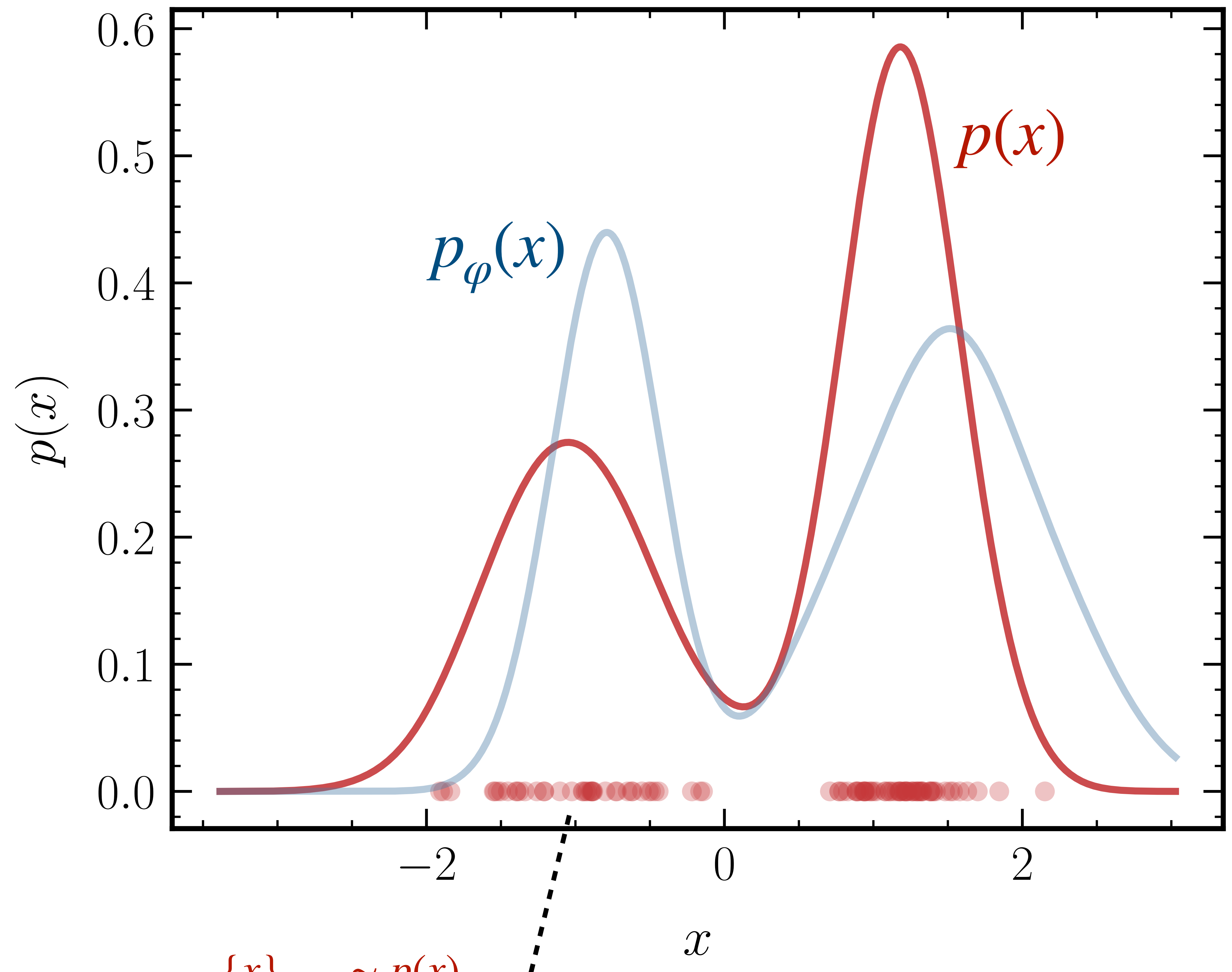




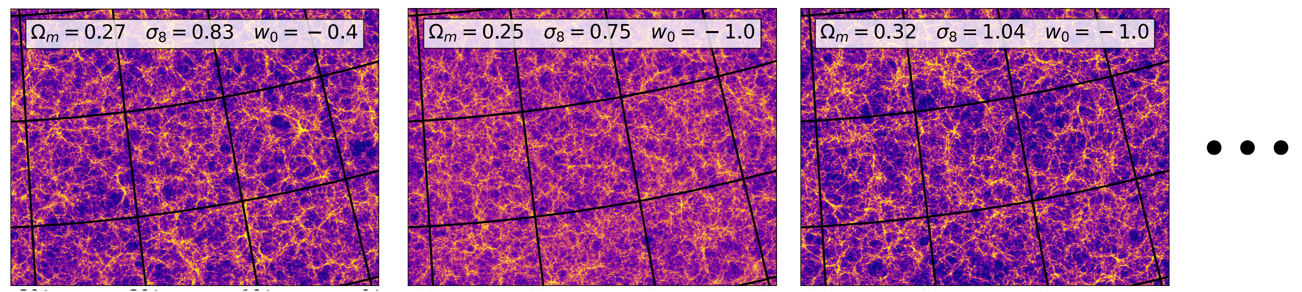
Generative modeling can efficiently enable these for a wide variety of scientific data/models!

Learning the data distribution

I'm sold! *How do I learn a generative model for my data?*



$\{x\}_{\text{train}} \sim p(x)$



1. Ingredients:

- A parameterized distribution $\boxed{p_\varphi(x)}$
- Samples from the data distribution $\{x\}_{\text{train}} \sim p(x)$

(empirical or simulated)

2. Maximize the likelihood of the model under the training data samples

$$\hat{\varphi} = \boxed{\arg\max_{\varphi}} \left[\log p_\varphi\left(\{x\}_{\text{train}}\right)\right]$$

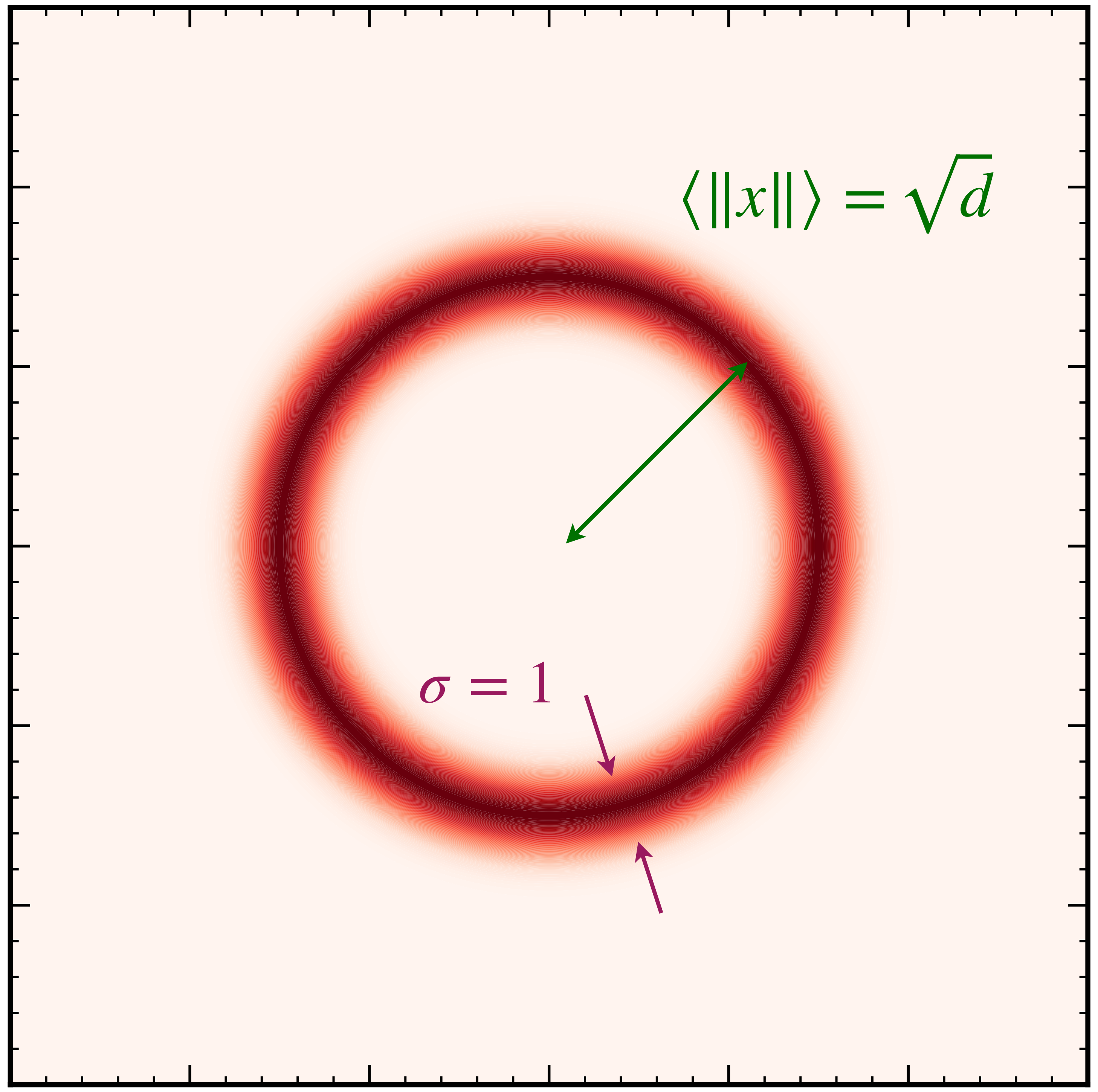
Not so fast...

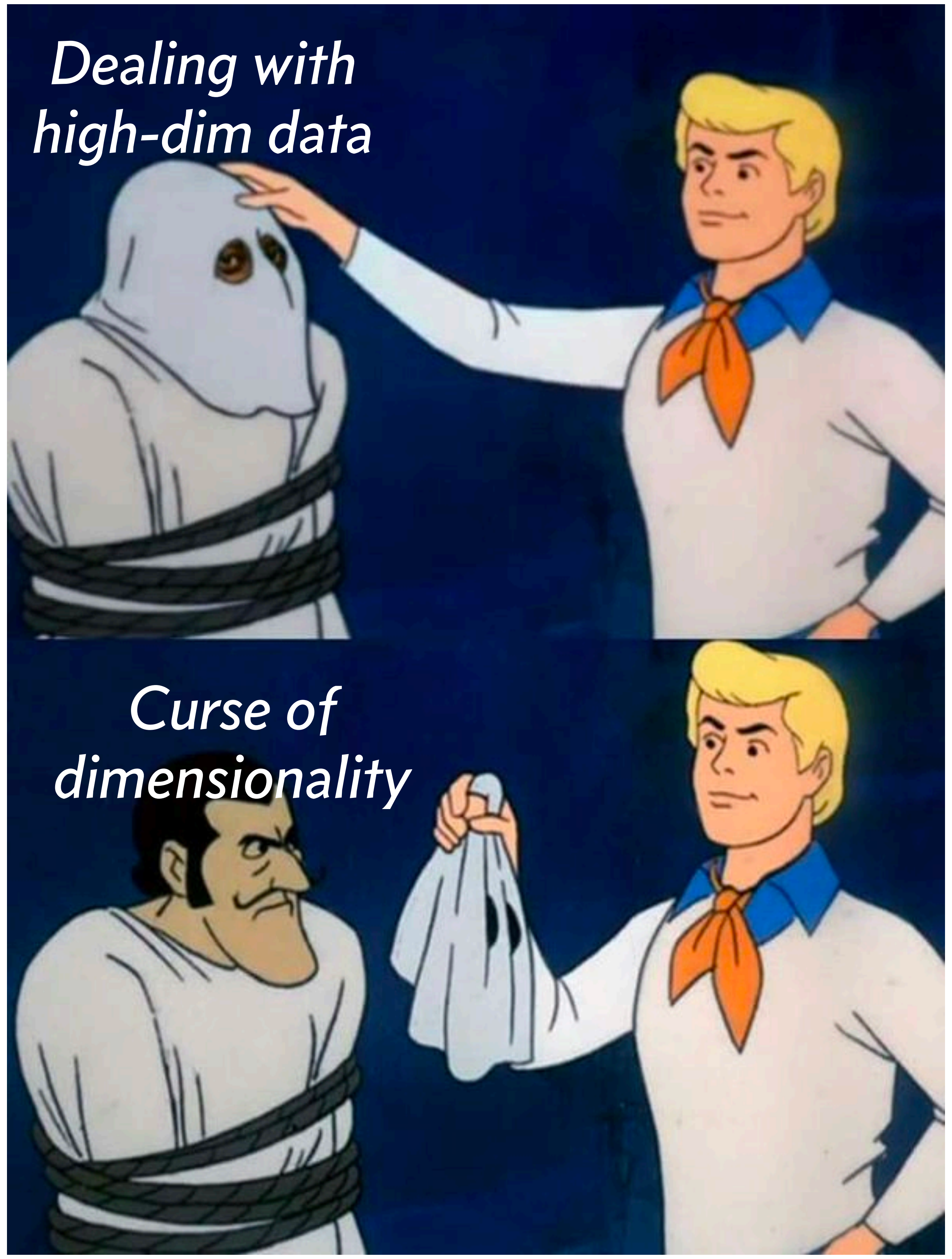
The curse of dimensionality

Where is most of the probability mass concentrated in high dimensions?

- In high dimensions, most of the probability density of a Gaussian distribution lies in a thin shell at distance $\sqrt{d}$ from the center
- Vanishingly small fraction of distribution support is actually occupied.

$$x \sim \mathcal{N}(0, \mathbb{I}_d)$$

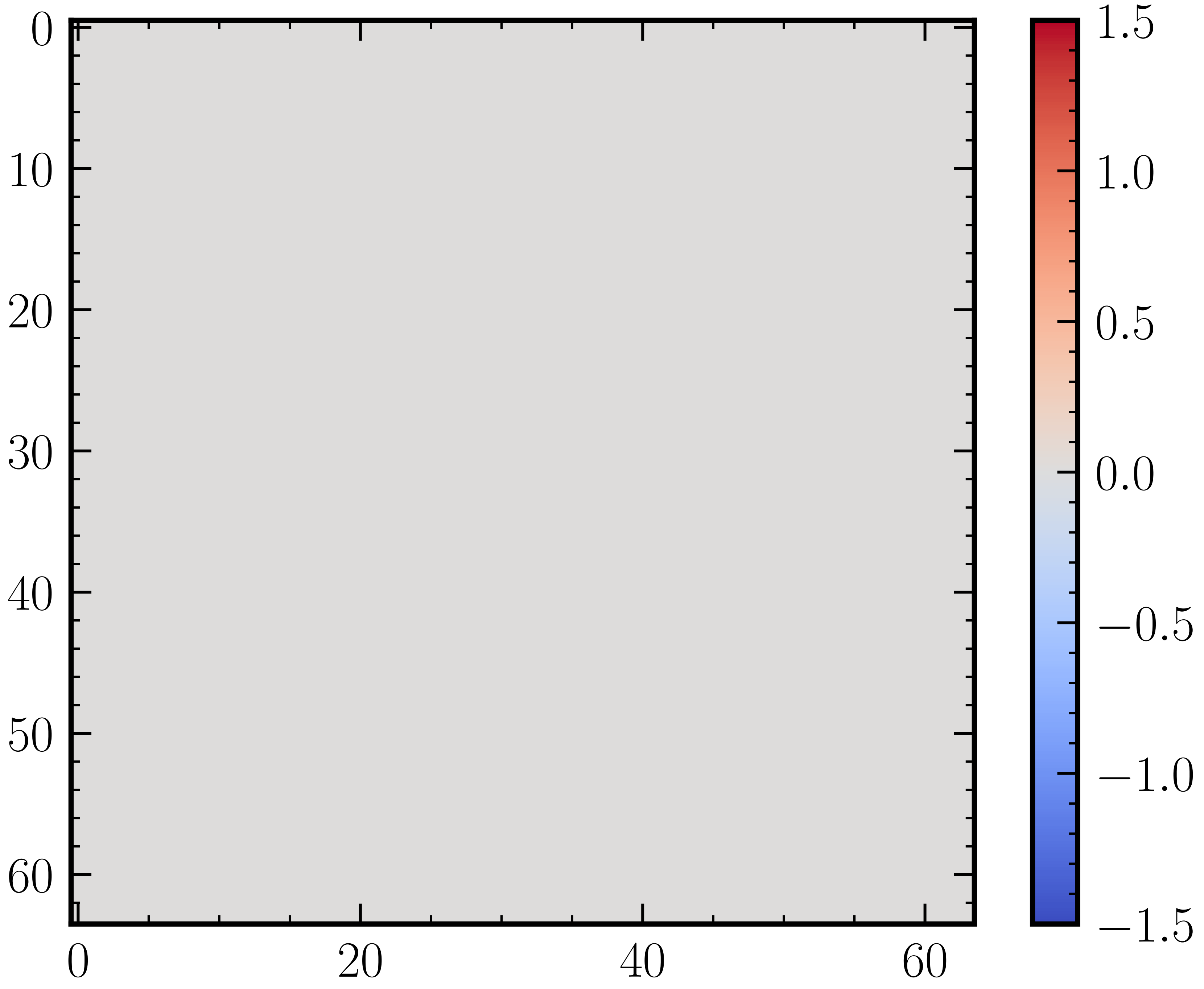




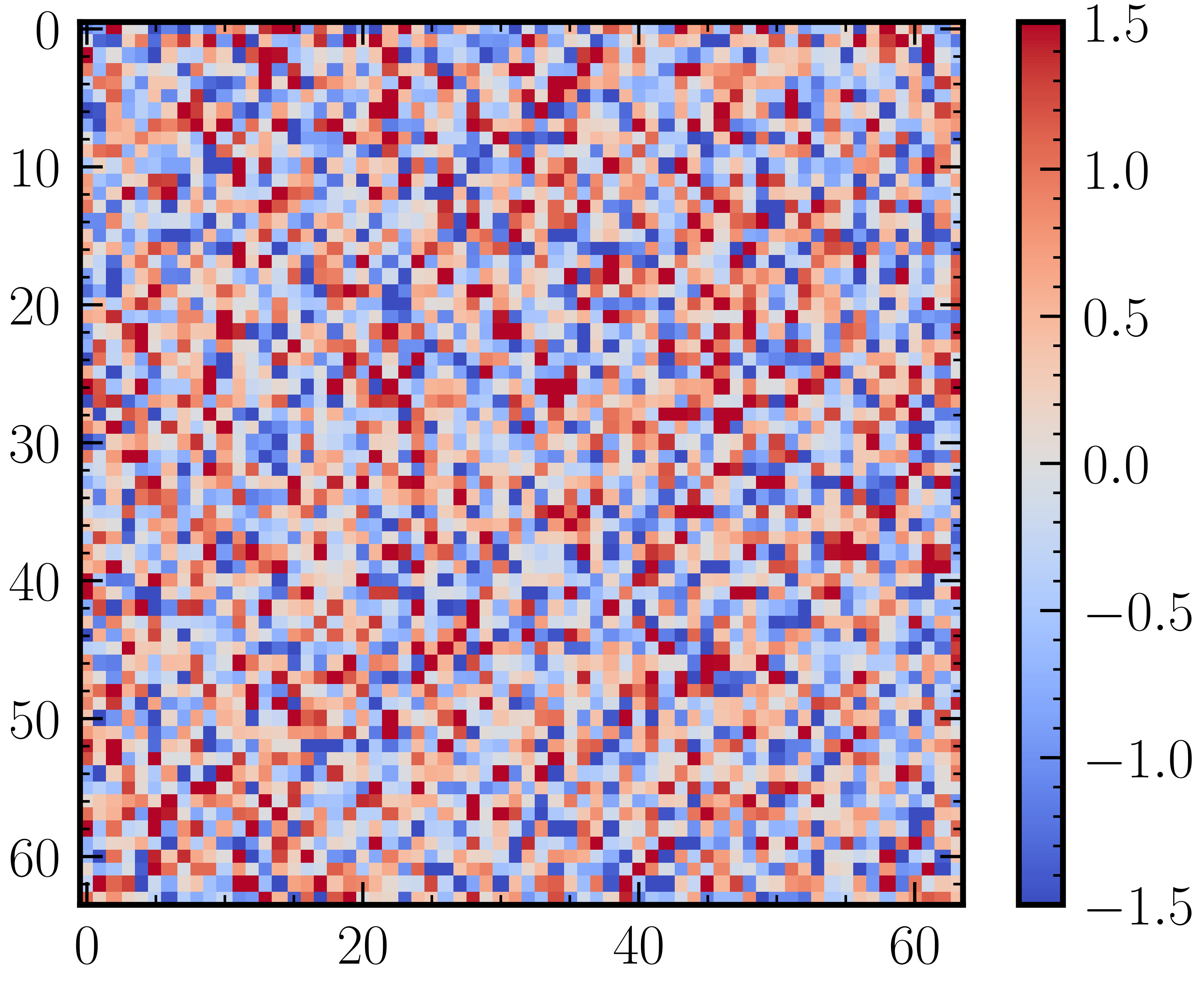
Learning high-dimensional distributions is challenging!

Typicality and likelihood of samples

Which of these samples have a higher likelihood under $\mathscr{L} = \mathcal{N}(0, \mathbb{I}_d)$?



$\log \mathscr{L} \approx -0.92\,\mathrm{nats/dim}$

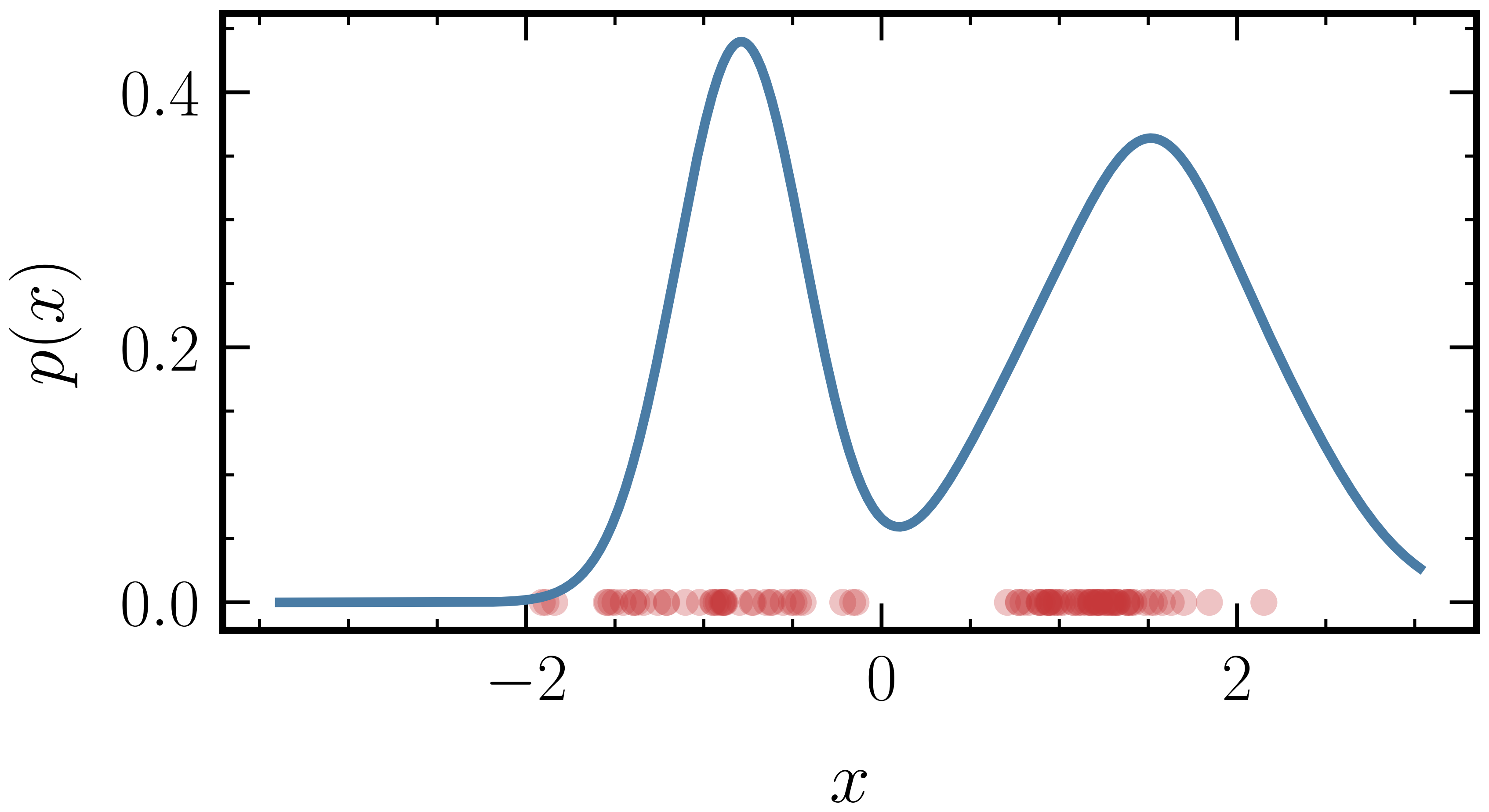


$\log \mathscr{L} \approx -1.43\,\mathrm{nats/dim}$

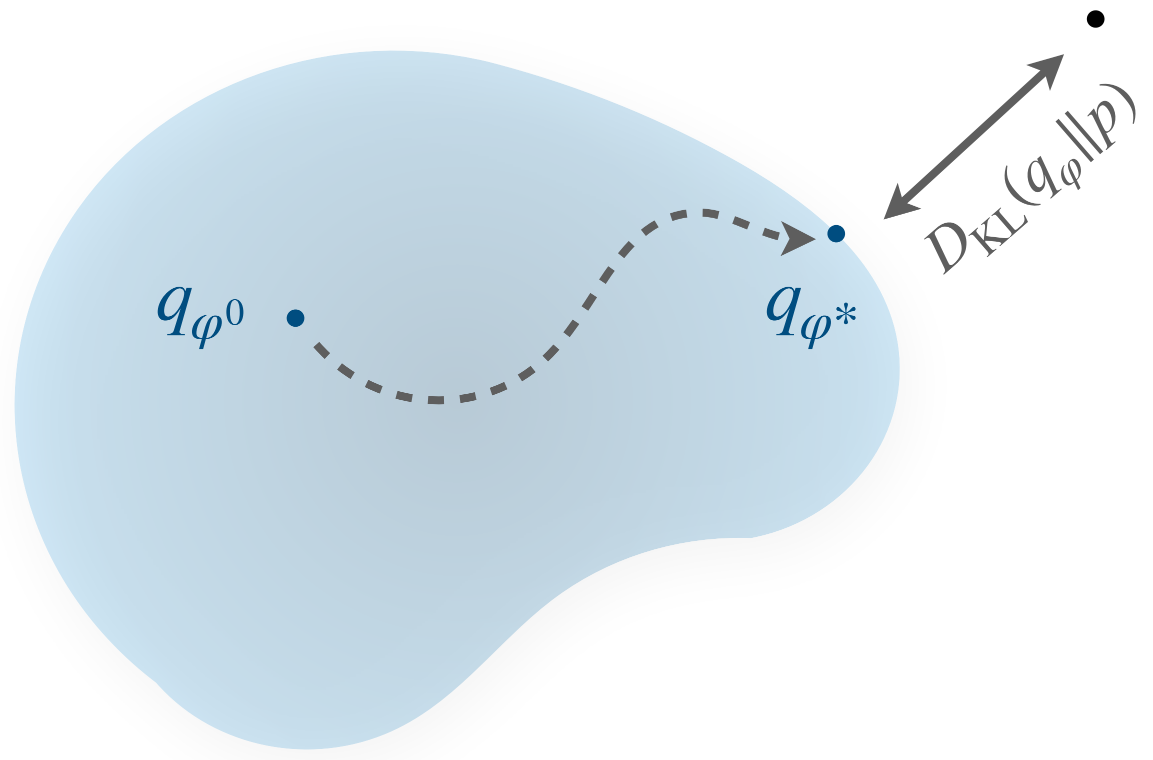
Evaluation of high-dimensional distributions is challenging!

(Some) Ways of training deep generative models

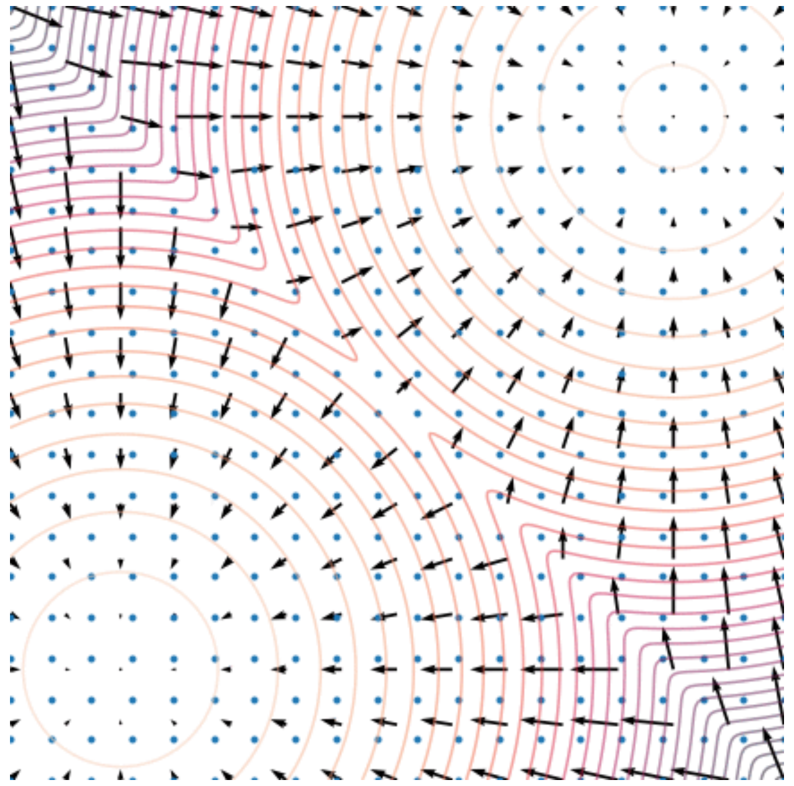
Maximum-likelihood



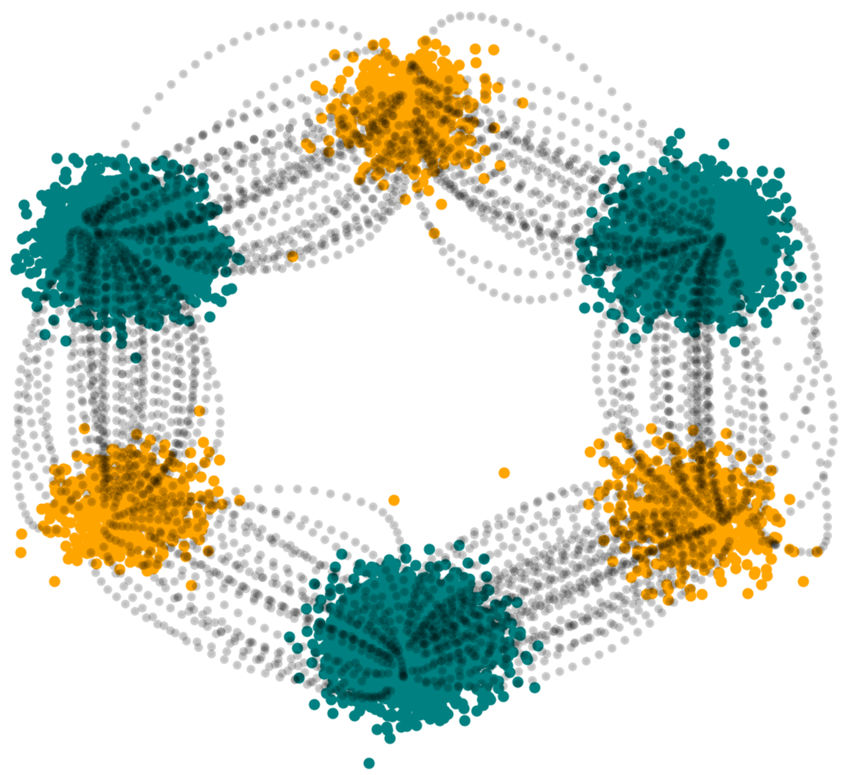
Optimizing a bound on the likelihood



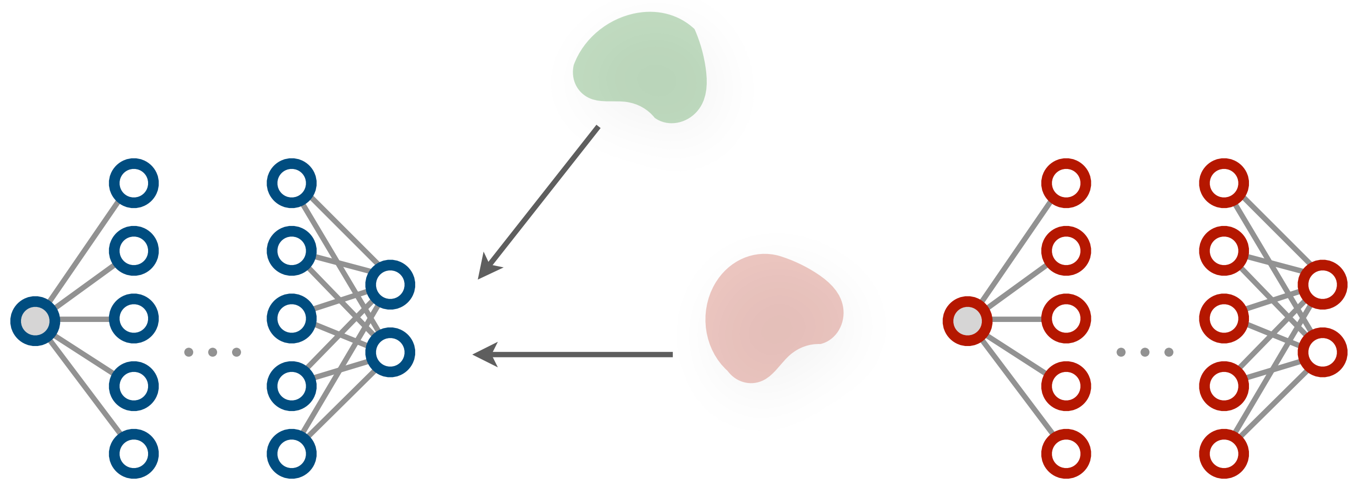
Score-matching



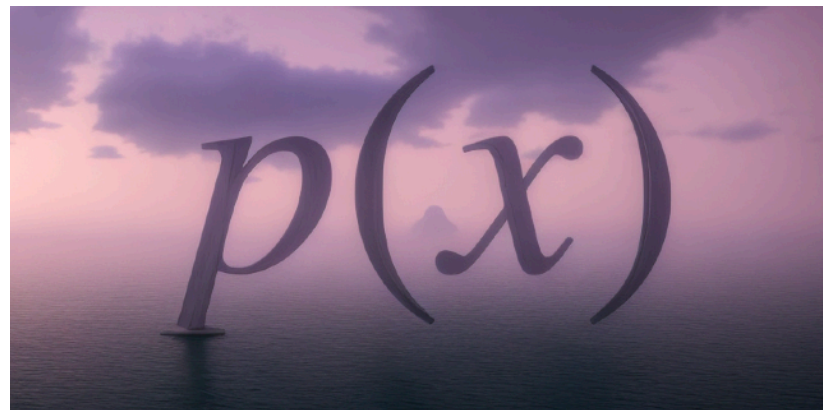
Optimal transport



Adversarial training

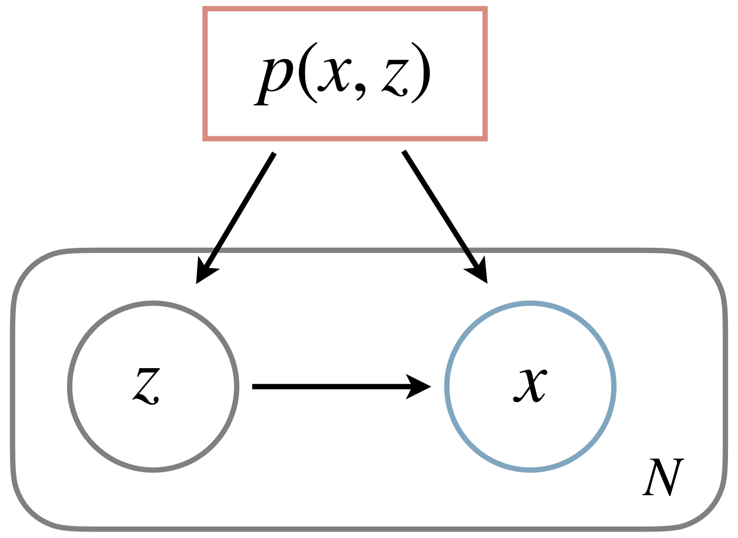


Outline



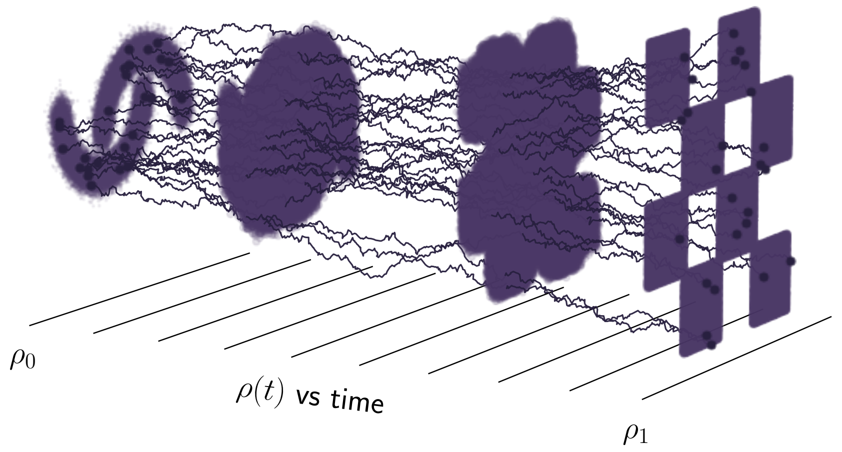
Why (deep) generative modeling?

What is it, and what can it do for you?



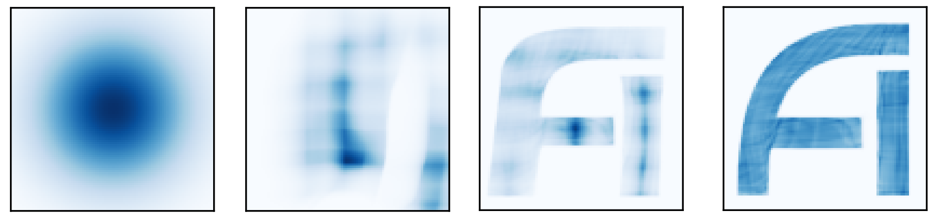
Variational auto encoders

Latent-variable modeling, and compression is all you need



Diffusion models

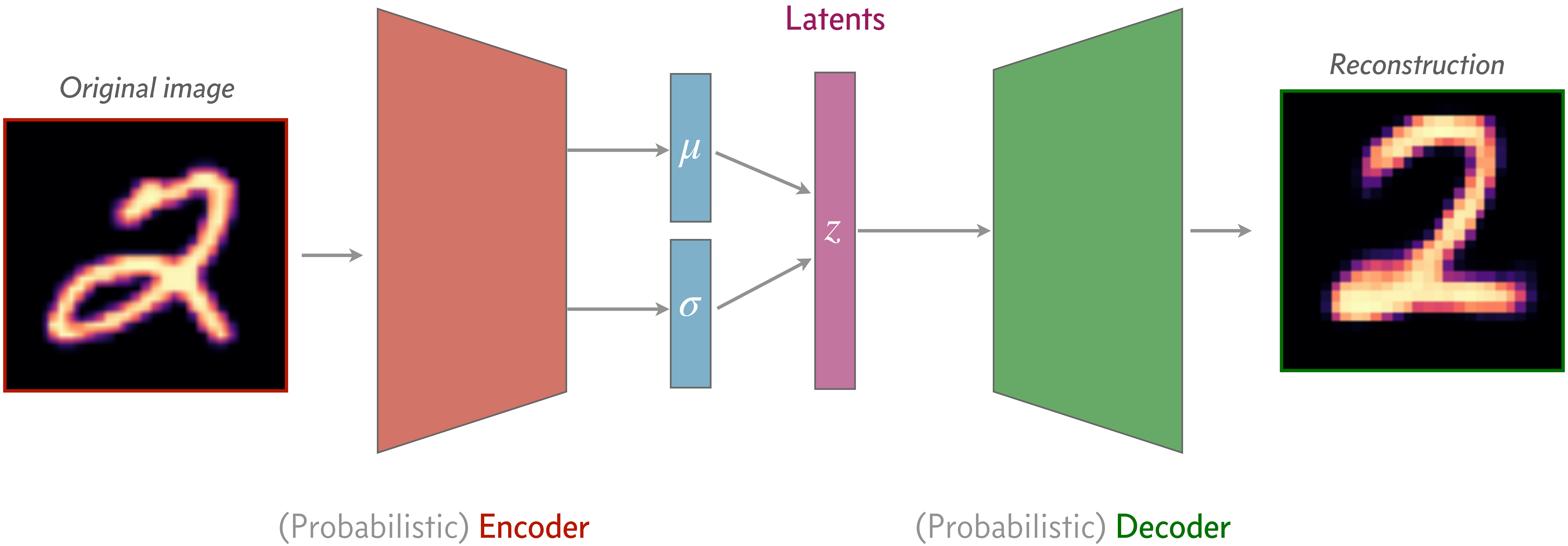
Models based on iterative refinement



Normalizing flows

Invertible transformations

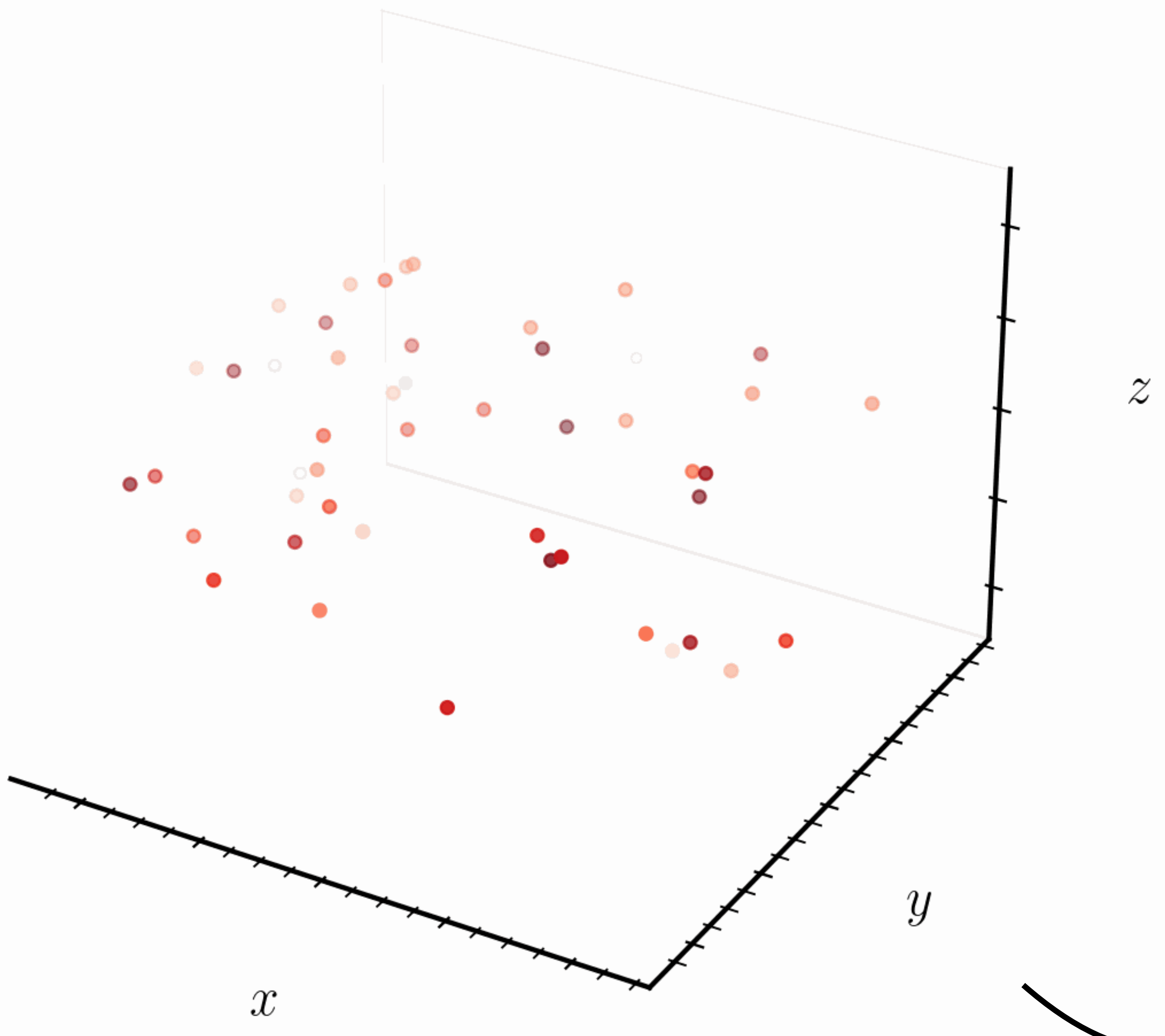
A bird-eye view



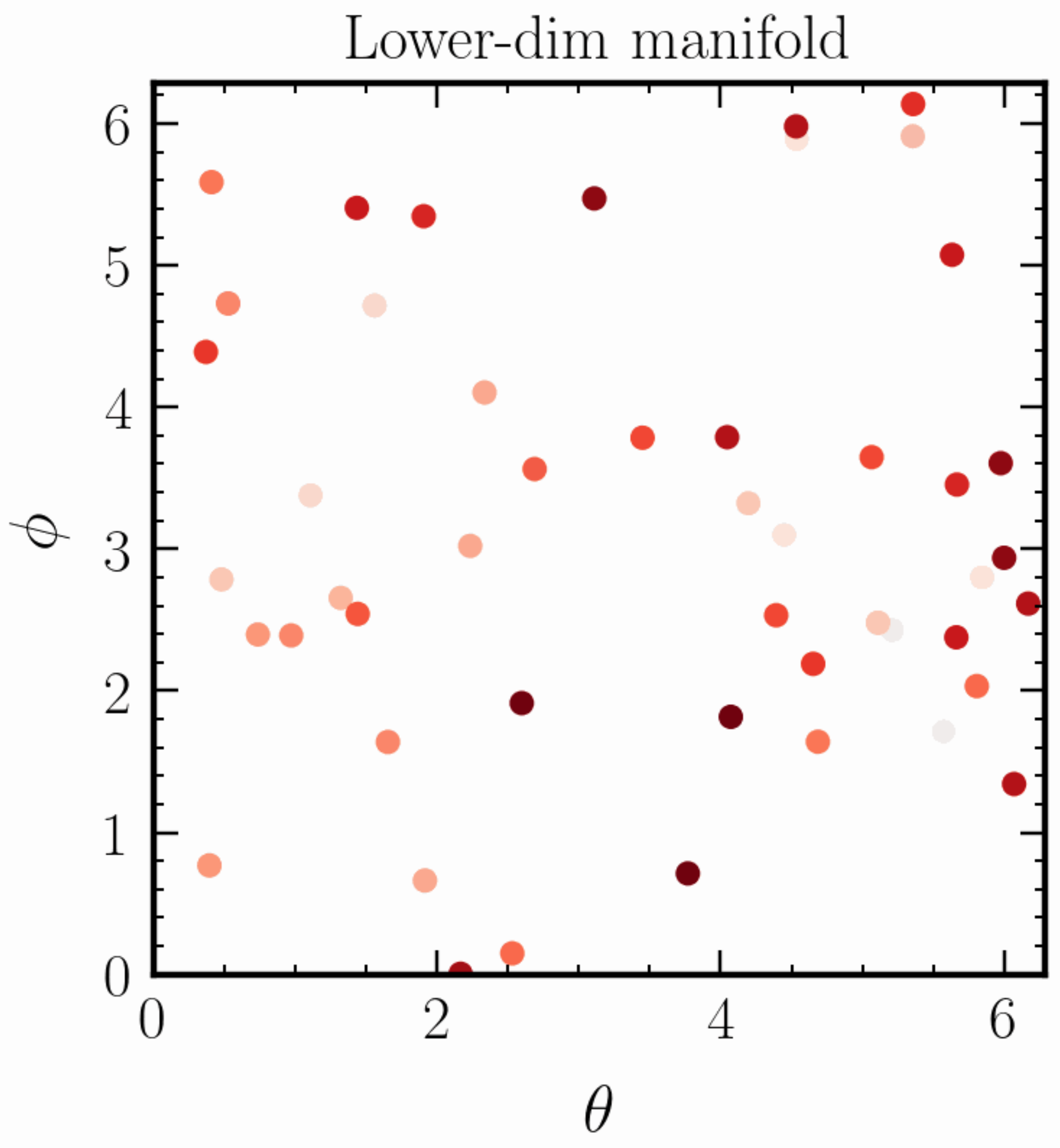
The pursuit of low-dimensional structure

Real-world datasets often live in structured low-dimensional manifolds

“Difficult to model” x



“Easy to model” z



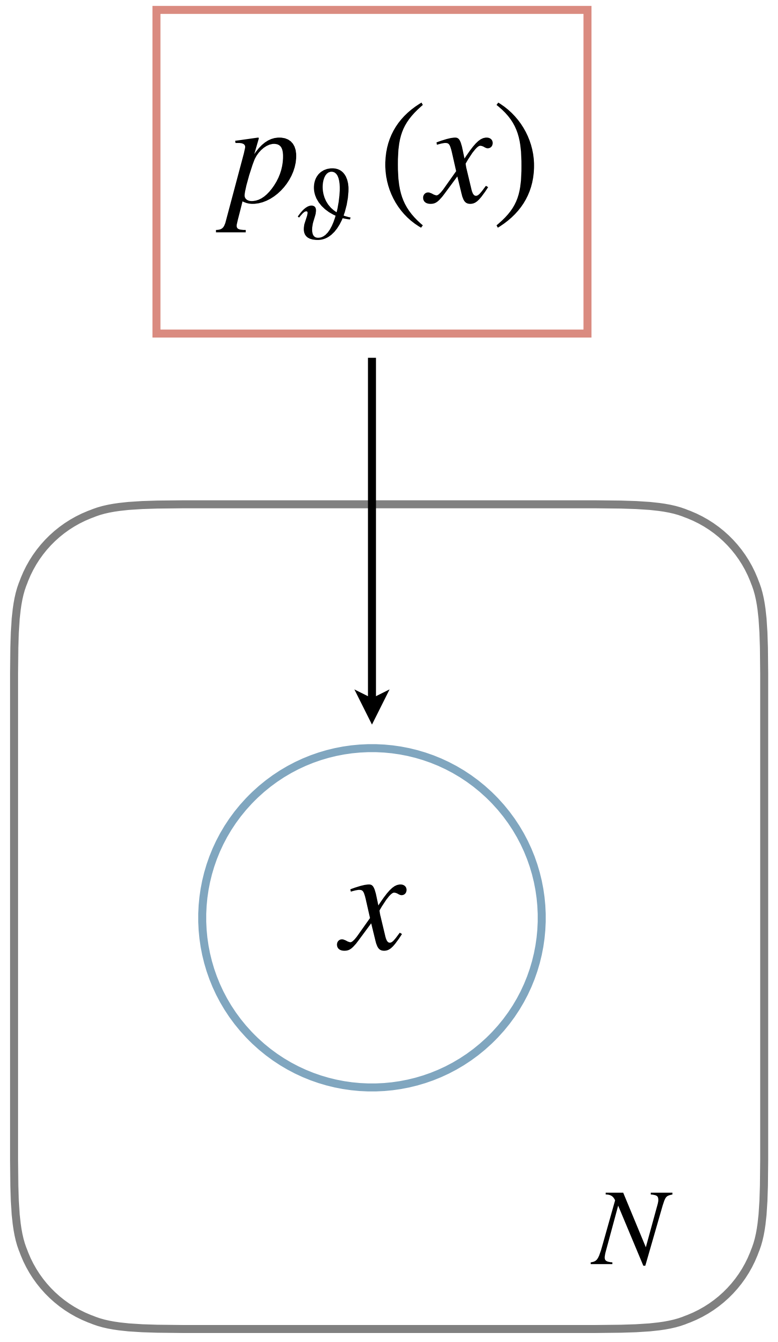
$$p(z \mid x)$$

Latent-variable modeling

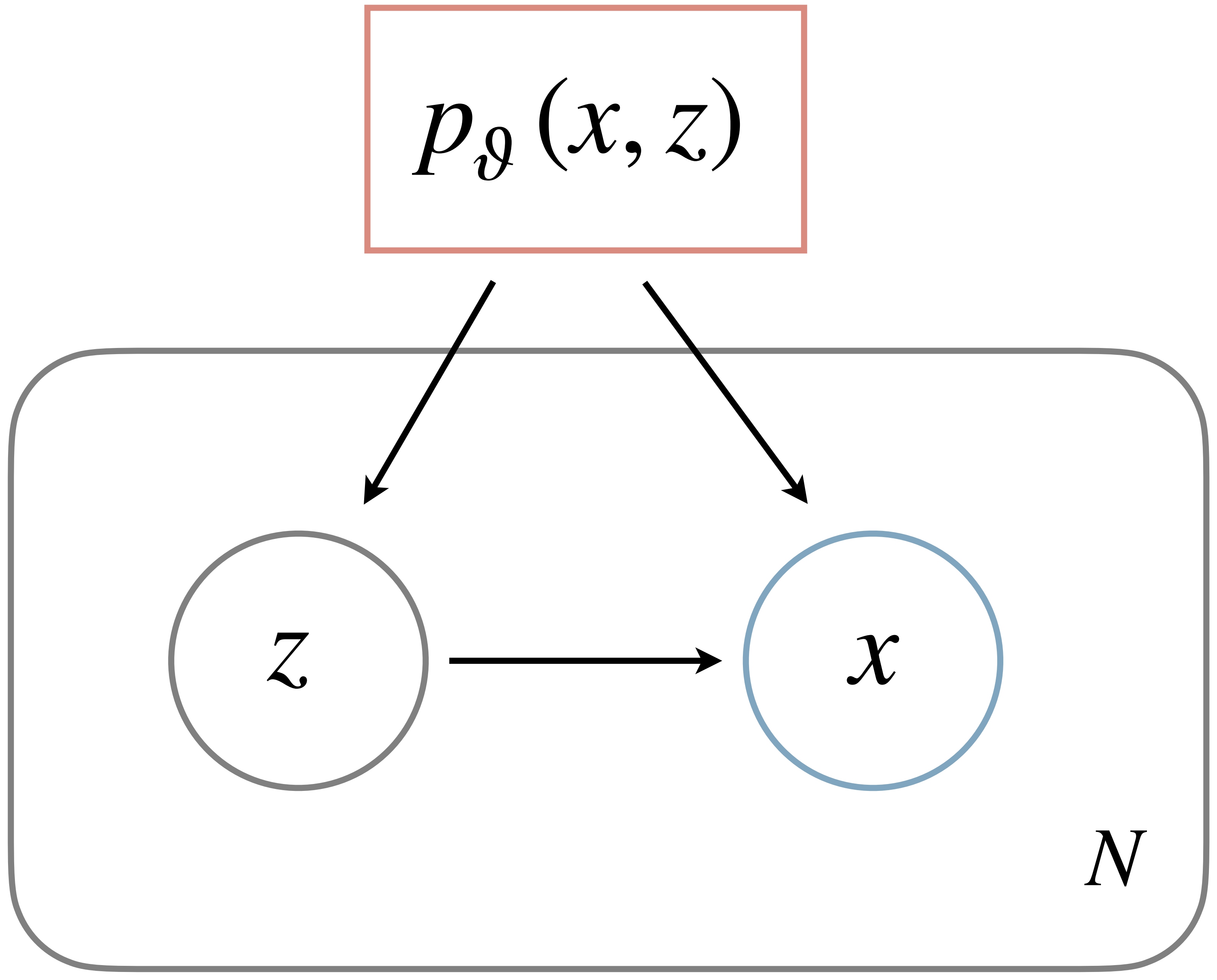
Learn lower-dimensional structure in the data distribution

Make the problem easier by making it "harder":

introduce *joint distribution* $p_\theta(x, z)$



Observed variables



Latent variables *Observed variables*

Common factorization:

$$p_\vartheta(x, z) = p(z) \cdot p_\vartheta\left(x \mid z\right)$$

Latent-variable modeling

Maximum-likelihood training?

$$
\begin{aligned}
\vartheta^* &= \arg\max_{\vartheta} p_\vartheta(x) \\
&= \arg\max_{\vartheta} \int p_\vartheta(x \mid z) p(z)\, \mathrm{d}z \\
&= \arg\max_{\vartheta} \left\langle p_\vartheta(x \mid z) \right\rangle_{p(z)}
\end{aligned}
$$

Difficult to build a good estimator!

The intractability of $p(x)$ is closely related to the intractability of the *posterior* $p(z \mid x)$

$$p(z \mid x) = \frac{p(x, z)}{p(x)}$$ (Bayes' theorem)

Kullback–Leibler (KL) divergence

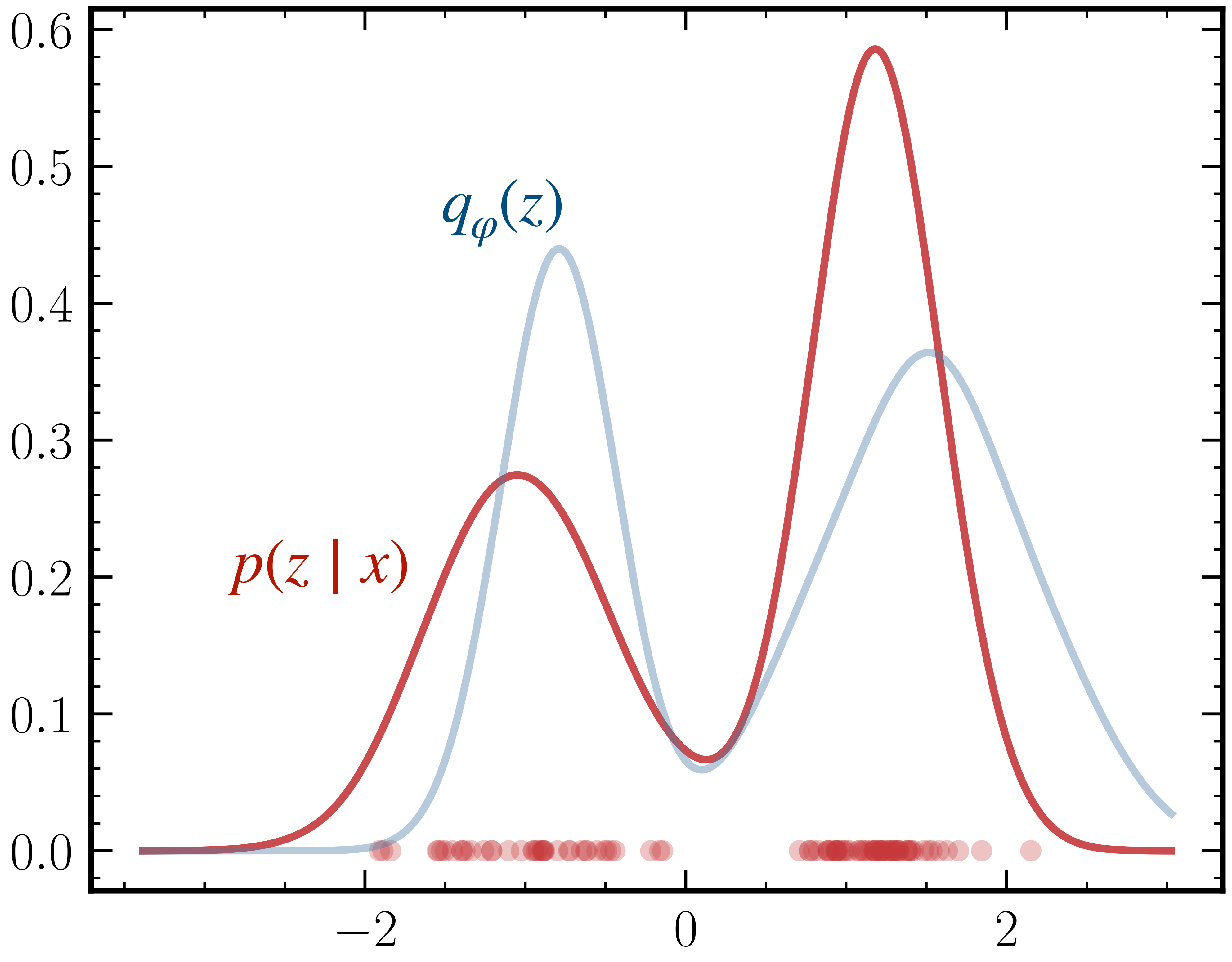
A measure of similarity between two probability distributions

$$D_{\mathrm{KL}}(P \| Q) = \int_{-\infty}^{\infty} \mathrm{d}x \, p(x) \, \log\left(\frac{p(x)}{q(x)}\right)$$

$$= \left\langle \log \frac{p(x)}{q(x)} \right\rangle_{x \sim p(x)}$$

$$= \underbrace{- \left\langle \log q(x) \right\rangle_{p(x)}}_{\text{Cross-entropy } \mathbb{H}(P, Q)} + \underbrace{\left\langle \log p(x) \right\rangle_{p(x)}}_{- \text{ (Self-)entropy } \mathbb{H}(P)}$$

Formally: *expected excess "surprise" from using Q as a model when the actual distribution is P*



KL-divergence

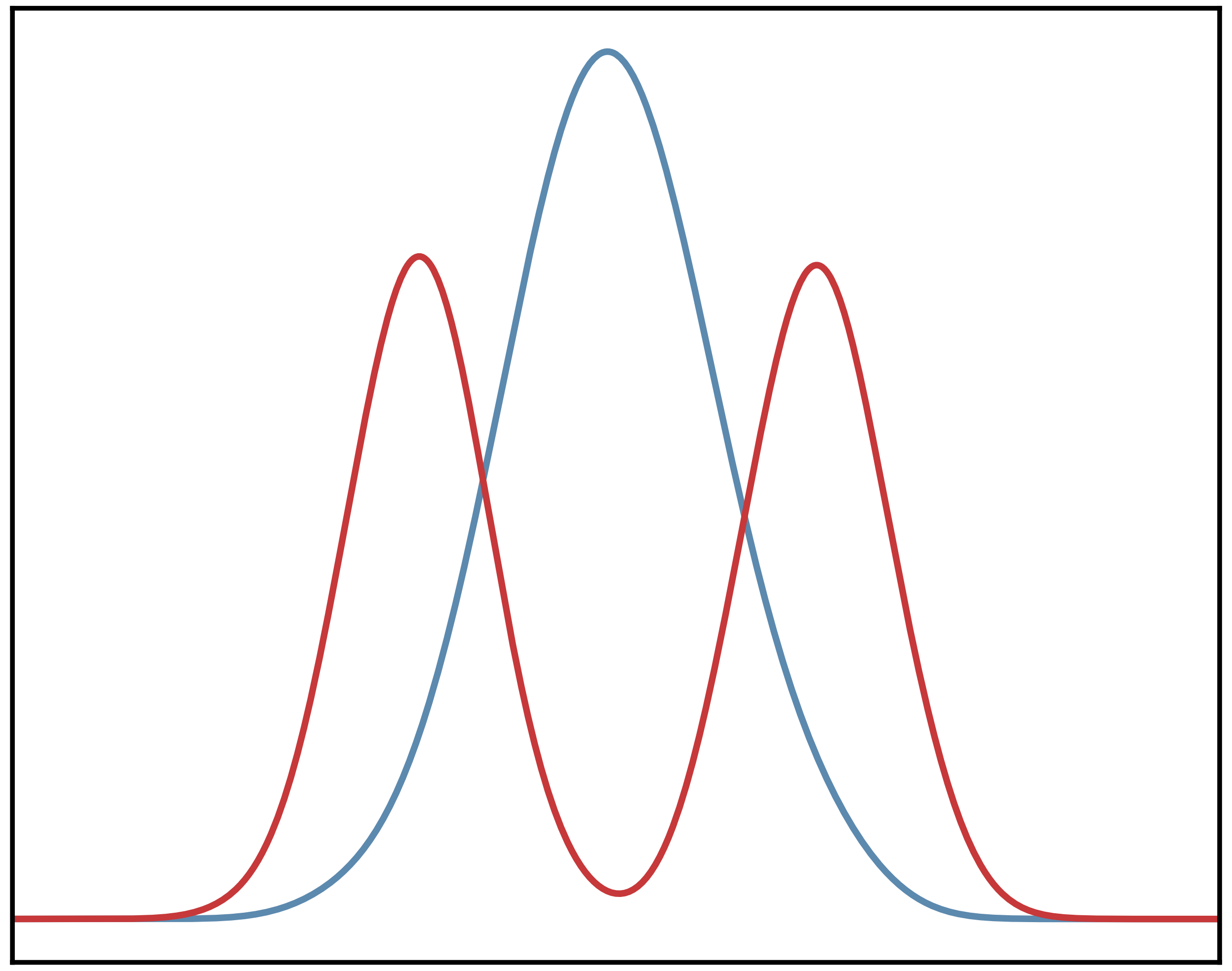
A measure of similarity between two probability distributions

$$D_{\mathrm{KL}}(Q\|P) = \int_{-\infty}^{\infty} \mathrm{d}x\, q(x)\, \log\left(\frac{q(x)}{p(x)}\right)$$

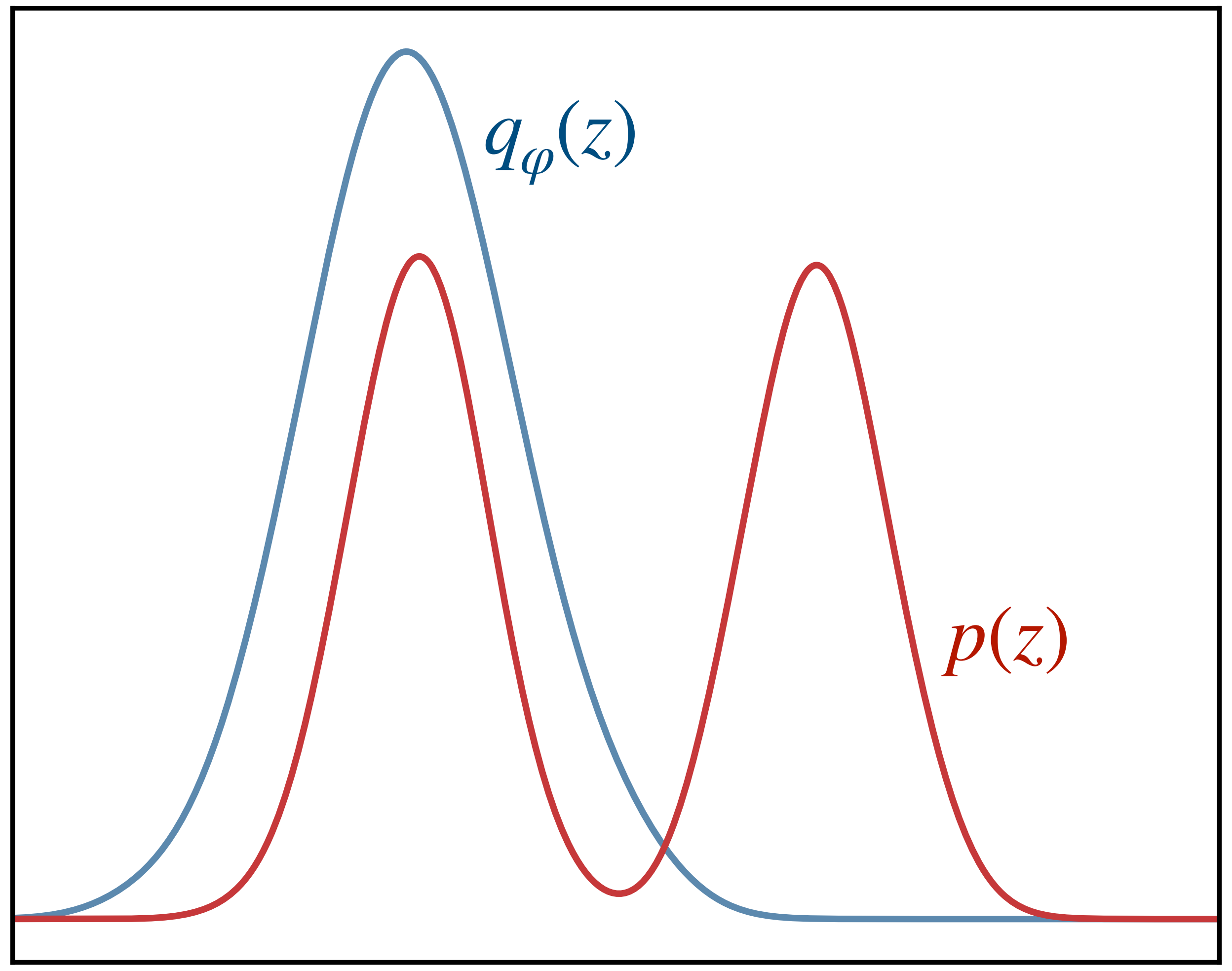
Not symmetric! $D_{\mathrm{KL}}(Q\|P) \neq D_{\mathrm{KL}}(P\|Q)$

"True" distribution

"Forward" KL $D_{\mathrm{KL}}(P\|Q)$



"Reverse" KL $D_{\mathrm{KL}}(Q\|P)$



Forward KL

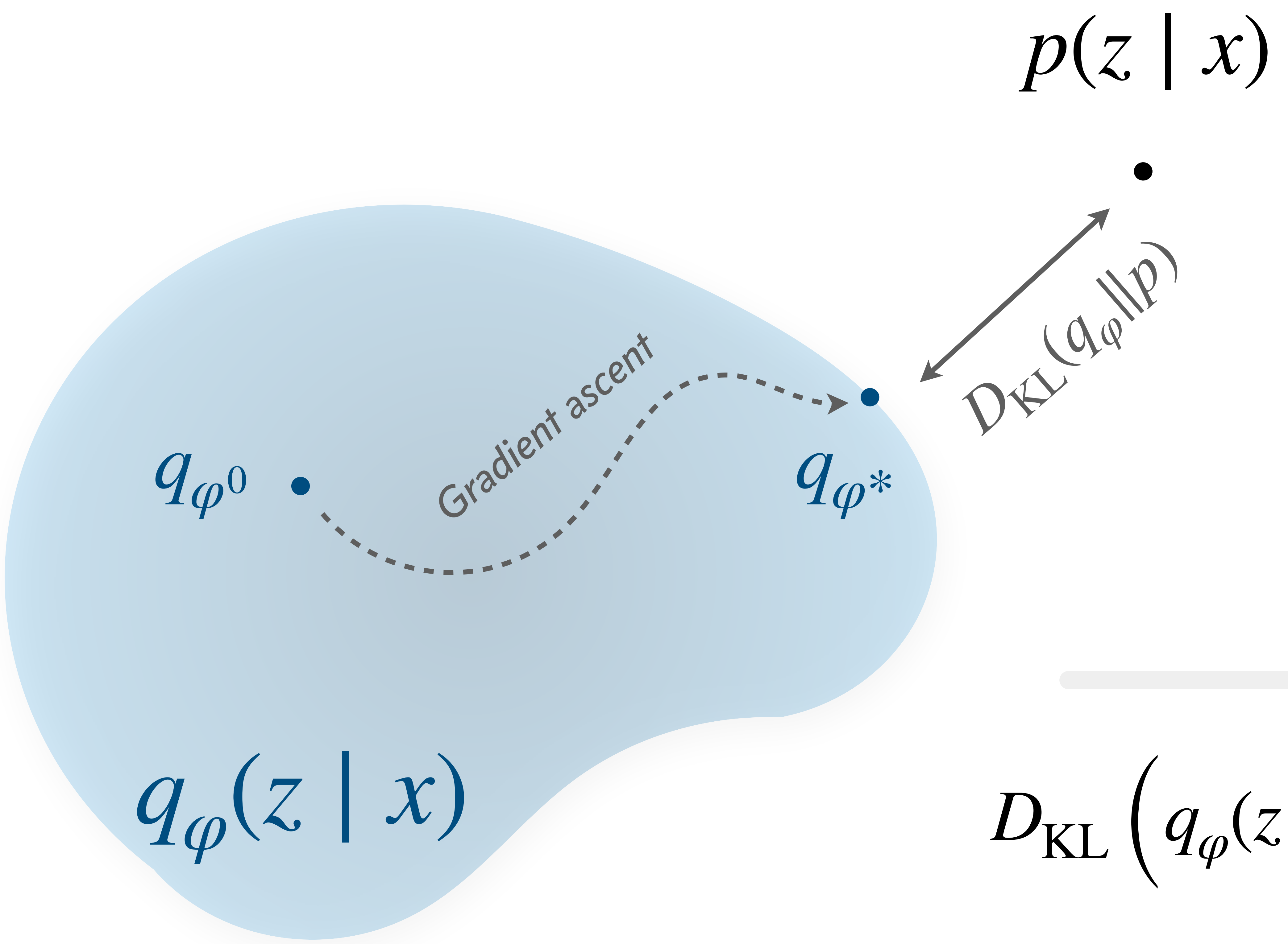
$$D_{\mathrm{KL}}(P_{\mathscr{D}}\|Q_\varphi) = -\left\langle \log q_\varphi(z) \right\rangle_{z\sim p_{\mathscr{D}}(z)} + \text{const}\,.$$

Maximum-likelihood inference is equivalent to minimizing the *forward* KL

Non-negative! $D_{\mathrm{KL}}(Q\|P) \geq 0$

Variational inference

Infer the posterior over the latent parameters



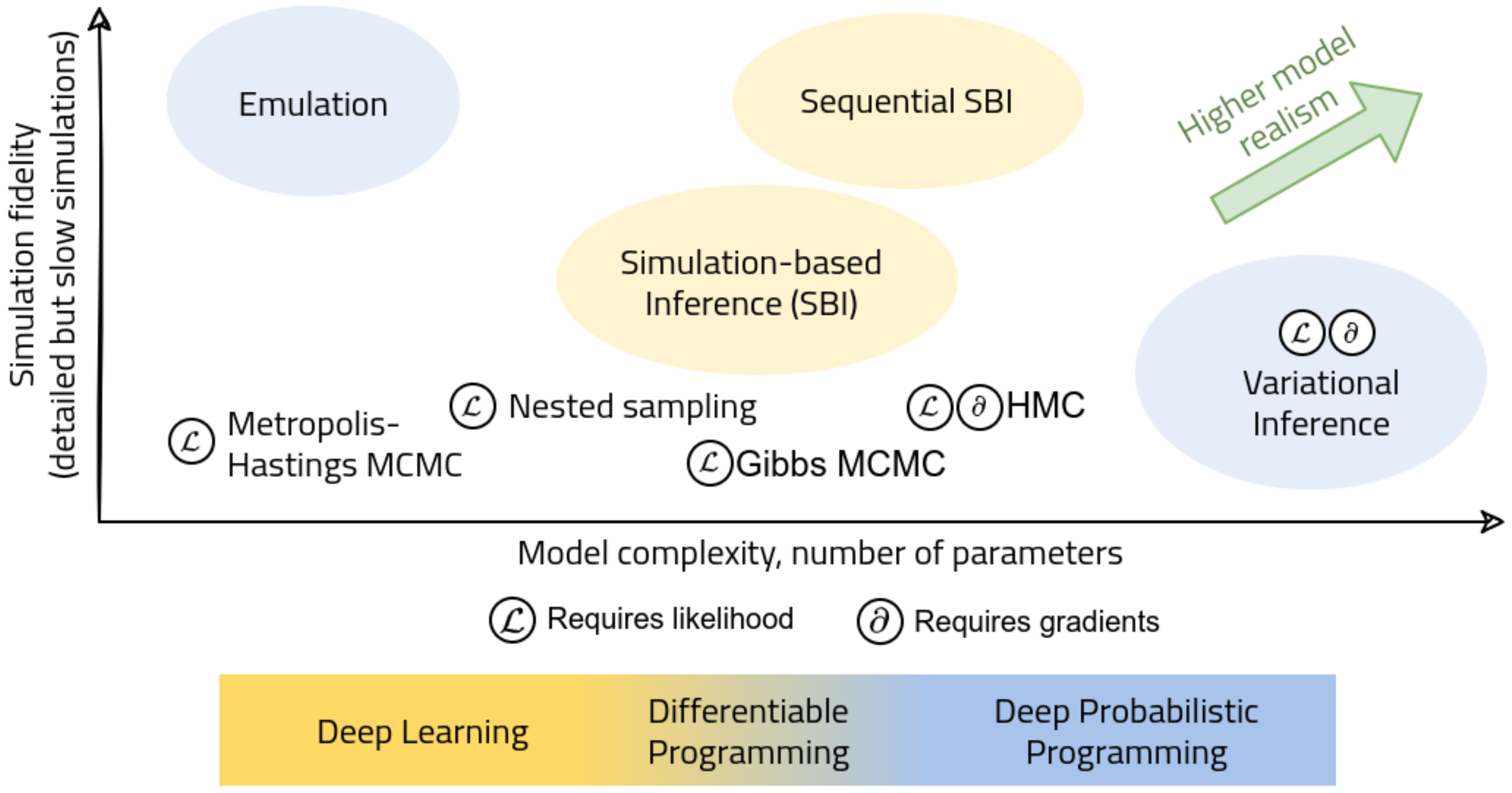
A two-for-one!

- ☑ Estimate approximate posterior $q_\varphi(z \mid x) \approx p(z \mid x)$
- ☑ Estimate likelihood/evidence $\mathrm{ELBO} \approx p(x)$

$$\underbrace{D_{\mathrm{KL}}\left(q_\varphi(z \mid x) \| p(z \mid x)\right)}_{\geq 0} = \underbrace{\log p(x)}_{\text{Evidence}} - \underbrace{\left\langle \log p_\vartheta(x, z) - \log q_\varphi(z) \right\rangle_{q_\varphi(z)}}_{\text{Evidence Lower BOund (ELBO)}}$$

Variational inference

A general-purpose technique for posterior estimation: *optimization* instead of *sampling*



[EuCAPT White Paper 2021]

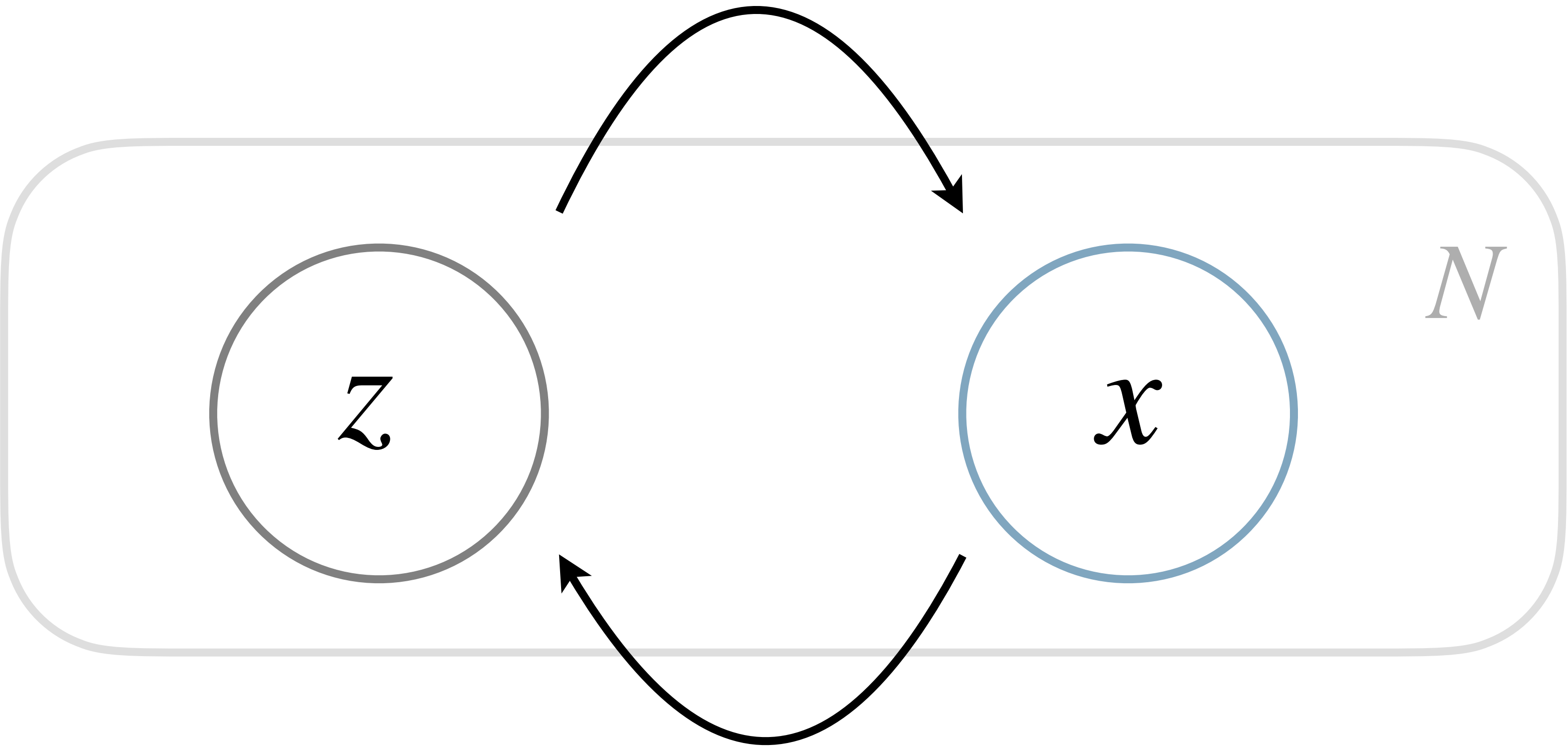
Can handle a huge number of parameters

A Bayesian latent-variable model optimized with variational inference

We're so back

Reverse process

$$p_\vartheta\left(x \mid z\right) \cdot p(z)$$



$$q_\varphi(z \mid x) \cdot p(x)$$

Forward process

It's so over

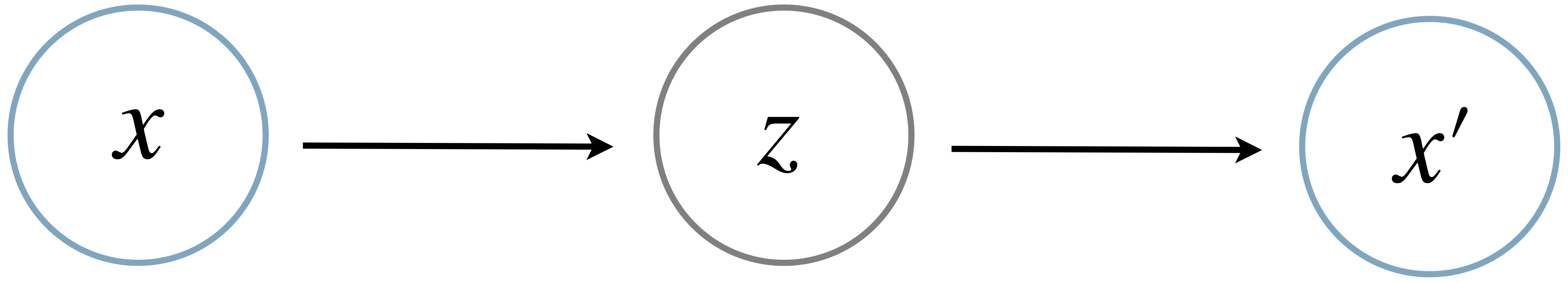
Maximizing ELBO

$\equiv$ Minimizing *reverse* KL

$\equiv$ "Aligning the forward and reverse processes"

Minimize $\left\langle \log \dfrac{q(x, z)}{p(x, z)} \right\rangle$

Forward process — Reverse process



Latents

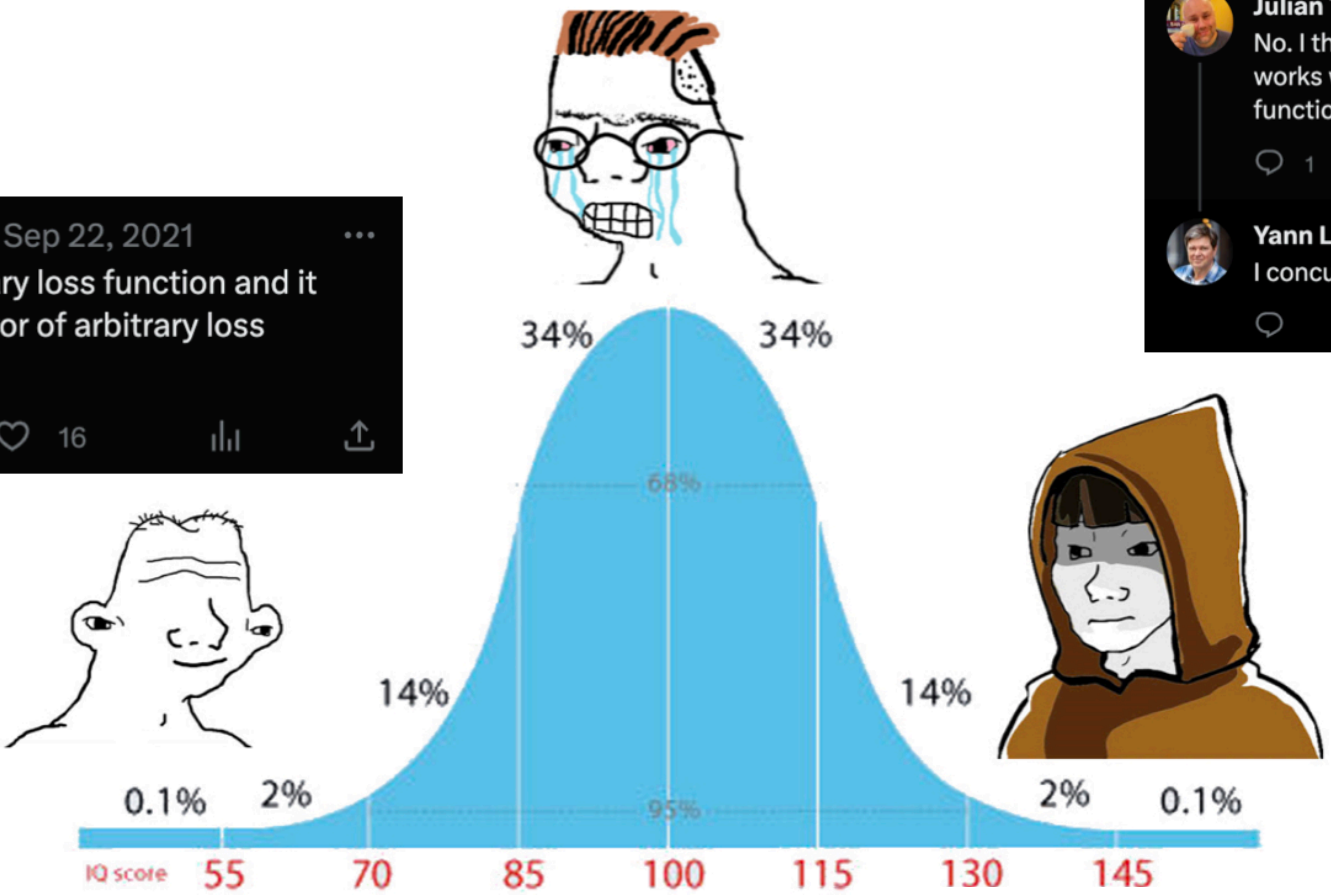
Christopher Yau
@cwcyau

People do realise that a variational autoencoder comes from the application of variational inference to a Bayesian latent variable model right? It isn't an arbitrary loss function with a KL term stuck on to it with a tweakable parameter to balance the two?

Julian Togelius @togelius · Sep 22, 2021
No. I think of it as an arbitrary loss function and it works well for me. I'm in favor of arbitrary loss functions.
1 1 16

Julian Togelius @togelius · Sep 22, 2021
No. I think of it as an arbitrary loss function and it works well for me. I'm in favor of arbitrary loss functions.
1 1 16

Yann LeCun @ylecun · Sep 22, 2021
I concur.
6

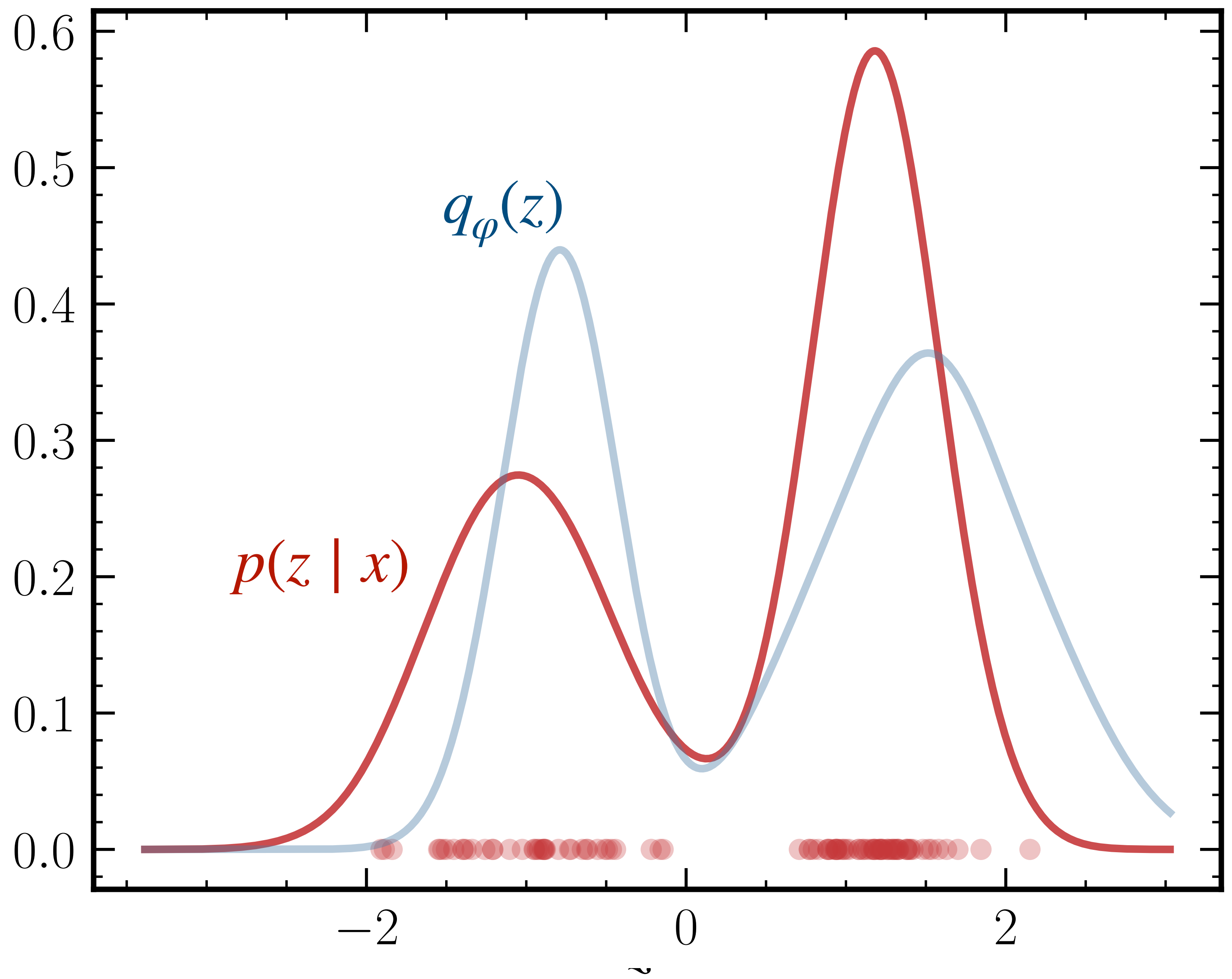


https://twitter.com/cwcyau/status/1440434674556227591

Variational inference

A general-purpose technique for posterior estimation

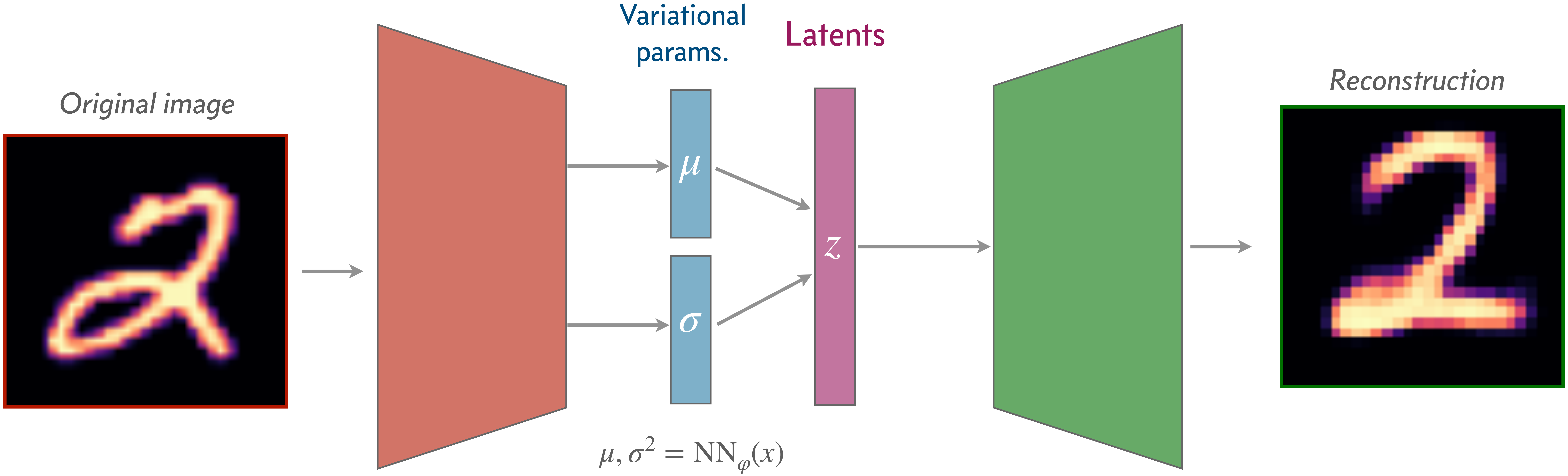
$$\overbrace{D_{\mathrm{KL}}\left(q_\varphi(z) \| p(z \mid x)\right)}^{\geq 0} = \overbrace{\log p(x)}^{\text{Evidence}} - \overbrace{\left\langle \log p_\vartheta(x, z) - \log q_\varphi(z) \right\rangle_{q_\varphi(z)}}^{\text{Evidence Lower BOund (ELBO)}}$$



$$\begin{aligned} \mathrm{ELBO} &= \left\langle \log p_\vartheta(x, z) - \log q_\varphi(z \mid x) \right\rangle_{q_\varphi} \\ &= \left\langle \log p_\vartheta(x \mid z) + \log p(z) - \log q_\varphi(z \mid x) \right\rangle_{q_\varphi} \\ &= \underbrace{\left\langle \log p_\vartheta(x \mid z) \right\rangle_{q_\varphi}}_{\text{"Reconstruction"}} - \underbrace{D_{\mathrm{KL}}\left(q_\varphi(z \mid x) \,\|\, p(z)\right)}_{\text{"Regularization"}} \end{aligned}$$

VAEs in practice

$p(z) = \mathcal{N}(z; 0, I)$



$\mu, \sigma^2 = \mathrm{NN}_\varphi(x)$

$x \sim p(x)$

$z \sim q_\varphi(z \mid x)$

$x' \sim p_\vartheta(x \mid z)$

(Probabilistic) Encoder

$q_\varphi(z \mid x) = \mathcal{N}(z; \mu, \sigma^2 \mathbb{I})$

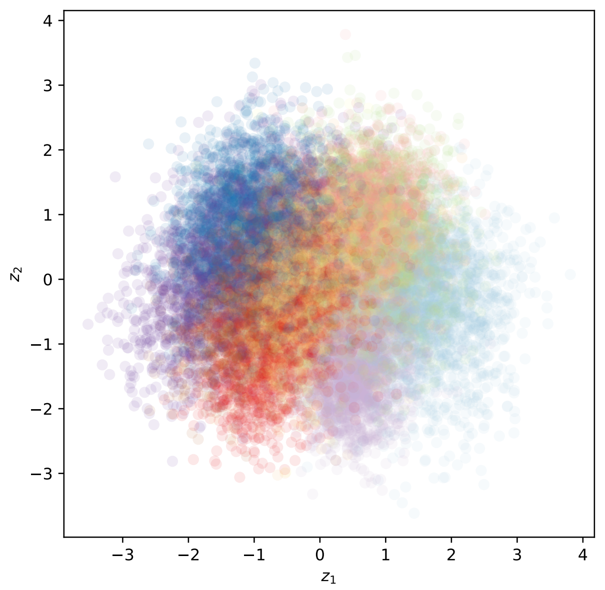
(Probabilistic) Decoder

Noise model / data likelihood

VAEs in practice

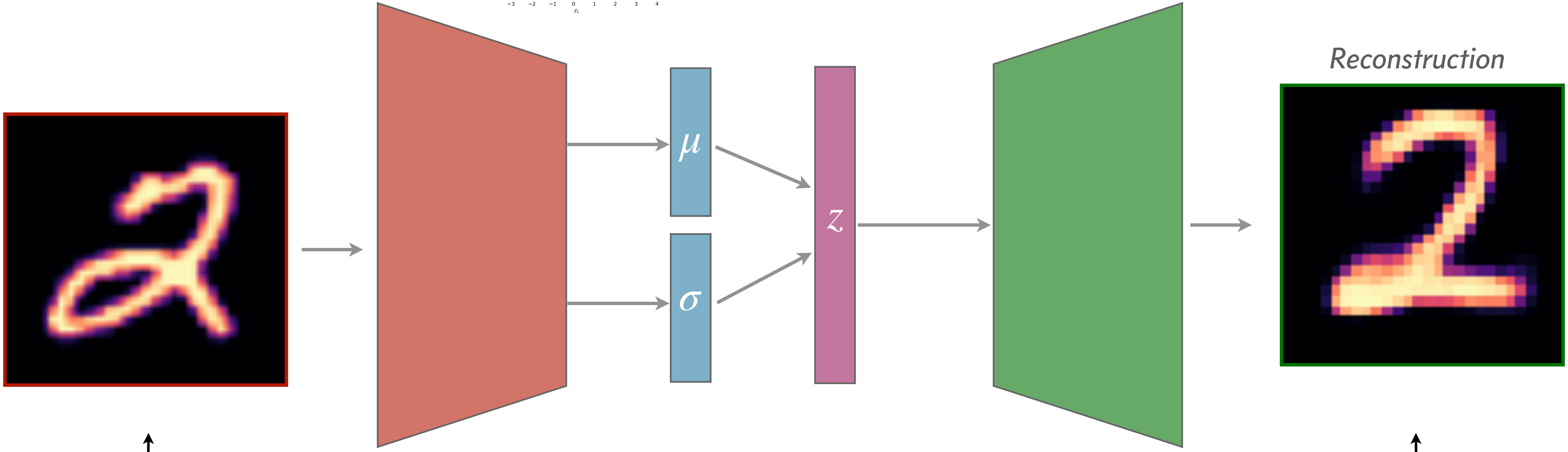
$$\mathrm{ELBO} = \left\langle \log p_\vartheta(x \mid z) \right\rangle_{q_\varphi} - D_{\mathrm{KL}}\left(q_\varphi(z \mid x) \parallel p(z)\right)$$

$q_\varphi(z \mid x)$



$$D_{\mathrm{KL}}\left(q_\varphi(z \mid x) \parallel p(z)\right)$$

Regularization



$$\left\langle \log p_\vartheta(x \mid z) \right\rangle_{q_\varphi}$$

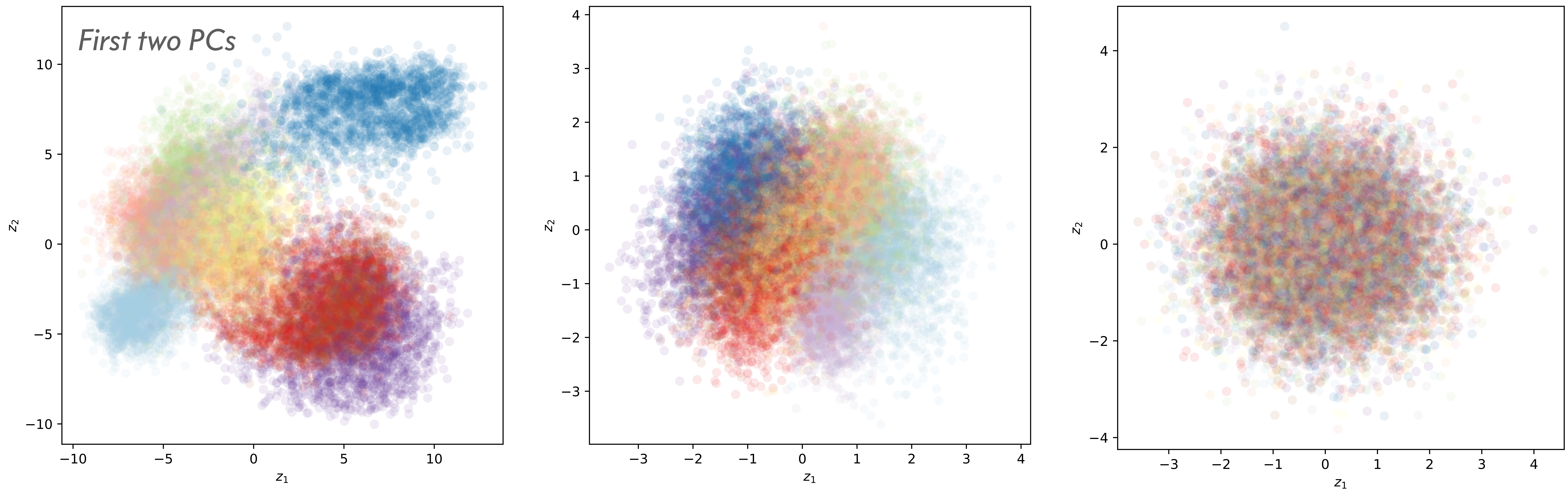
Reconstruction (e.g., MSE, …)

$\|x - x'\|_2^2$

A semantically meaningful latent space

The KL-term enforces simplicity in the latent space, encouraging learned semantic structure and *disentanglement*

Pure reconstruction ⟷ *More latent regularization*



Neural compression: *Rate-distortion theory*

Autoencoding is a form of (neural) compression!

$$-\mathrm{ELBO} = -\left\langle \log p_\vartheta(x \mid z) \right\rangle_{q_\varphi} + D_\mathrm{KL}\left(q_\varphi(z \mid x) \,\|\, p(z)\right)$$

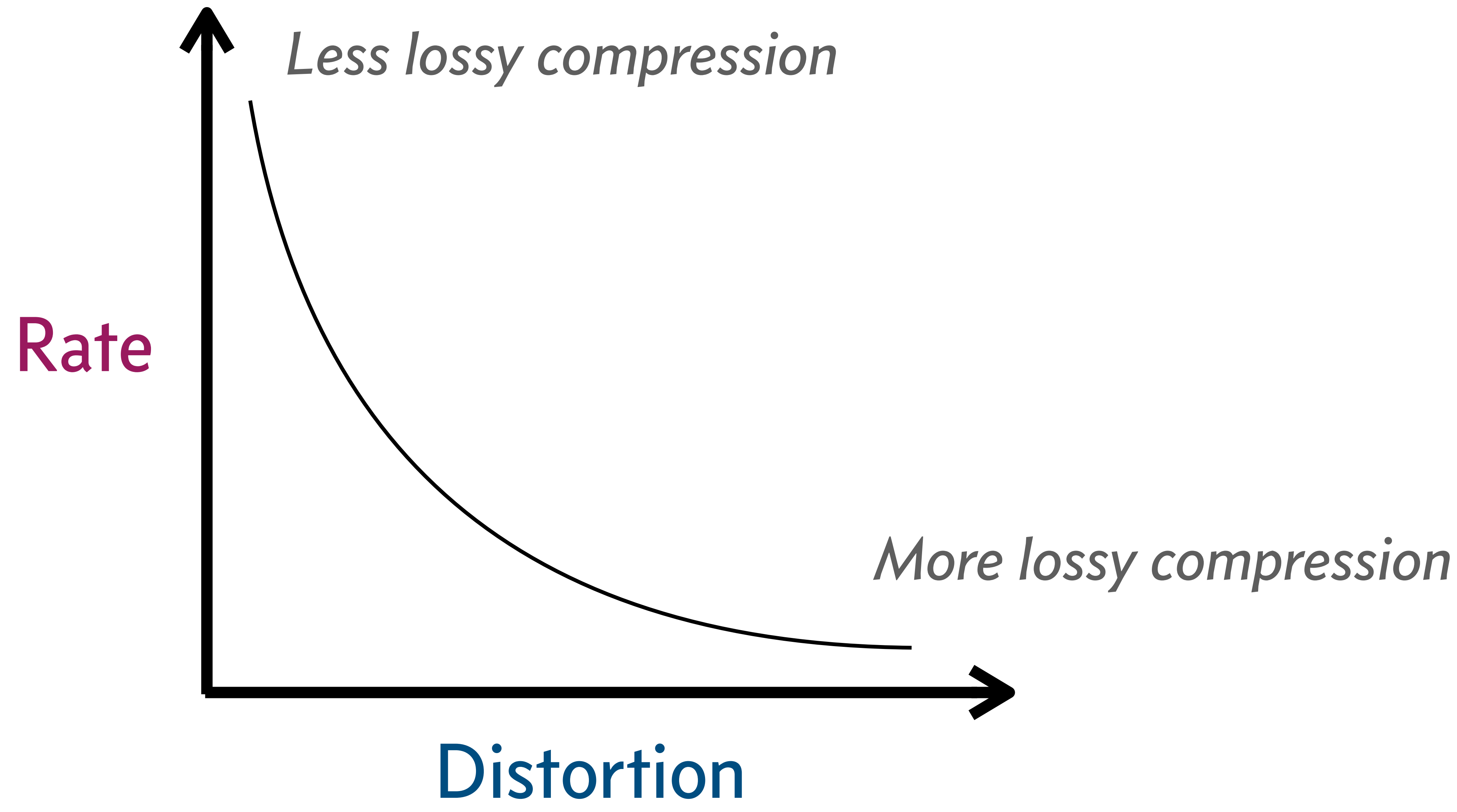
Distortion

"Reconstruction loss"

Rate

"Amount of compression"

Rate-distortion curve quantified this tradeoff



Controlling compression and disentanglement: β-VAEs

$$-\text{ELBO} = -\left\langle \log p_\vartheta(x \mid z) \right\rangle_{q_\varphi} + \beta \cdot D_{\text{KL}}\left(q_\varphi(z \mid x) \,\|\, p(z)\right)$$

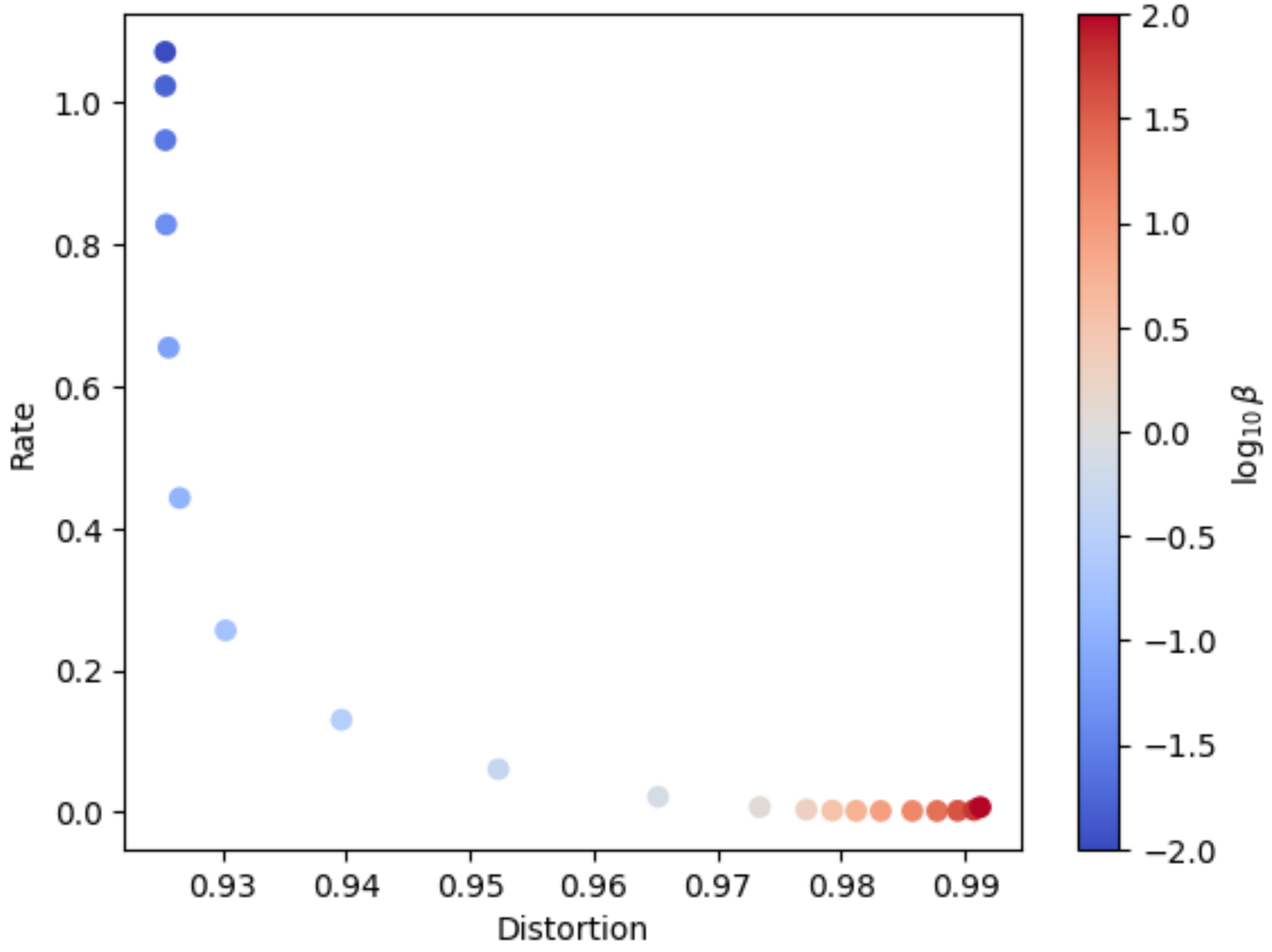
Distortion

Rate

If the data-generating process is associated with a principled noise model, by using it (the *likelihood*) as the reconstruction loss we are aiming to reconstruct the mean data.

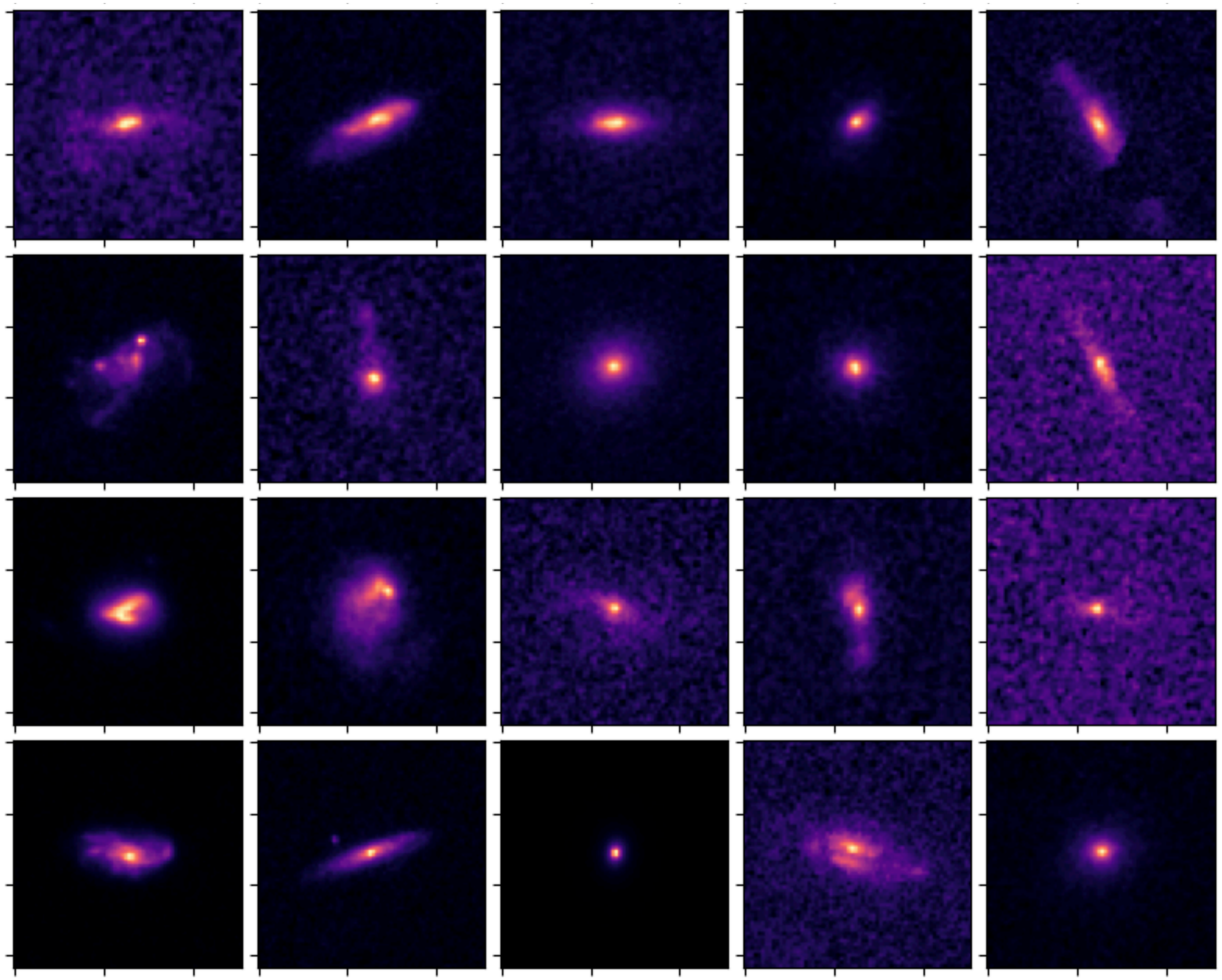
$$\log p(x \mid z; x') = -\frac{1}{2}\left(\frac{x - x'}{\sigma}\right)^2 + \log\left(\frac{1}{\sigma\sqrt{2\pi}}\right)$$

- Larger σ: More of the data variation is attributed to the likelihood → larger "β", more compression
- Smaller σ: Latents z try to capture more of the variation in the data (e.g. small perceptual features)



Tutorials 1 and 2: variational inference and VAEs

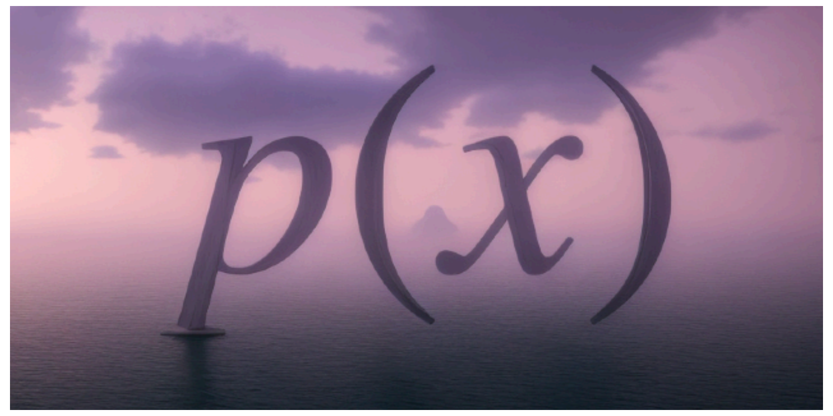
Lead: Carol Cuesta-Lazaro



[Mandelbaum et al; https://zenodo.org/record/3242143]

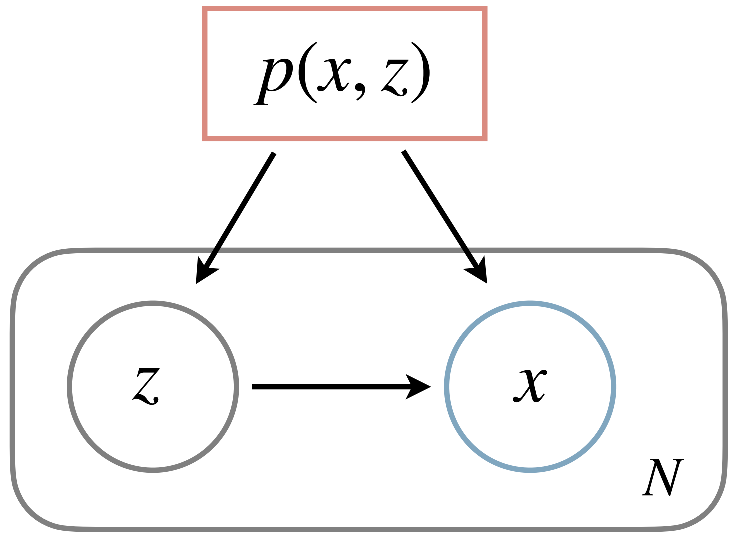
- Implement the ELBO objective for variational inference
- Construct a VAE and use it to build a generative model of galaxy images using samples form the HST COSMOS dataset
- Boilerplate code for training/reconstruction/ sampling for quick iteration
- Experiment with trade-offs between pure reconstruction and a latent space regularization

Outline



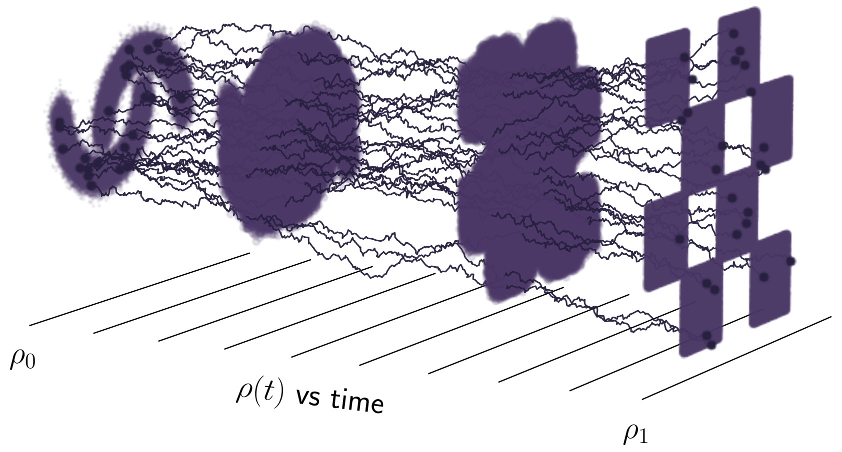
Why (deep) generative modeling?

What is it, and what can it do for you?



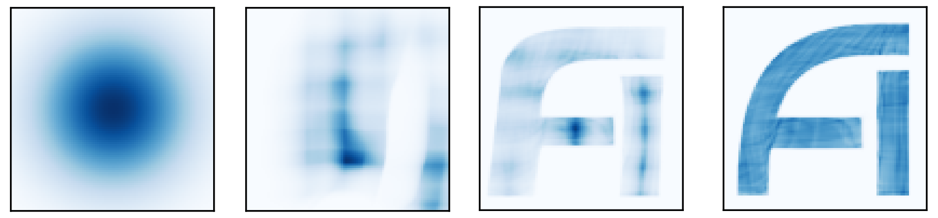
Variational auto encoders

Latent-variable modeling, and compression is all you need



Diffusion models

Models based on iterative refinement



Normalizing flows

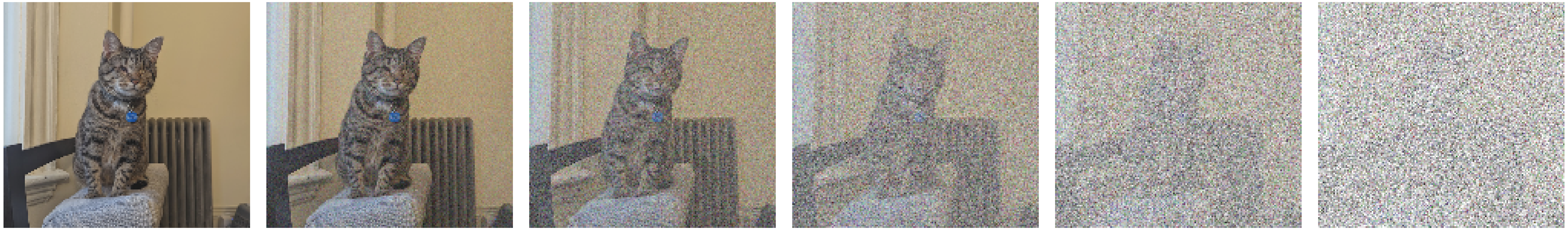
Invertible transformations

Diffusion models: overview

Forward process *(adding noise)*

$x(t=0) \sim p(x)$

$x(t=1) \sim \mathcal{N}(0,1)$



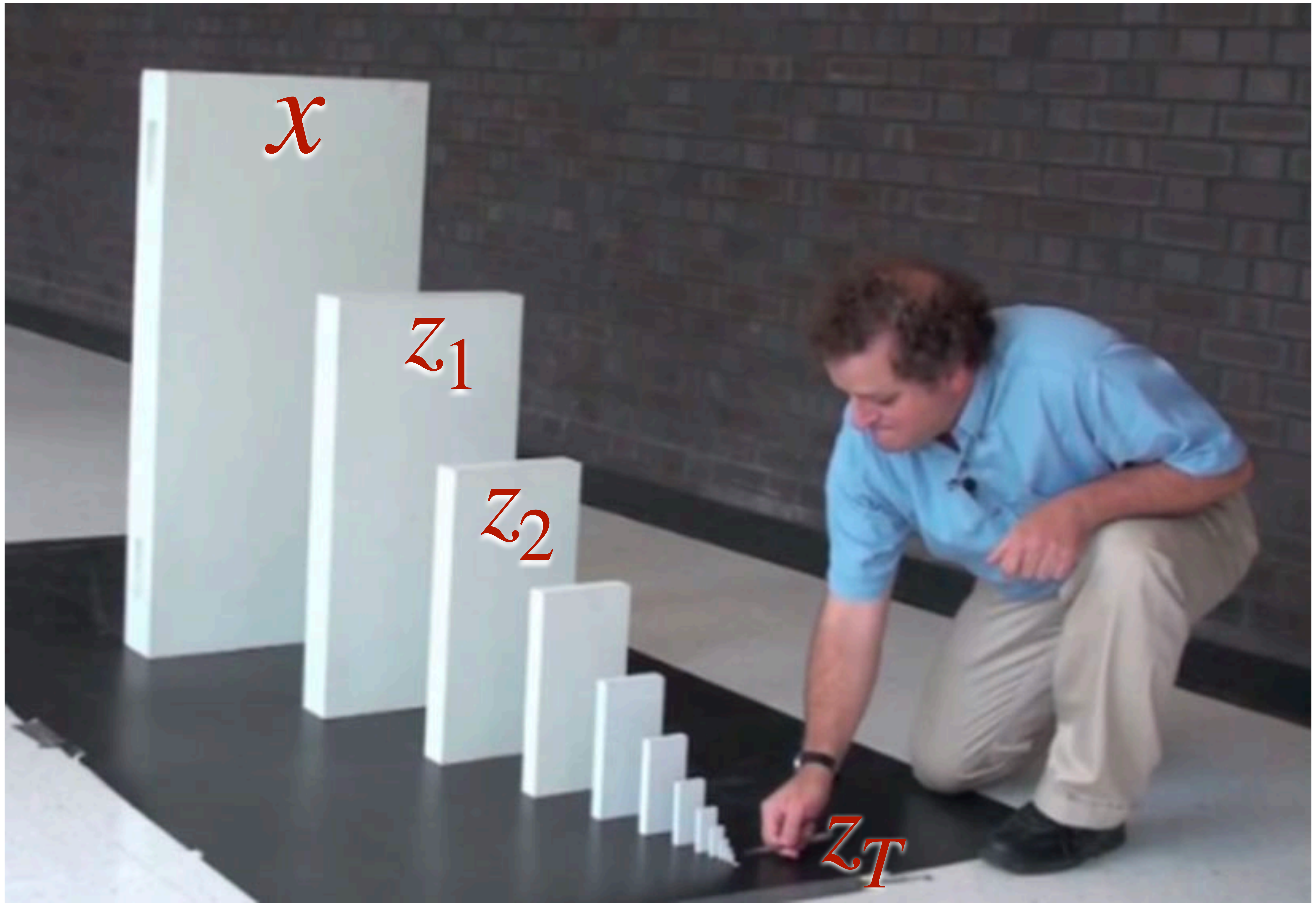
$x_{t-1} \sim p(x_{t-1} \mid x_t)$

Reverse process *(denoising)*

Prompt: *"A cat perched on an Ikea Poang chair"*

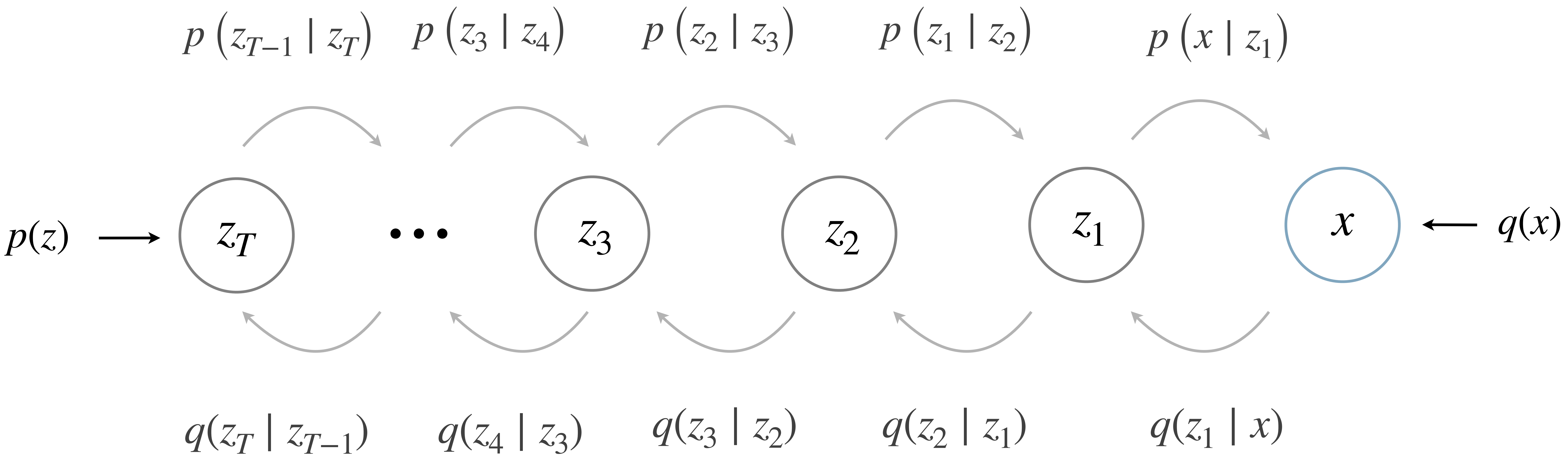
image ~ *p*(image | text prompt)

Towards diffusion: hierarchical VAEs



Towards diffusion: (Markovian) hierarchical VAEs

Reverse process $$p\left(x, z_1, z_2, \cdots, z_T\right) = p\left(z_T\right) p\left(z_{T-1} \mid z_T\right) \cdots p\left(z_1 \mid z_2\right) p\left(x \mid z_1\right)$$



Forward process $$q\left(x, z_1, z_2, \cdots, z_T\right) = q(x)\, q\left(z_1 \mid x\right)\, q\left(z_2 \mid z_1\right) \cdots q\left(z_T \mid z_{T-1}\right)$$

Towards diffusion: (Markovian) hierarchical VAEs

Diffusion models can be seen as hierarchical VAEs with a few restrictions:

- The forward *(encoding)* distribution prescribed as a Markov chain of Gaussians; it is not learned

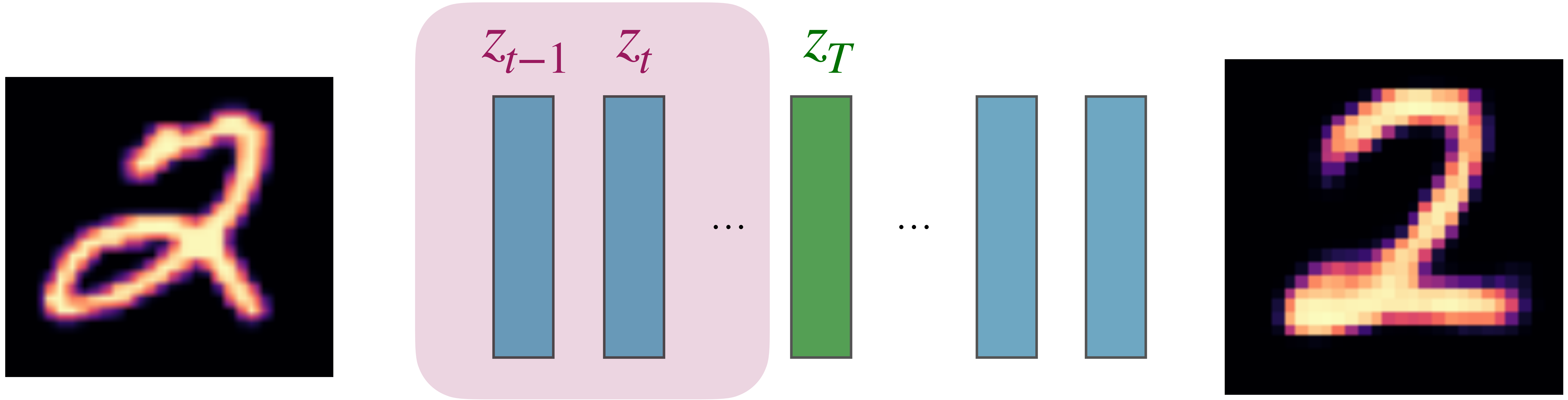
$$q\left(z_t \mid z_{t-1}\right) = \mathcal{N}\left(z_t; \alpha_t z_{t-1}, \beta_t\right)$$

- Distributions of latents at the final timestep T is a standard (unit) Gaussian

$$q(z_T \mid z_{T-1}, \ldots x) = \mathcal{N}(z_T; 0, \mathbb{I})$$

- The dimensionality of latents is the same as the data dimensionality

$$\dim(z_t) = \dim(x)$$

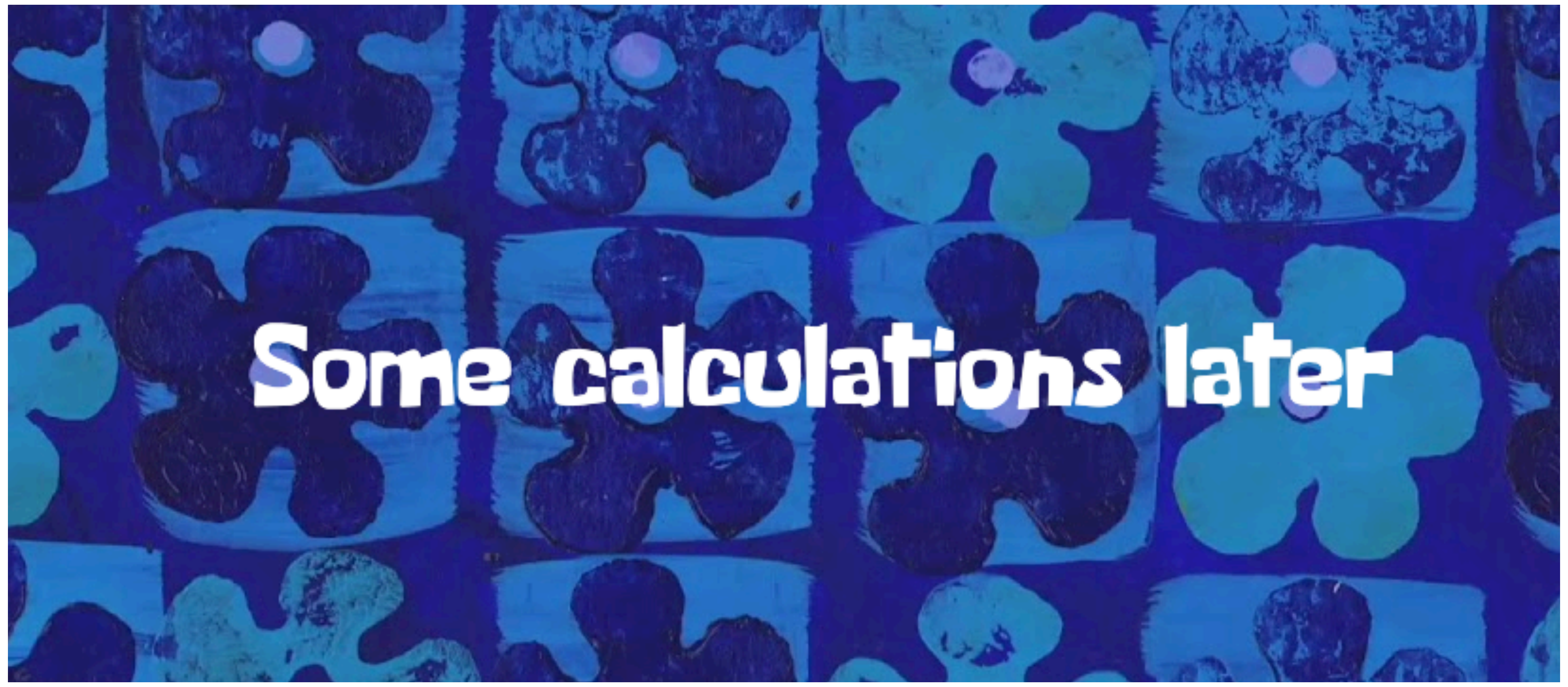


Variational diffusion models

[Kingma et al 2021]
[Gory details: Luo 2022; 2208.11970]

Align the forward and reverse distributions; variational lower bound (ELBO) as before

$$L = \left\langle \log \frac{q\left(x, z_1, z_2, \cdots, z_T\right)}{p\left(x, z_1, z_2, \cdots, z_T\right)} \right\rangle_{q(x)}$$



$$L = \left\langle \log p_\vartheta\left(x \mid z_1\right) \right\rangle_{q(z_1|x)} - D_{\mathrm{KL}}\left(q\left(z_T \mid x\right) \| p\left(z_T\right)\right) - \sum_{t=2}^{T} \left\langle D_{\mathrm{KL}}\left(q\left(z_{t-1} \mid z_t, x\right) \| p_\vartheta\left(z_{t-1} \mid z_t\right)\right) \right\rangle_{q(z_t|x)}$$

Reconstruction

(Noise model; no trainable parameters)

Prior regularization

(No trainable parameters)

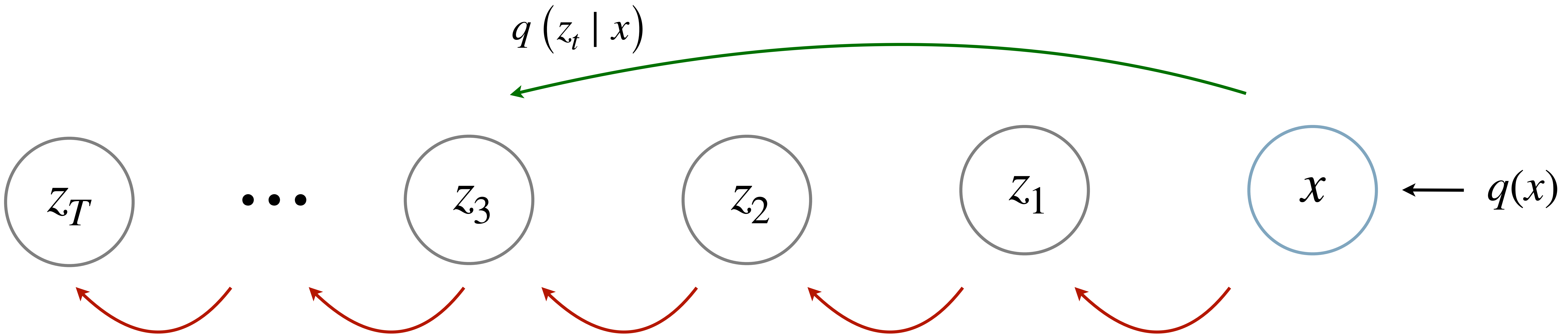
Denoising matching

ELBO! Bound on $p(x)$

The forward process and diffusion kernel

$$\sum_{t=2}^{T} \left\langle D_{\mathrm{KL}}\left(q\left(z_{t-1} \mid z_t, x\right) \| p_\vartheta\left(z_{t-1} \mid z_t\right)\right)\right\rangle_{q(z_t|x)}$$

Predict arbitrary timestep without Markovian sampling



Variance-preserving noise schedule

$$q\left(z_t \mid z_{t-1}\right) = \mathcal{N}\left(\sqrt{1-\beta_t} \cdot z_{t-1}, \beta_t\right)$$

$$z_t = \sqrt{1-\beta_t} \cdot z_{t-1} + \sqrt{\beta_t} \cdot \varepsilon$$

Diffusion kernel $\alpha_t = 1 - \beta_t$

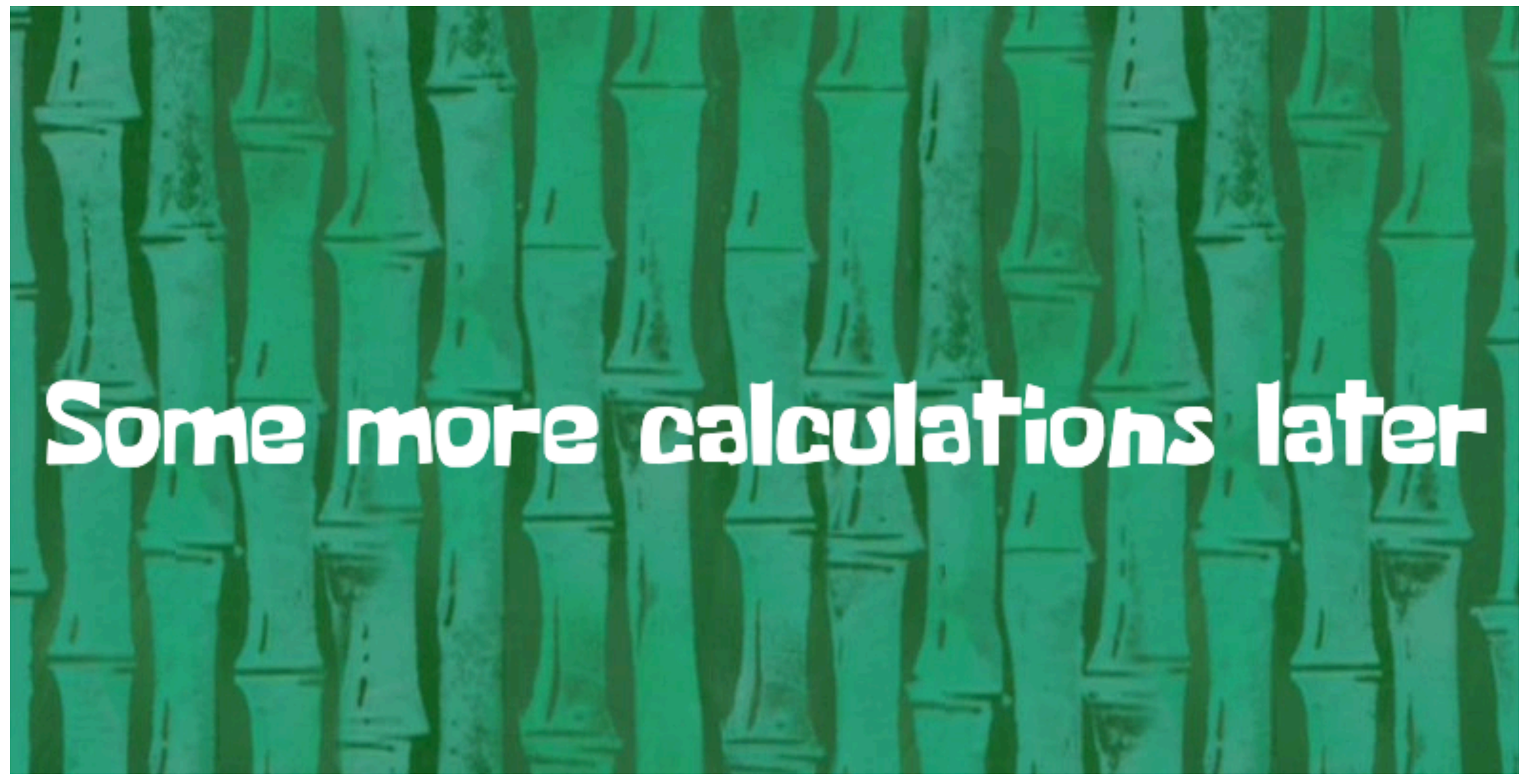
$$q\left(z_t \mid x\right) = \mathcal{N}\left(\sqrt{\bar{\alpha}_t} \cdot x, \sqrt{1-\bar{\alpha}_t}\right)$$

$$\bar{\alpha}_t = \prod_{i=1}^{t} \alpha_i$$

The denoising objective

Given the nature of the forward (noising) process, $q\left(z_{t-1} \mid z_t, x\right)$ can be computed analytically

$$\sum_{t=2}^{T} \left\langle D_{\mathrm{KL}}\left(q\left(z_{t-1} \mid z_t, x\right) \| p_\vartheta\left(z_{t-1} \mid z_t\right)\right)\right\rangle_{q(z_t|x)}$$



$$q\left(z_{t-1} \mid z_t, x\right) = \mathcal{N}\left(z_{t-1}; \mu_q(x_t, x_0), \sigma_q(t)\mathbb{I}\right)$$

Match *Set equal*

$$p_\vartheta\left(z_{t-1} \mid z_t, x\right) = \mathcal{N}\left(z_{t-1}; \mu_\vartheta(x_t, x_0), \sigma_\vartheta(t)\mathbb{I}\right)$$

Learnable denoising distribution; assume Gaussian

Denoising loss

$$\frac{1}{2\sigma_q^2(t)} \frac{\bar{\alpha}_{t-1}\left(1-\alpha_t\right)^2}{\left(1-\bar{\alpha}_t\right)^2}\left[\left\| \hat{x}_\theta\left(z_t, t\right) - x \right\|^2\right]$$

[Ho et al 2020]

The denoising objectives

x-prediction; MLE

$$\frac{1}{2\sigma_q^2(t)} \frac{\bar{\alpha}_{t-1}\left(1-\alpha_t\right)^2}{\left(1-\bar{\alpha}_t\right)^2}\left[\left\| \hat{x}_\theta\left(z_t, t\right) - x \right\|^2\right]$$

ϵ-prediction; MLE

$$\frac{1}{2\sigma_q^2(t)} \frac{\left(1-\alpha_t\right)^2}{\left(1-\bar{\alpha}_t\right)\alpha_t}\left[\left\| \epsilon - \hat{\epsilon}_\theta\left(x_t, t\right) \right\|^2\right]$$

ϵ-prediction; “simple”

$$\left\| \epsilon - \hat{\epsilon}_\theta\left(x_t, t\right) \right\|^2$$

Typical objective for training image diffusion models: *SOTA on many tasks!*

Simple objectives as a weighted sum of ELBOs

Kingma and Gao (2023) showed that common objectives can be written as a weighted sum (across different noise levels) of ELBOs

$$L_w(x) = \left\langle w(t) \cdot w_{\mathrm{ML}}(t) \left\| \epsilon - \hat{\epsilon}_\theta\left(z_t, t\right) \right\|^2 \right\rangle_{t,\epsilon}$$

Additional weighting (w_{ML}^{-1} for ϵ-prediction)

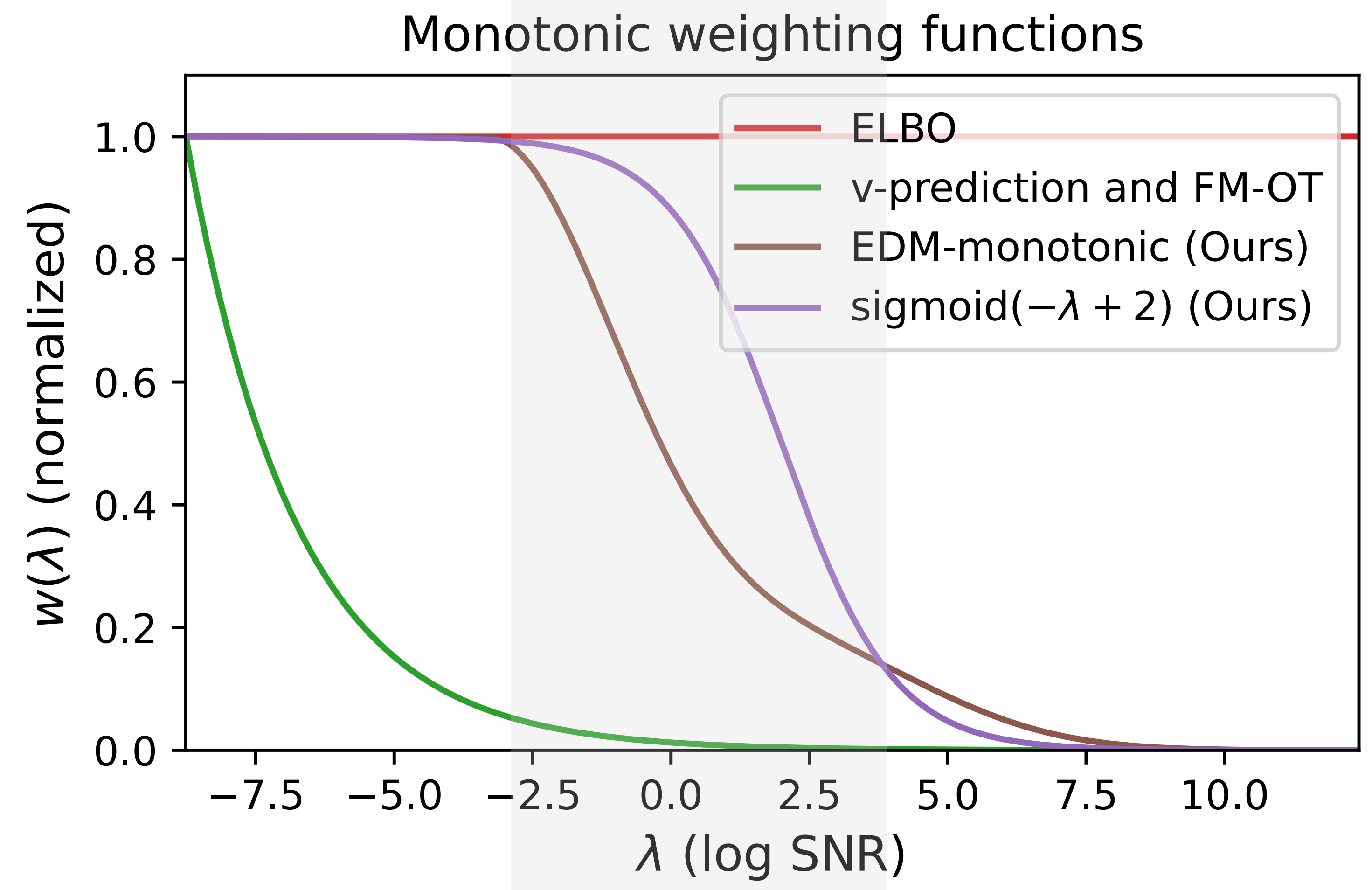
Weighting for ELBO/ ML objective

$$L(t;x) \equiv D_{\mathrm{KL}}\left(q\left(z_{t:1} \mid x\right) \| p\left(z_{t:1}\right)\right)$$

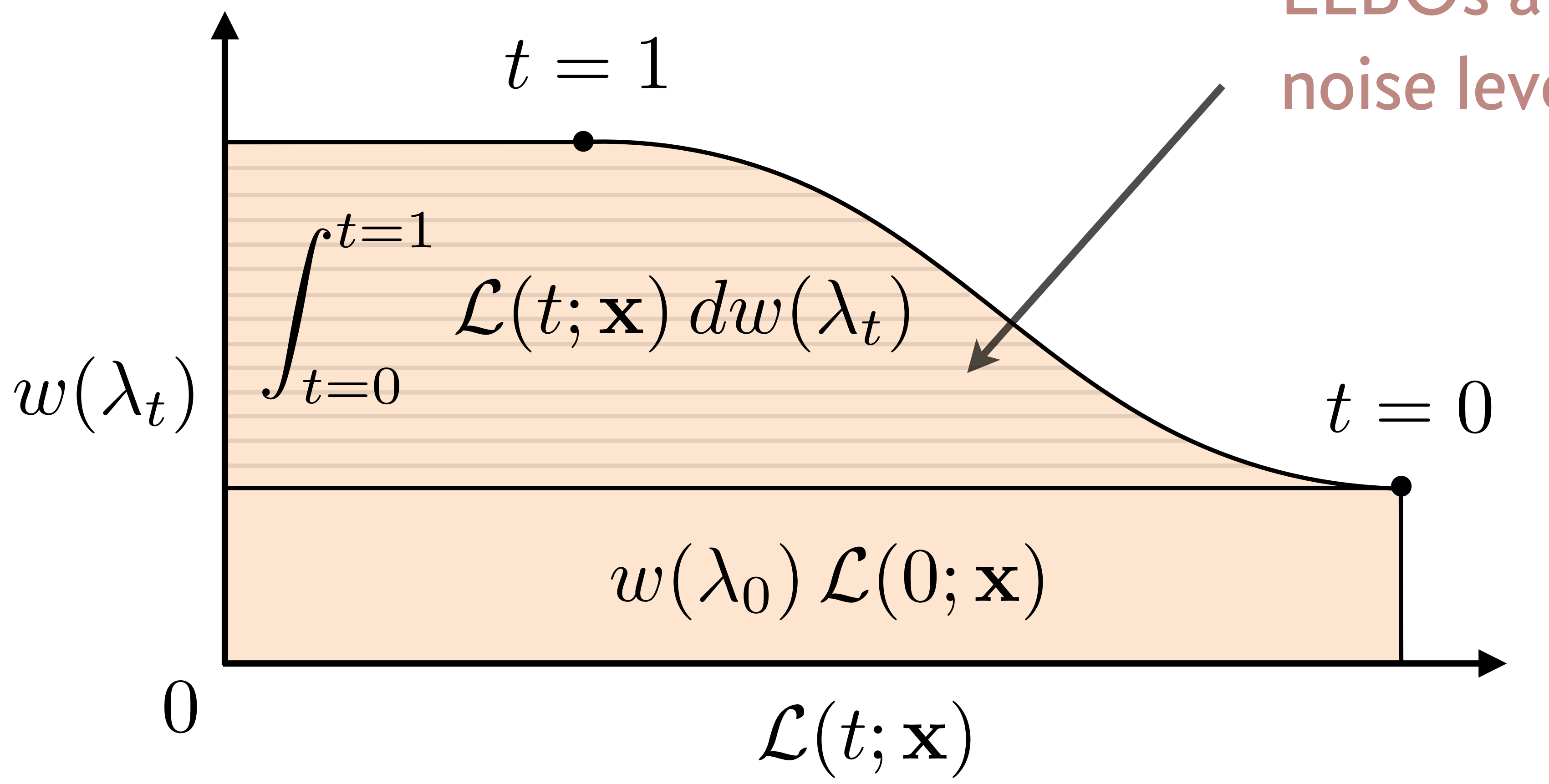
$$L_w(x) \propto \int_0^1 \frac{d}{dt} w(t)\, L(t;x)\, \mathrm{d}t + w(t_0)\, L(0;x)$$

Interpretation: *data augmentation with additive Gaussian noise / data-distribution smoothing*

More important for perceptual quality?



ELBOs at different noise levels



Continuous-time/SDE formulation

$$x_t = \sqrt{1-\beta_t} \cdot x_{t-1} + \sqrt{\beta_t} \cdot \varepsilon$$

In the limit of infinite time steps, $\Delta_t \to 0$ and the forward diffusion process can be written as

$$\begin{aligned} x_t &= \sqrt{1-\beta(t)\Delta_t}\, x_{t-1} + \sqrt{\beta(t)\Delta_t}\,\mathcal{N}(0,\mathbb{I}) \\ &\approx x_{t-1} - \frac{\beta(t)\Delta_t}{2} x_{t-1} + \sqrt{\beta(t)\Delta_t}\,\mathcal{N}(0,\mathbb{I}) \end{aligned}$$

Which is an update rule corresponding to the Euler-Murayama discretization of the stochastic differential equation (SDE)

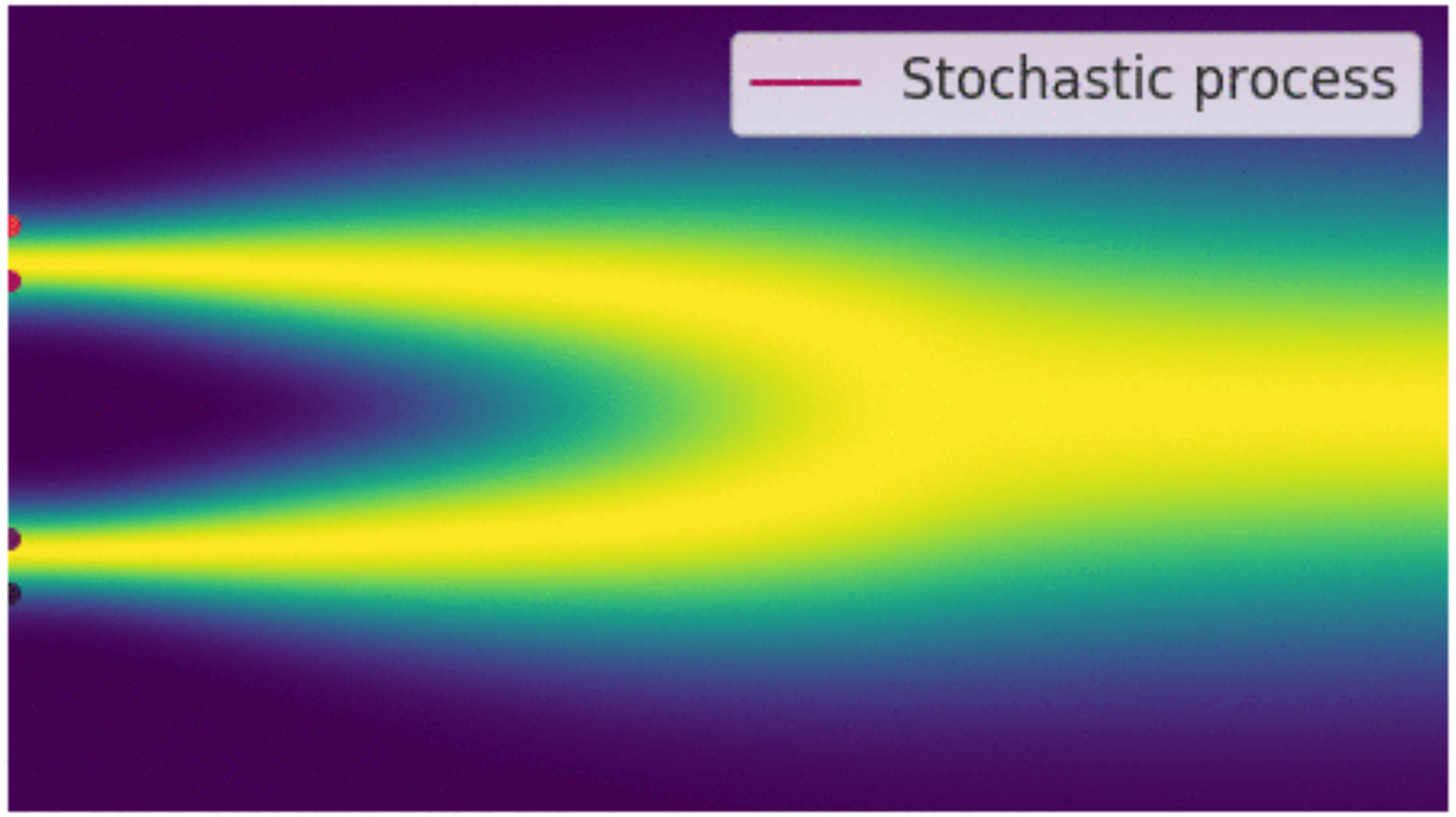
$$\mathrm{d}x_t = -\frac{1}{2}\beta(t) x_t \,\mathrm{d}t + \sqrt{\beta(t)}\,\mathrm{d}w_t$$

Continuous-time/SDE formulation

[Song et al 2021]

https://yang-song.net/blog/2021/score/

The forward diffusion process defined by an SDE

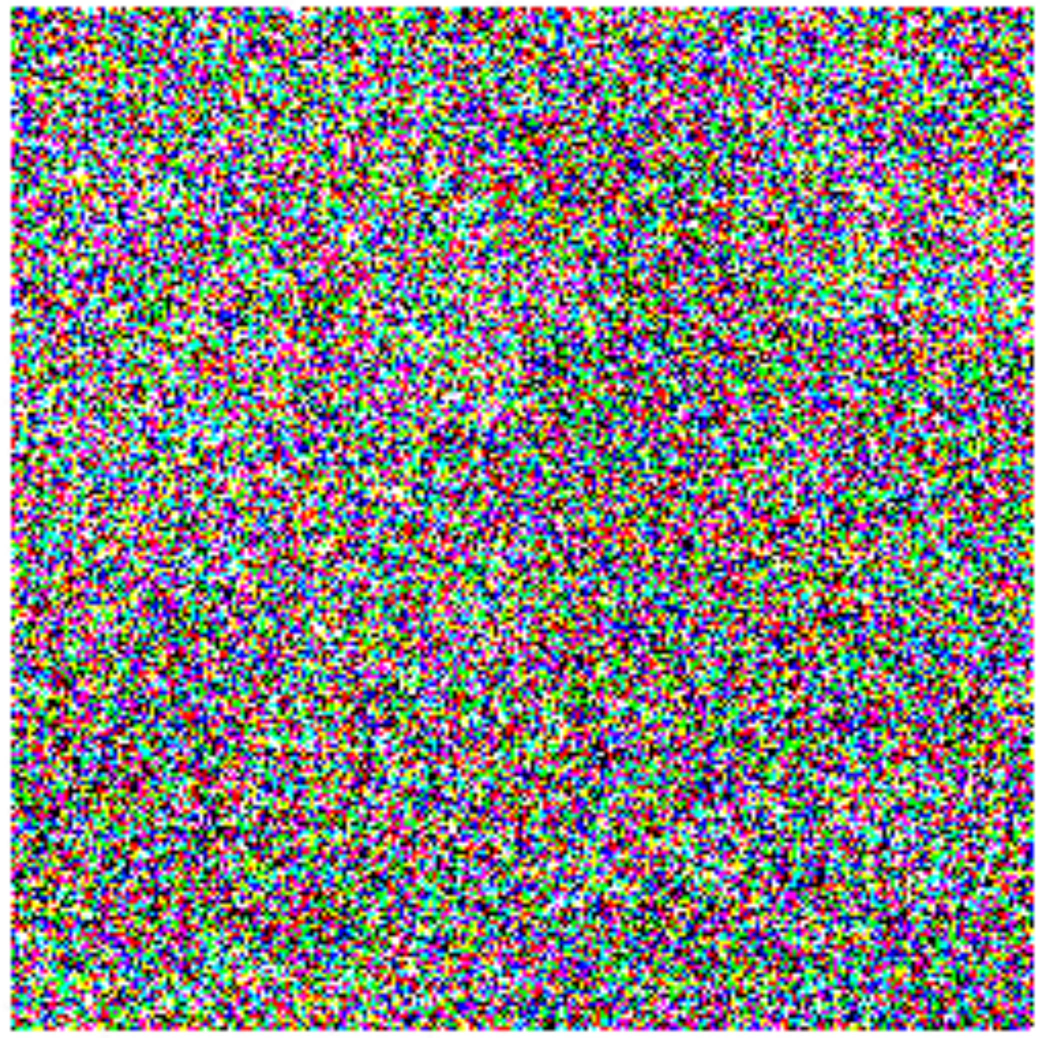


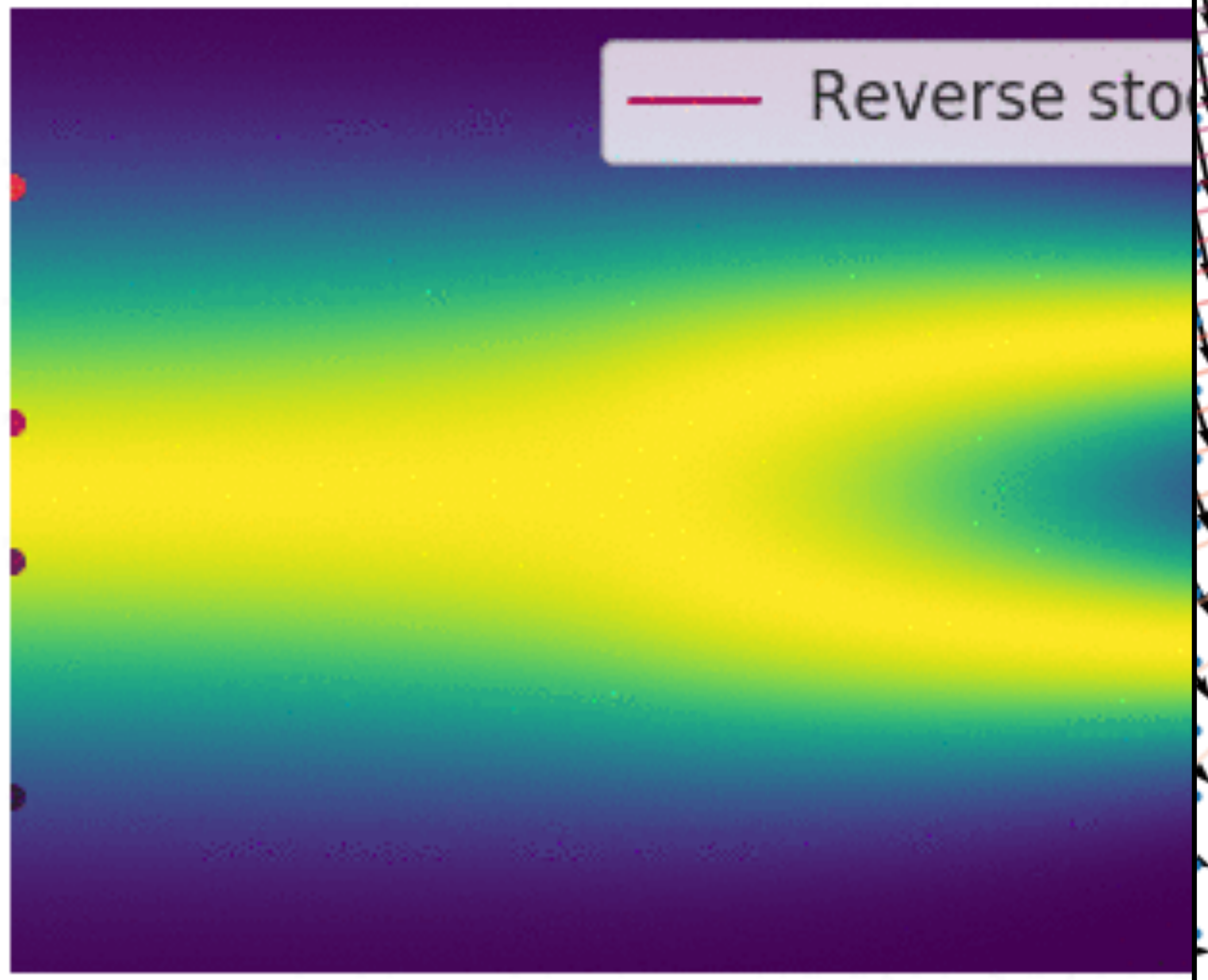
$$\mathrm{d}x_t = -\frac{1}{2}\beta(t)x_t\,\mathrm{d}t + \sqrt{\beta(t)}\mathrm{d}w_t$$

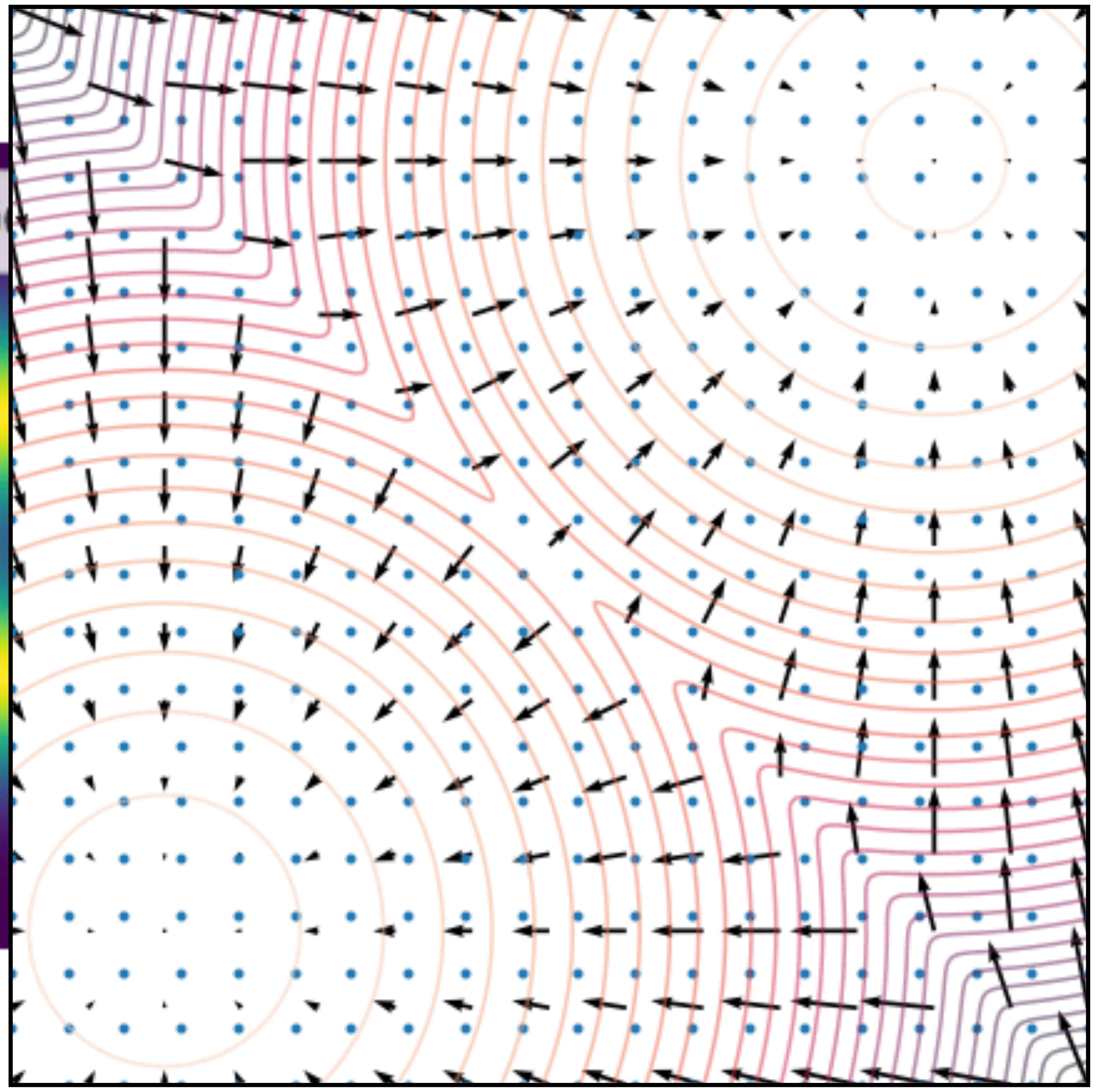
The reverse SDE

https://yang-song.net/blog/2021/score/

The reverse process satisfies a reverse-time SDE that can be derived from the forward SDE and the score of the marginal distribution, $\nabla_{x_t} \log q(x_t)$







$$dx_t = \left[-\frac{1}{2}\beta(t)x_t - \beta(t)\nabla_{x_t}\log q\left(x_t\right)\right]dt + \sqrt{\beta(t)}dw_t$$

Denoising score matching

* x conditioning disappears when taking expectation wrt x to give marginal score

Need to compute the score $\nabla_{x_t} \log q(x_t)$

The *conditional* score $\nabla_{x_t} \log q(x_t \mid x)$ can be computed using the diffusion kernel

$$\nabla_{x_t} \log q(x_t \mid x) = -\frac{(x_t - x)}{\sigma_t^2} = -\frac{\epsilon}{\sigma_t}$$

Noise-prediction

$$\frac{1}{2\sigma_q^2(t)} \frac{\left(1-\alpha_t\right)^2}{\left(1-\bar{\alpha}_t\right)\alpha_t} \left[\left\| \epsilon - \hat{\epsilon}_\theta\left(x_t, t\right) \right\|^2 \right]$$

$\Longleftrightarrow$

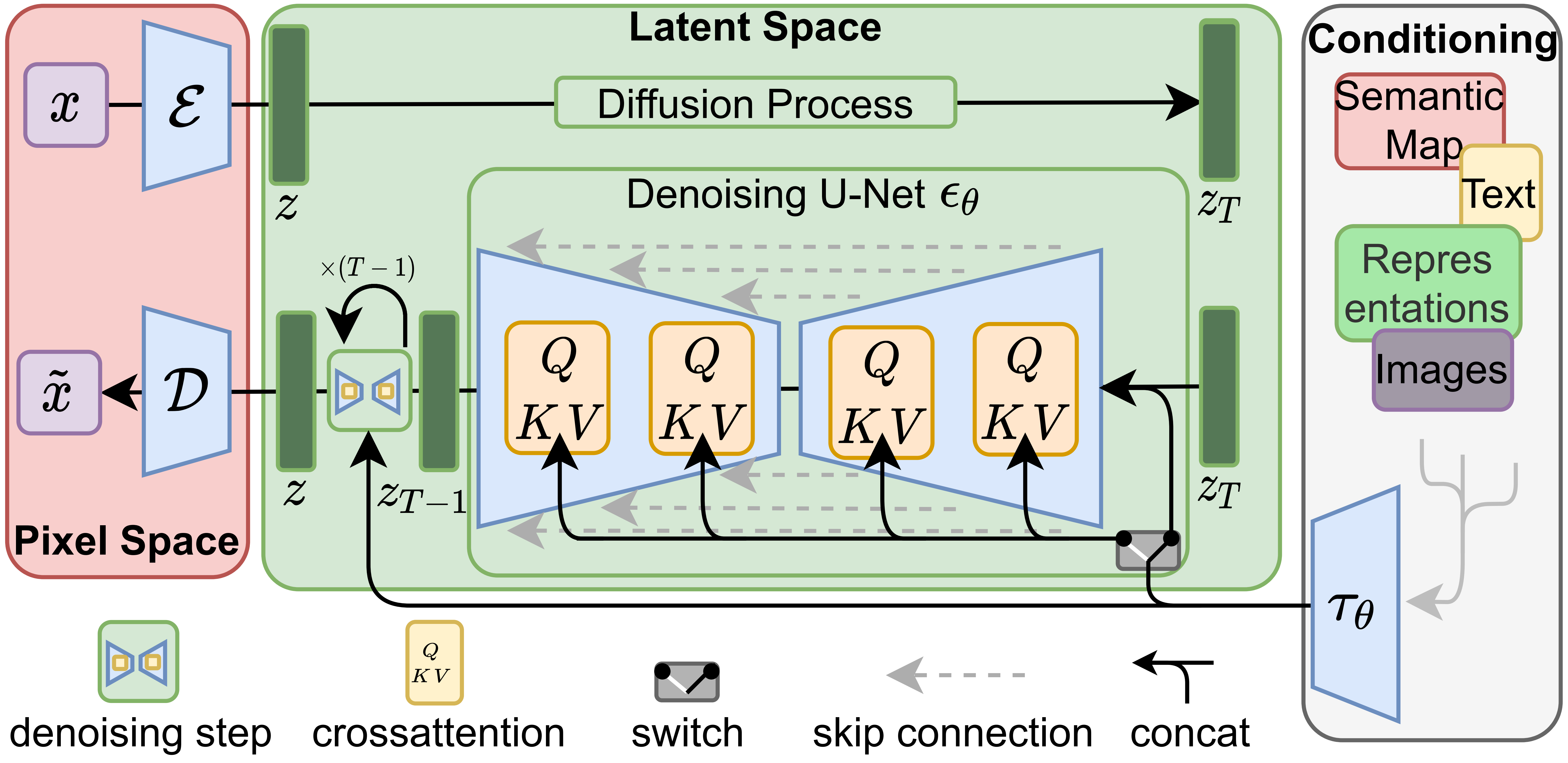
Score-matching *

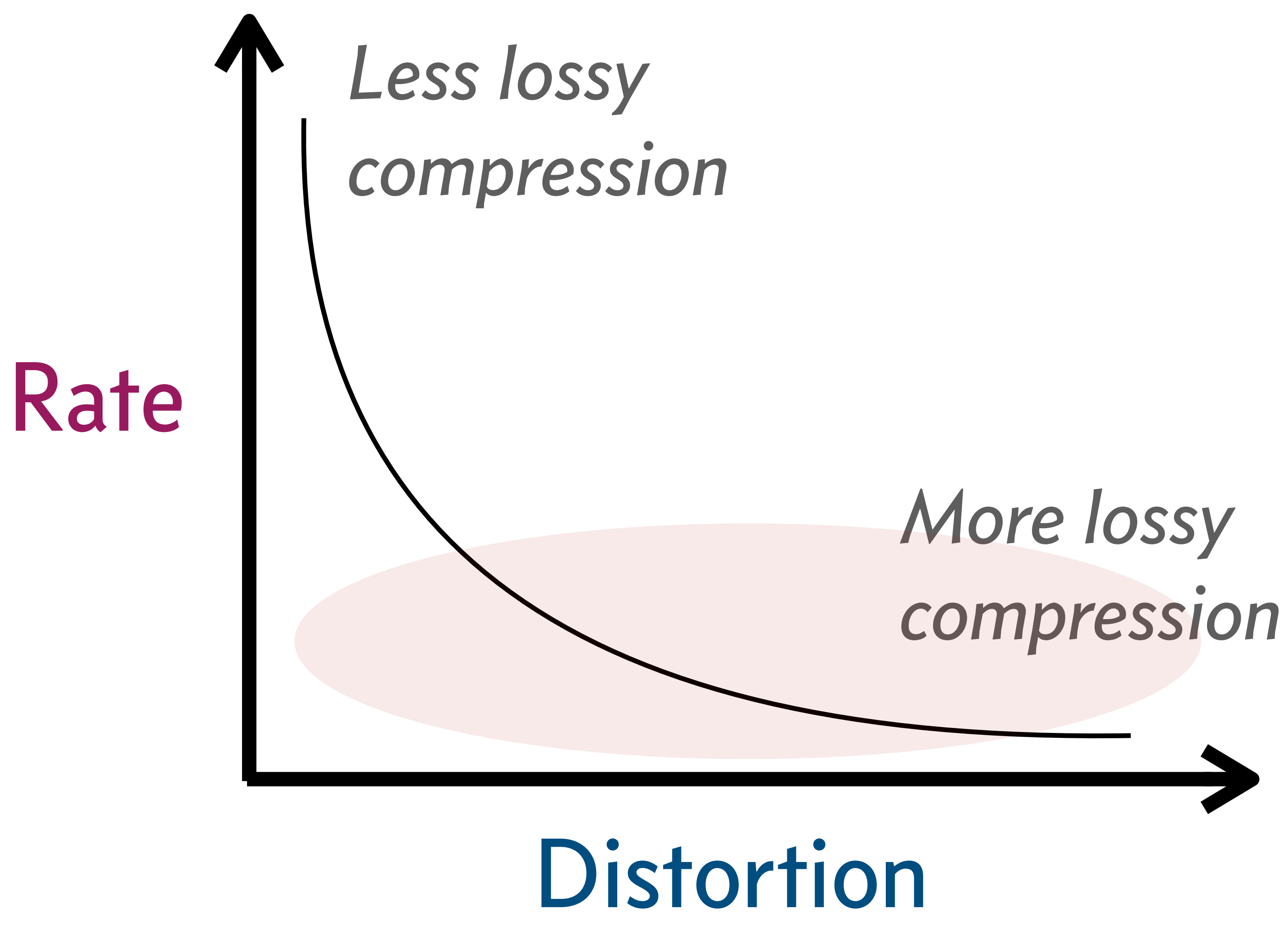
$$\frac{1}{2\sigma_q^2(t)} \frac{\left(1-\alpha_t\right)^2}{\alpha_t} \left[\left\| s_\theta\left(x_t, t\right) - \nabla \log q(x_t) \right\|^2 \right]$$

The noise- and score-prediction networks are equivalent up to a std-scaling

The noise/score-prediction model and *latent diffusion*

[Rombach et al 2021]

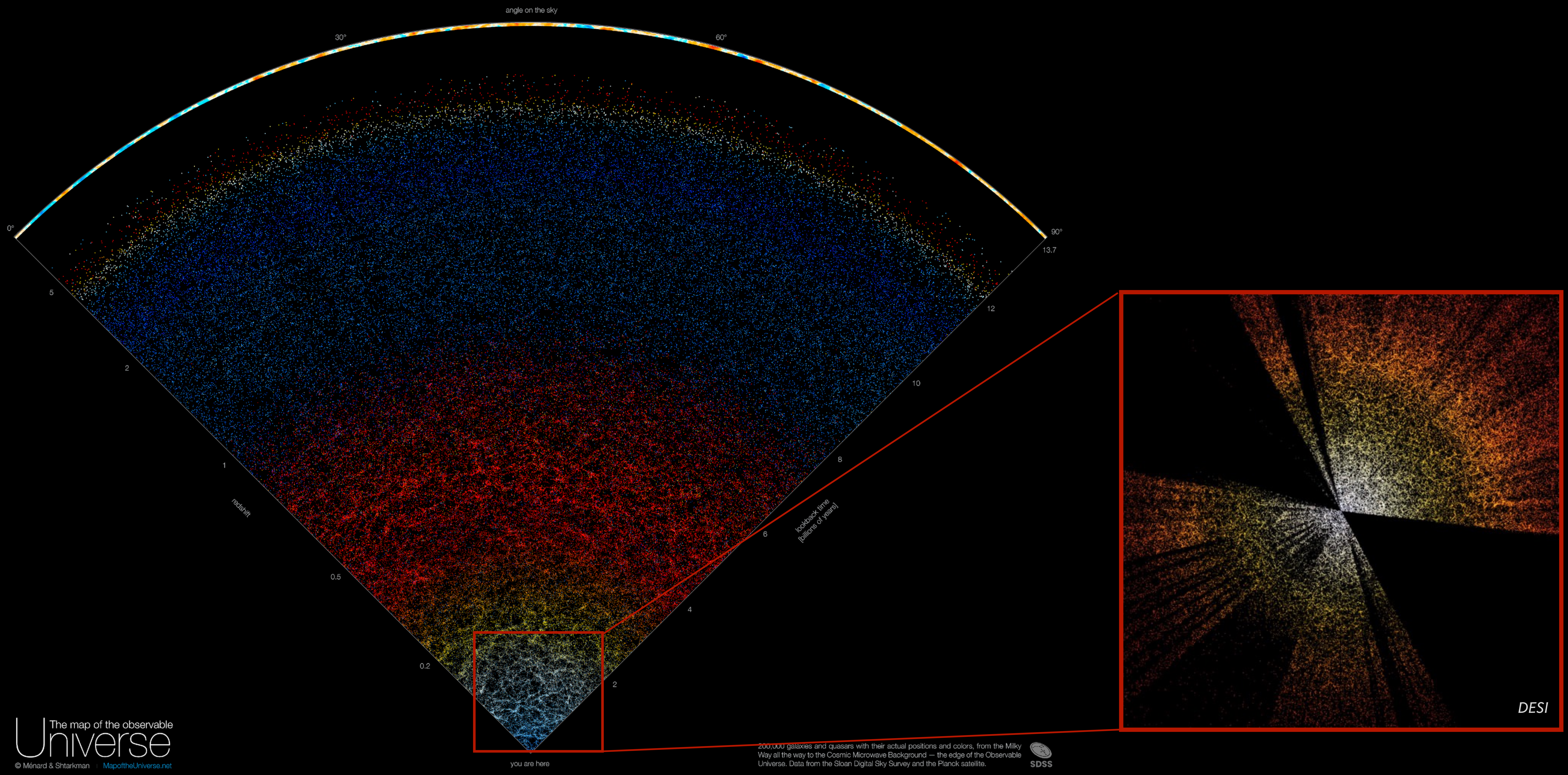




Perceptual compression while retaining semantically meaningful information

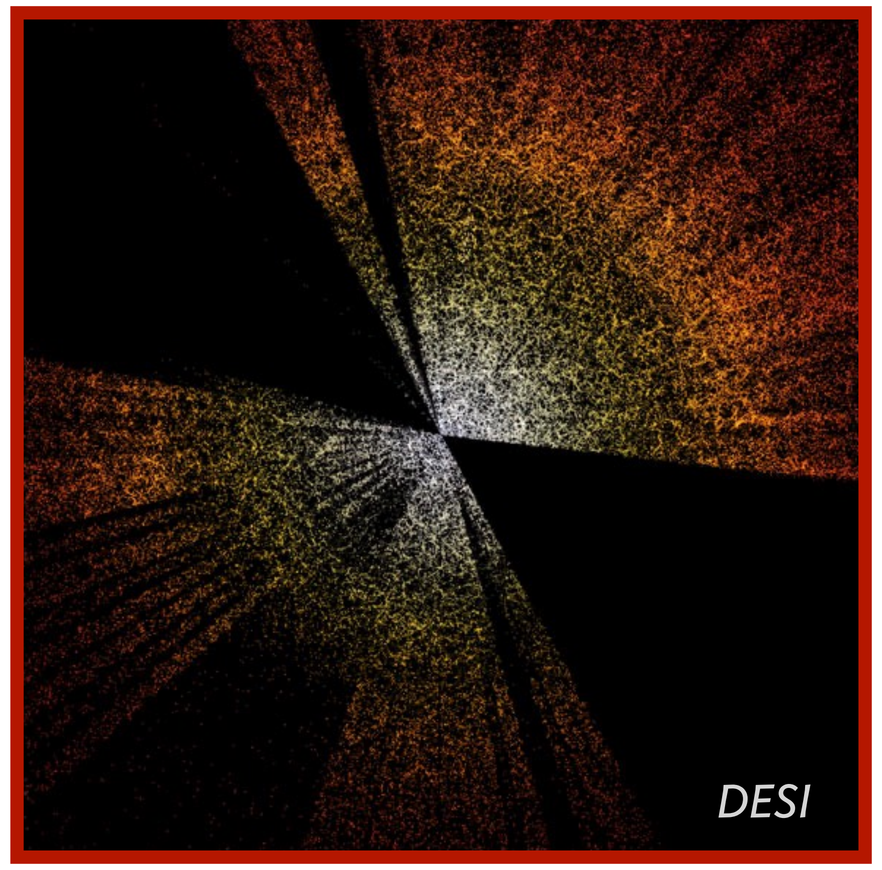
An application to *galaxy clustering*

Work with Carol Cuesta-Lazaro [MIT/IAIFI]



angle on the sky
0°
30°
60°
90°
13.7
12
10
8
6
4
2
lookback time [billions of years]
5
2
1
0.5
0.2
redshift
you are here
DESI
The map of the observable Universe
© Ménard & Shtarkman
MapoftheUniverse.net
200,000 galaxies and quasars with their actual positions and colors, from the Milky Way all the way to the Cosmic Microwave Background — the edge of the Observable Universe. Data from the Sloan Digital Sky Survey and the Planck satellite.
SDSS

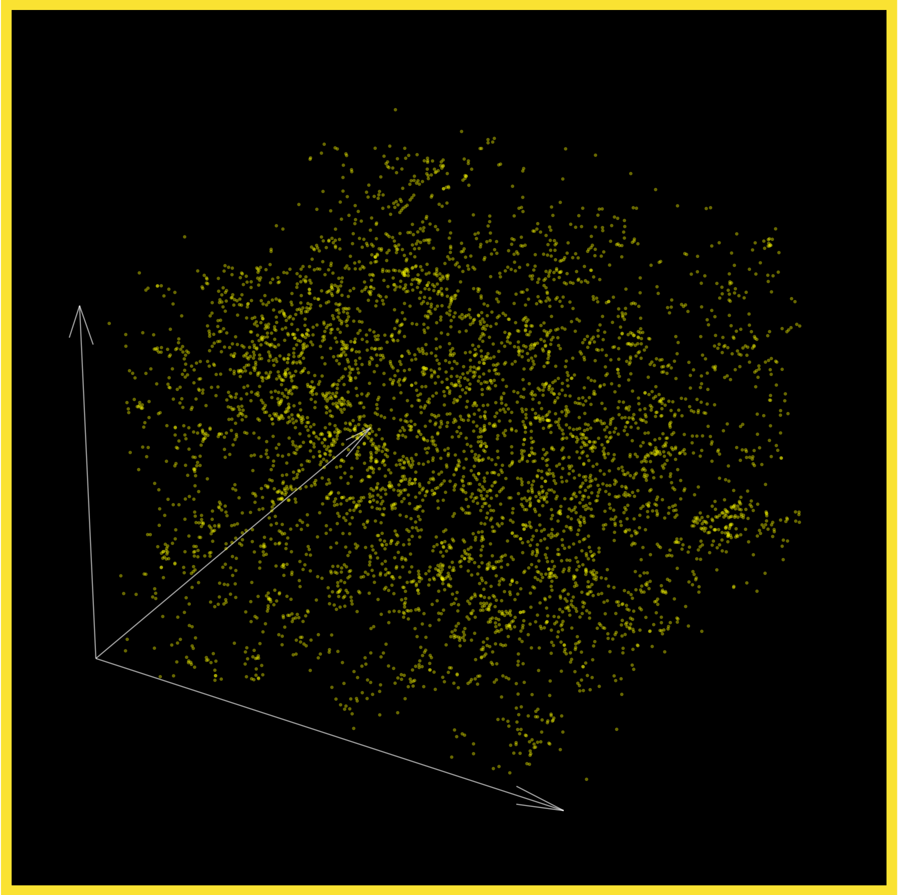
The likelihood of a galaxy field

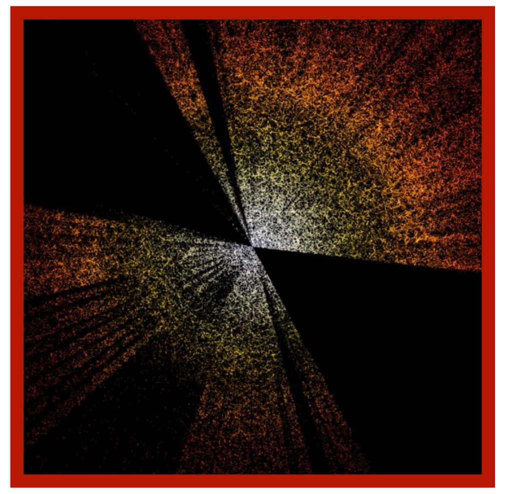
$p($  $\mid$ Cosmology parameters $)$

Simplify this *and/or this*

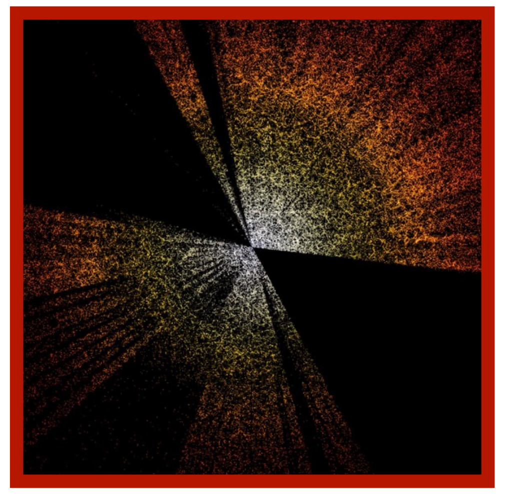
Intractable!

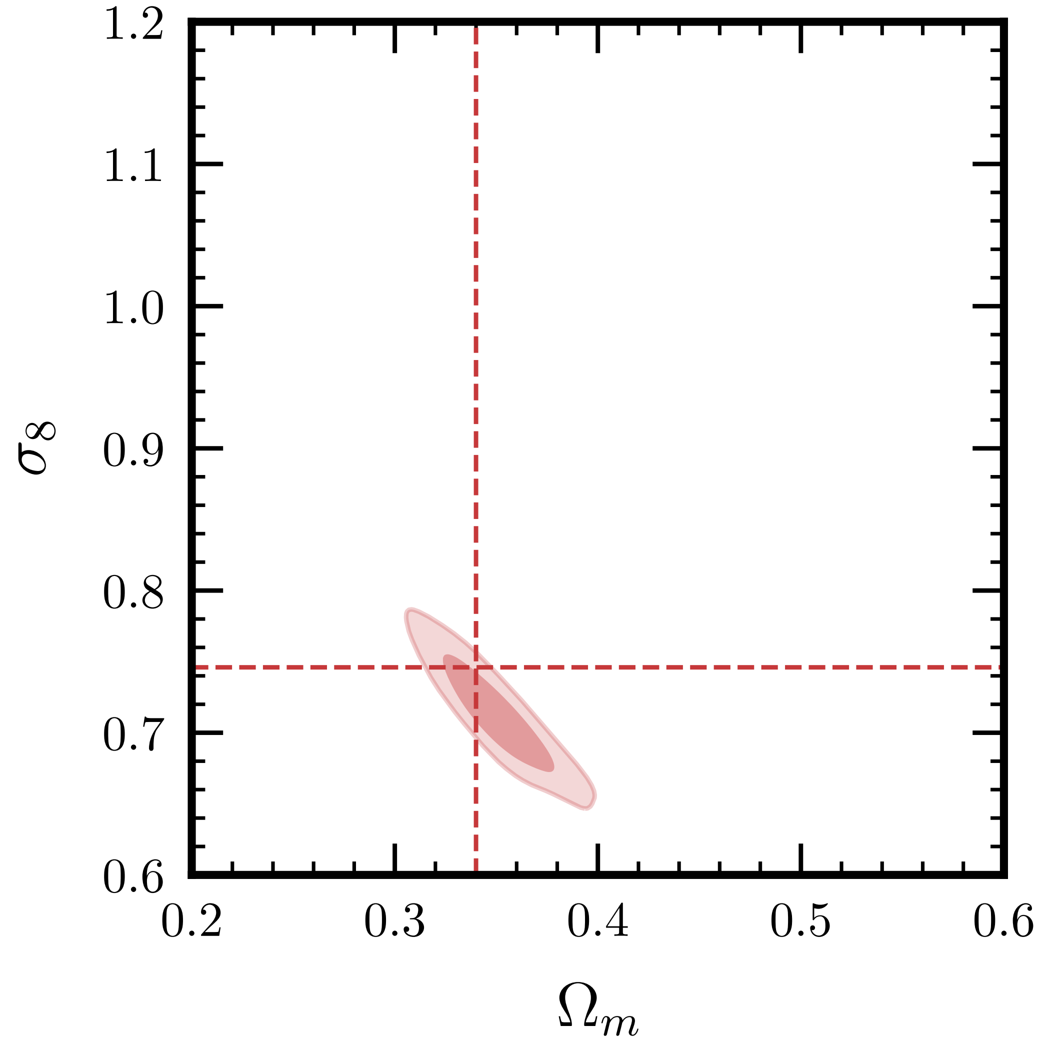
Emulation and inference



$\sim p($  $|$ Cosmology $)$

Emulation/ sampling

$p($ Cosmology Ω_m, σ_8 $|$  $)$



Parameter estimation

$\nabla_{\{\Omega_m,\sigma_8\}} p$

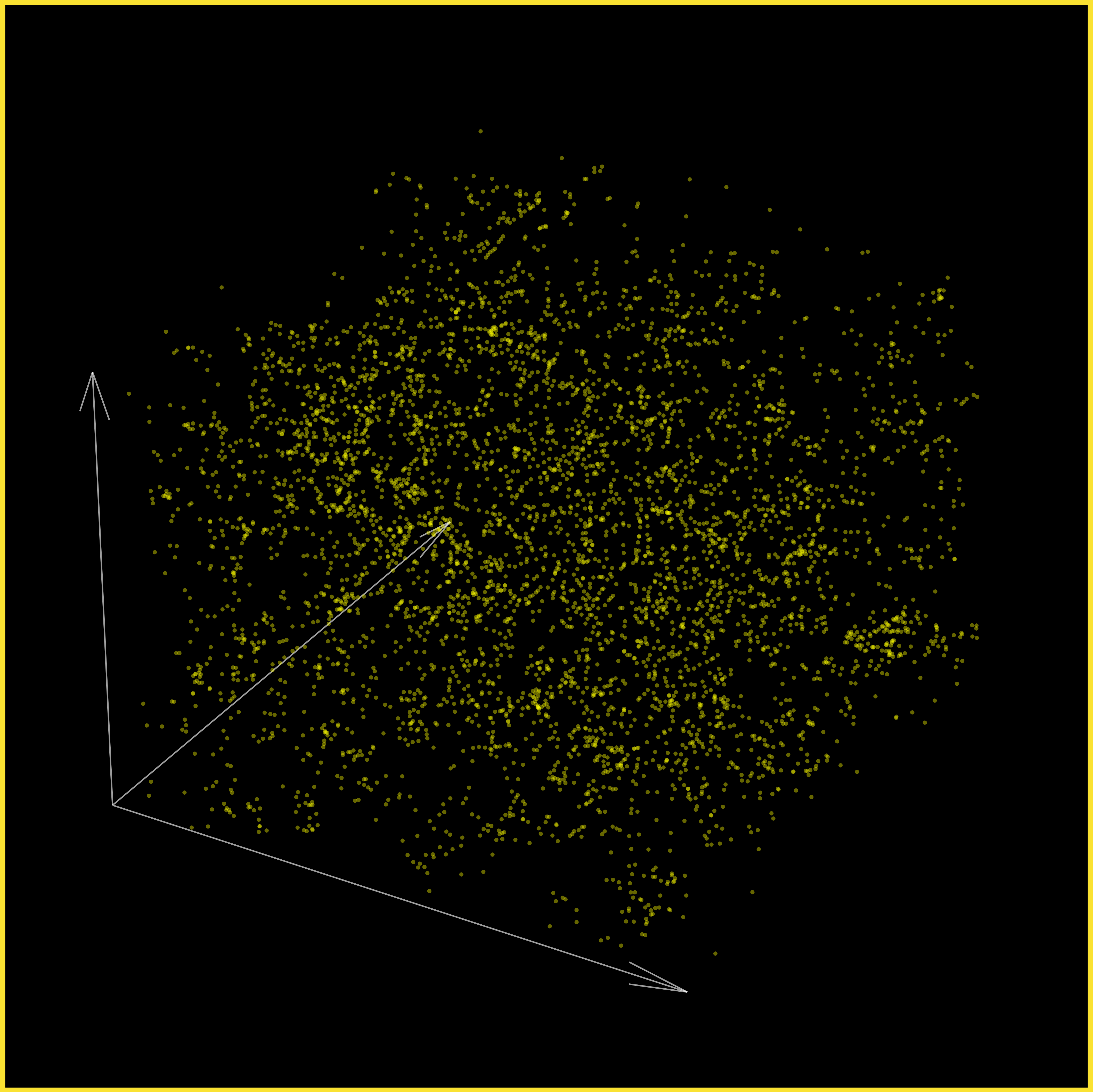
Differentiable likelihood → even better!

The diffusion score model

Want a score model that

- Operates on *sets* of varying cardinality
- Is permutation equivariant
- Efficiently captures correlation structure of point cloud

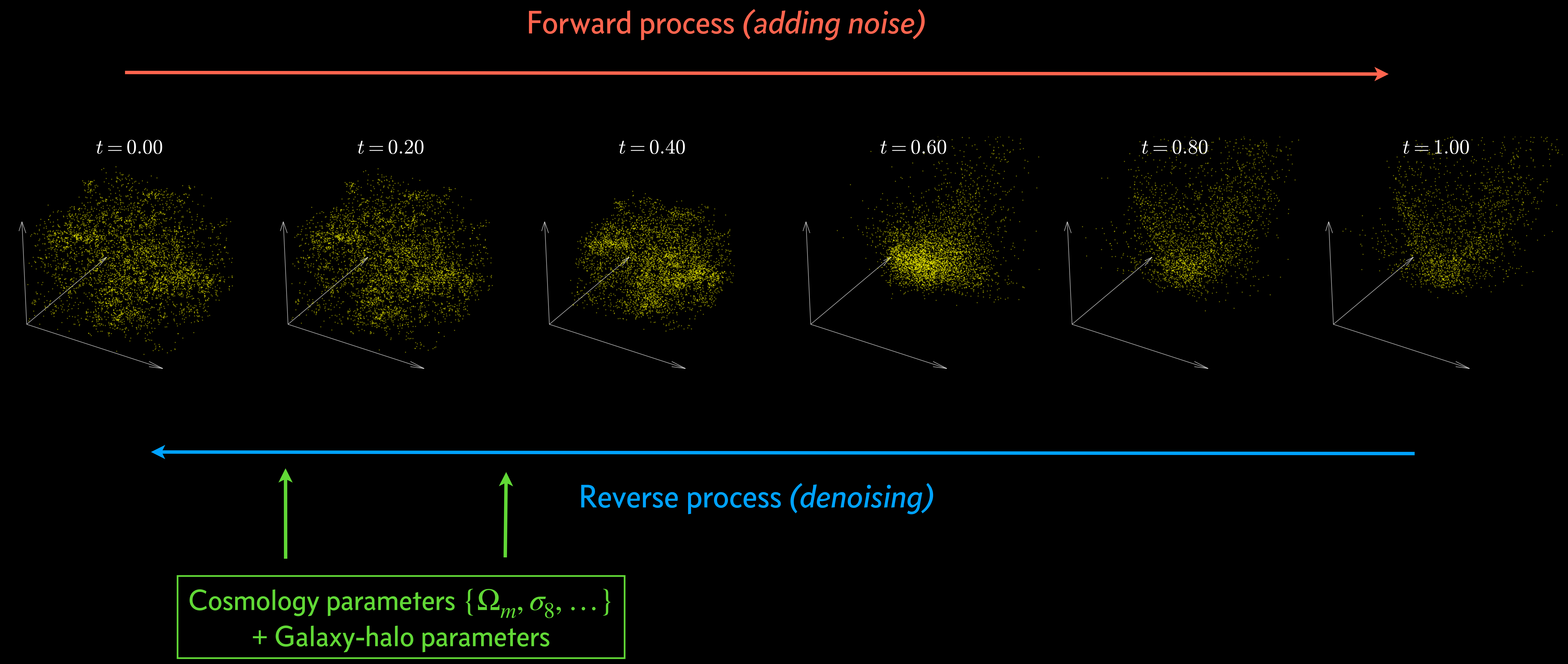
✓ Tranformers
✓ Graph neural networks



Graph neural network-guided diffusion on galaxies

SM, Cuesta-Lazaro [ICML ML4Astro]

Samples from *Quijote* [Villaescusa-Navarro et al, 2021].

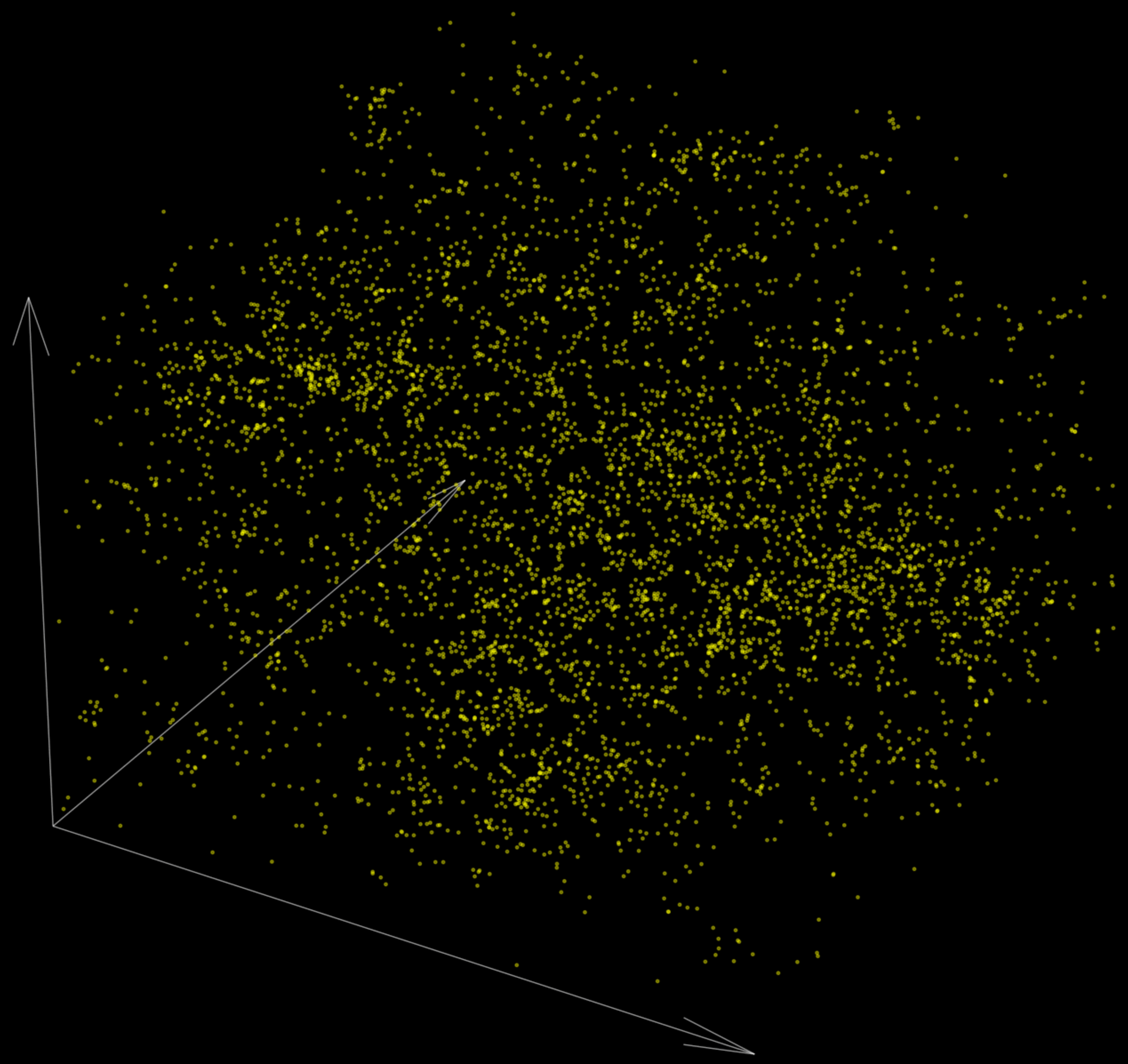


Diffusion on galaxies

SM, Cuesta-Lazaro [ICML ML4Astro]

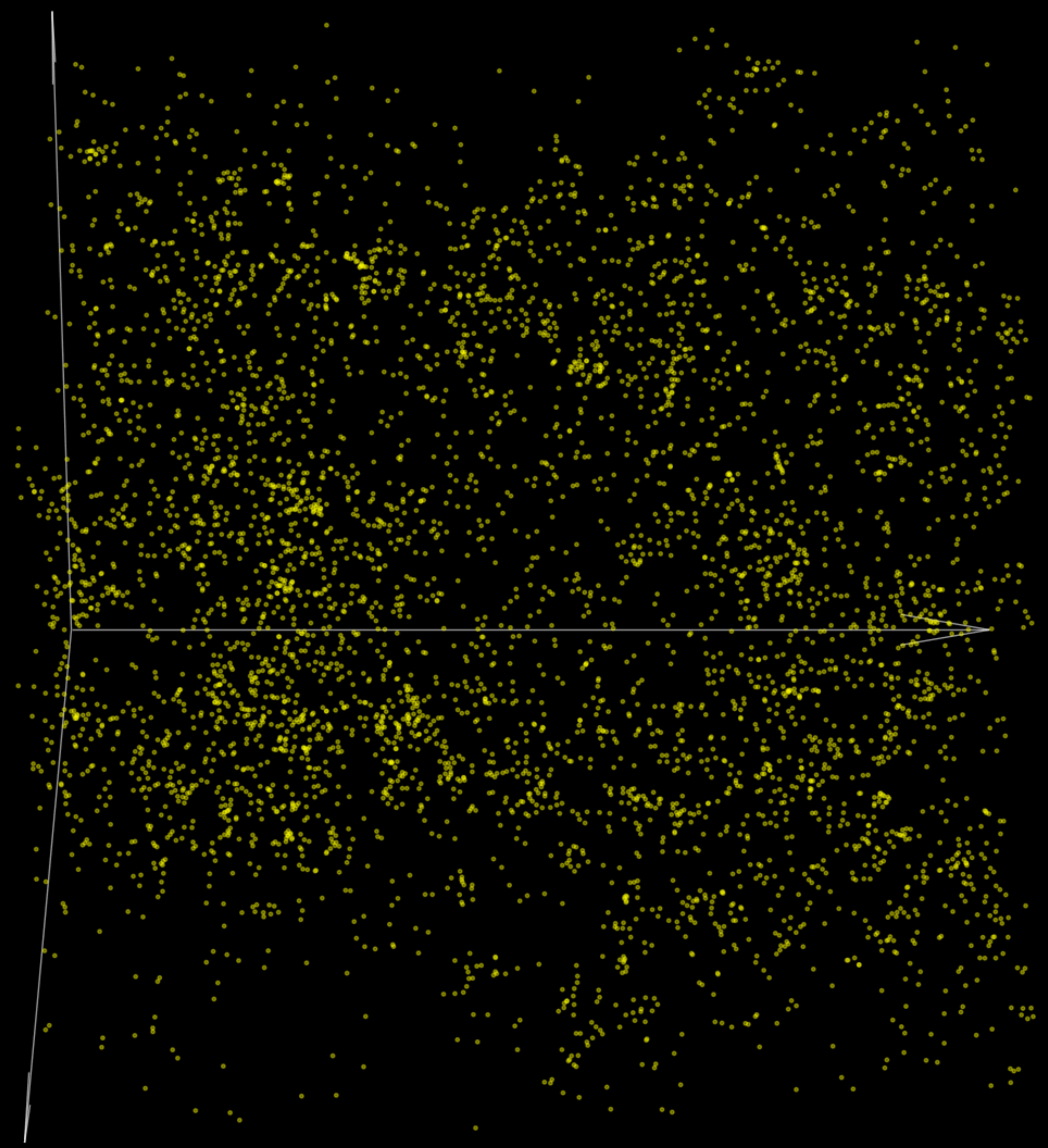
Diffusion process

$t = 0.00$



Conditional generation $x \sim p(x \mid \Omega_m, \sigma_8)$

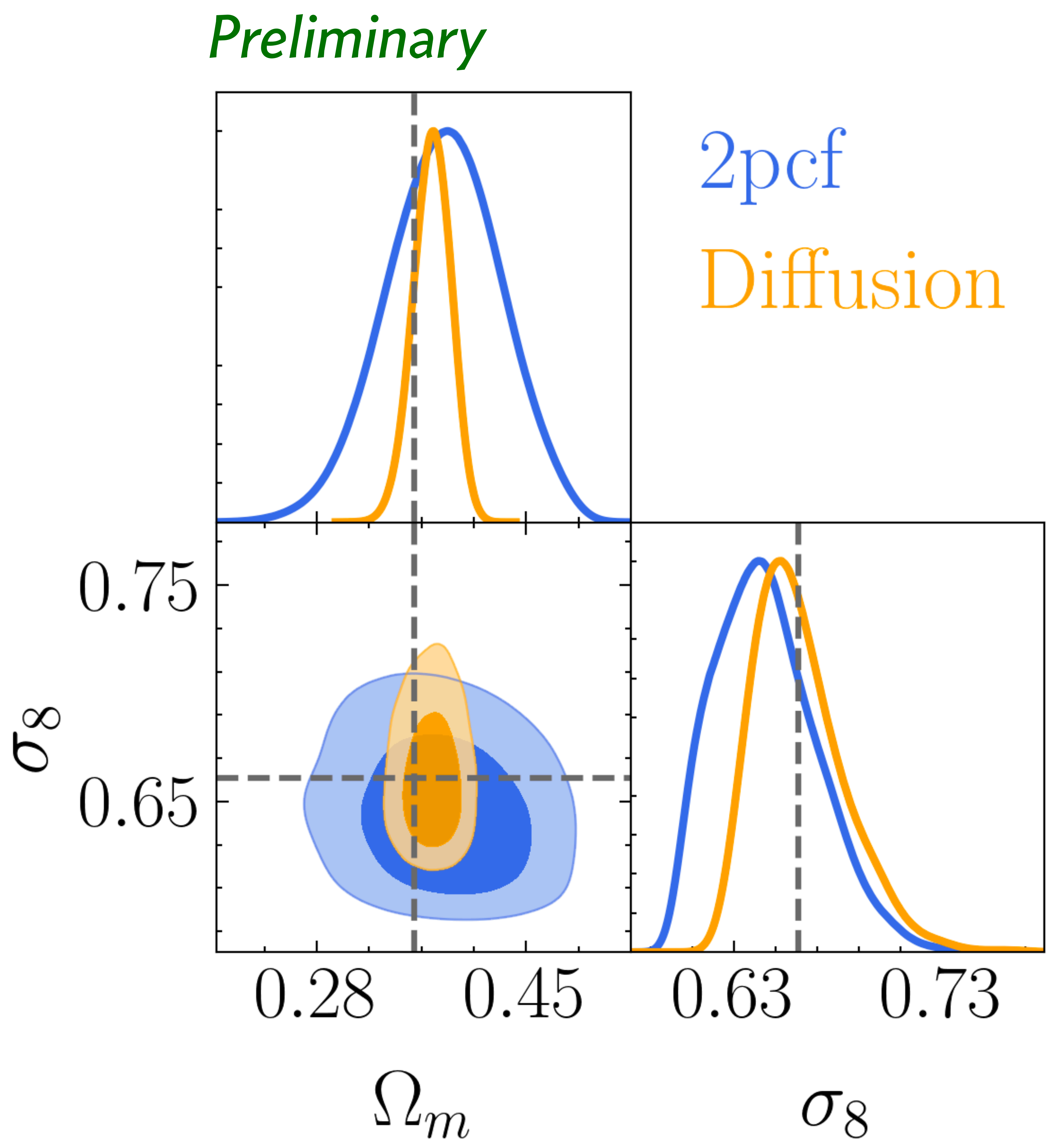
$\Omega_m = 0.10, \sigma_8 = 0.60$



Likelihoods and parameter inference

For a given dataset, can use the likelihood $p(x \mid \theta)$ for posterior parameter inference

- Monte Carlo sampling (MCMC, nested sampling, HMC...)
- Variational inference



Another application: *as a galaxy prior for gravitational lensing*

[Adam, Coogan, Malkin et al 2022]

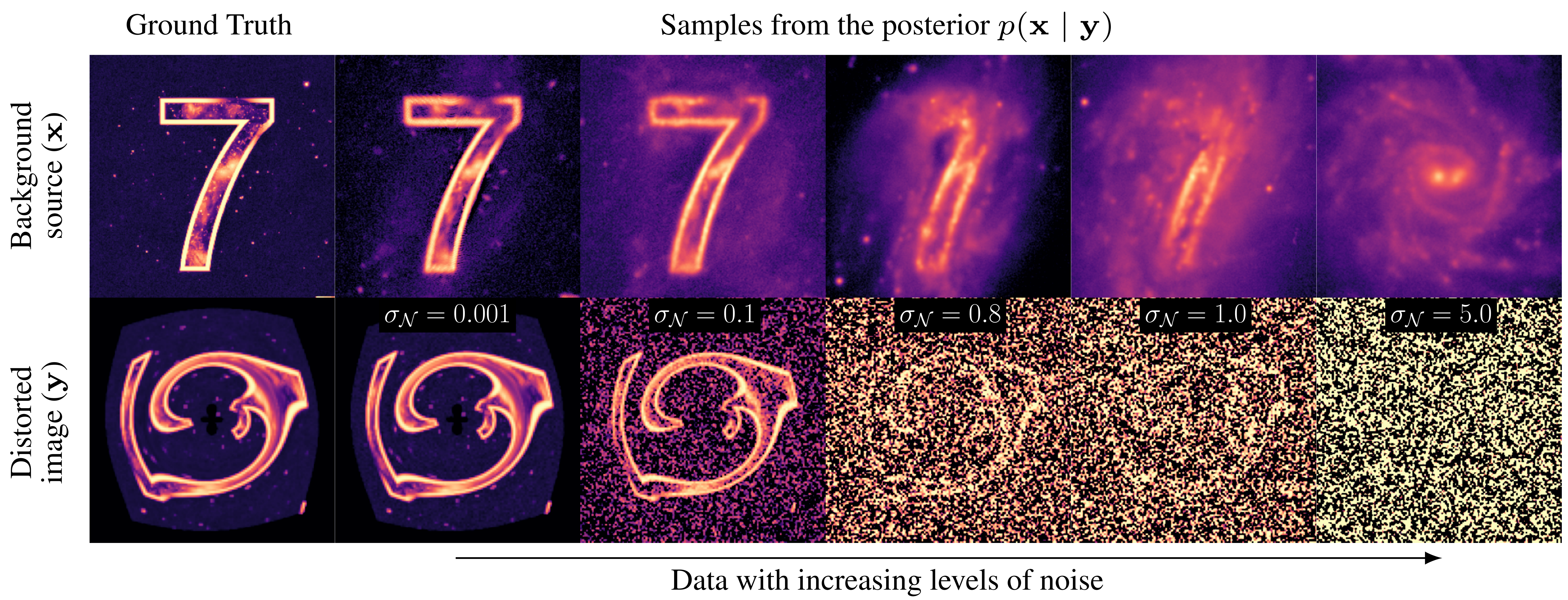
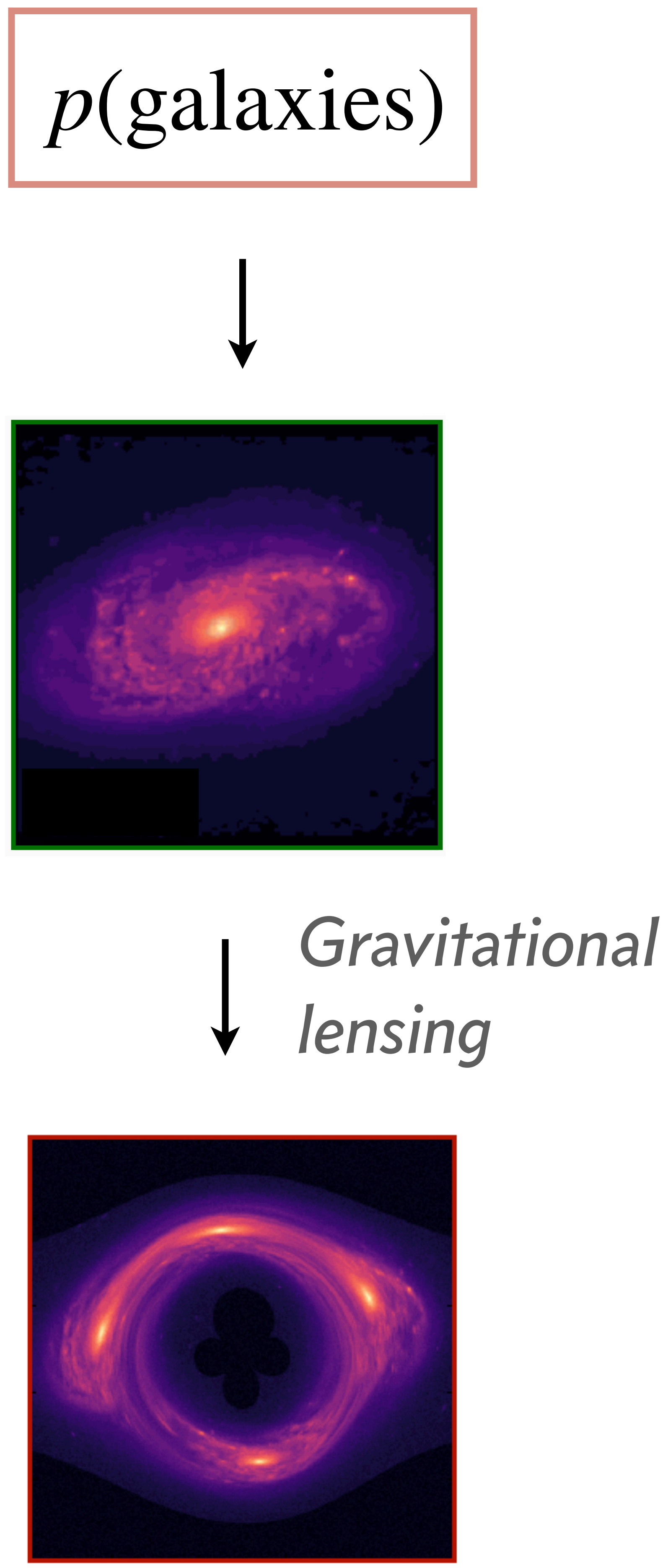
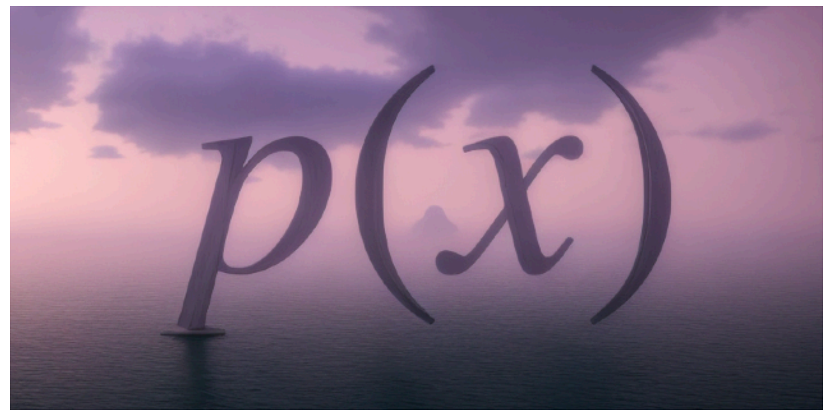


Figure 2: Application of the method to a lensing system with a highly out-of-distribution source. The ground truth is given in the leftmost panel. Other panels show increasingly noisy data (lower row) and a sample from their corresponding source posterior (upper row). As the likelihood becomes less informative, the prior dominates, making the sources increasingly look like galaxies.

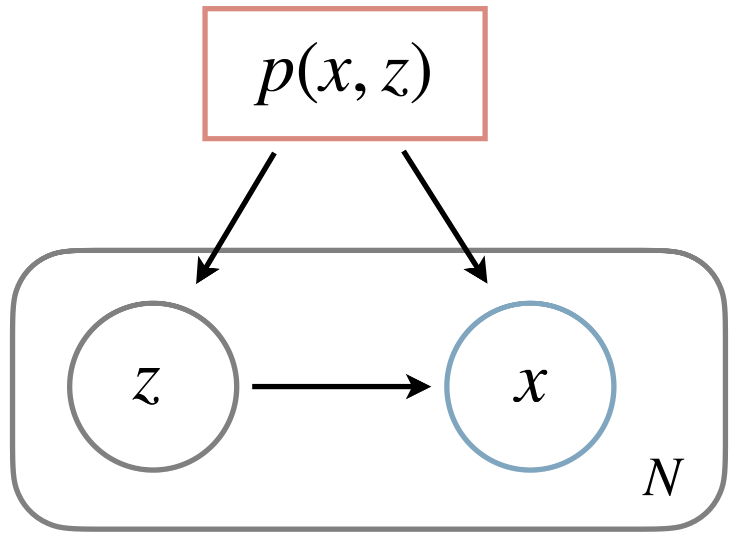


Outline



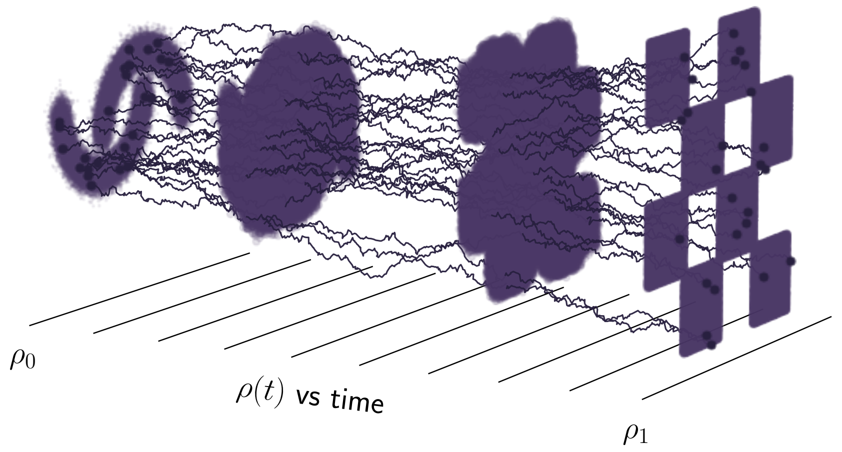
Why (deep) generative modeling?

What is it, and what can it do for you?



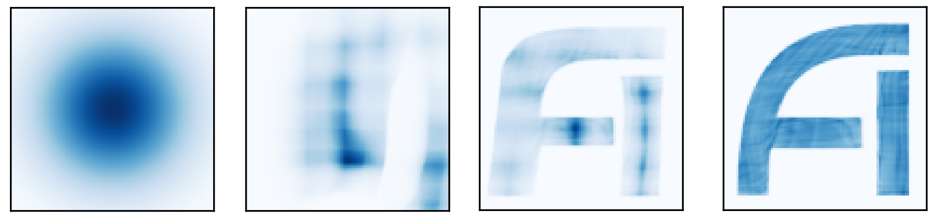
Variational auto encoders

Latent-variable modeling, and compression is all you need



Diffusion models

Models based on iterative refinement

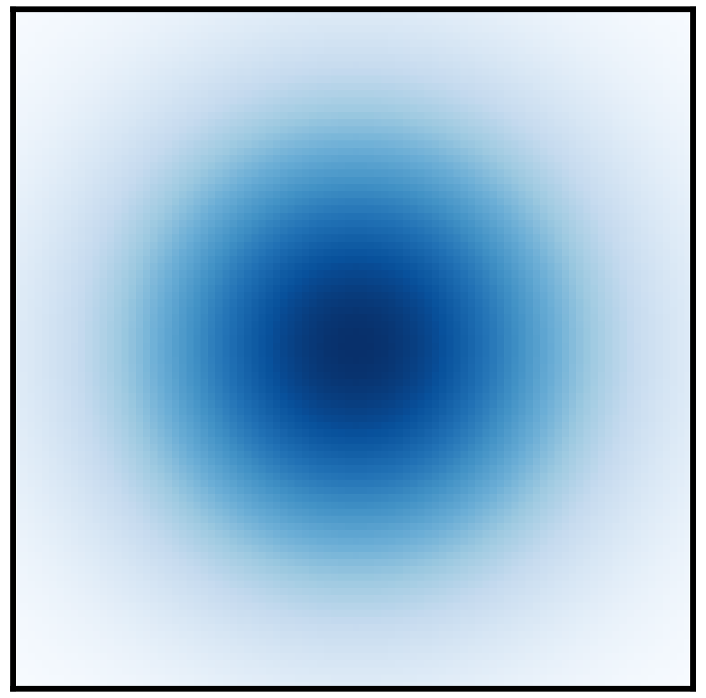


Normalizing flows

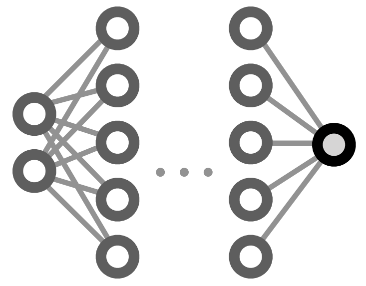
Invertible transformations

Normalizing flows

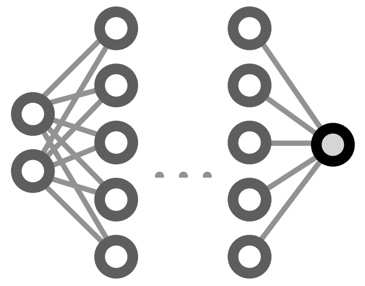
Base density



$p_z(z)$



$\theta = f(z)$



One-to-one transformation

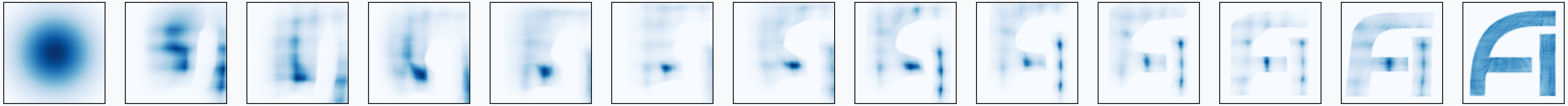
Tractable f^{-1} and $\det \nabla f$

(IAIFI logo)

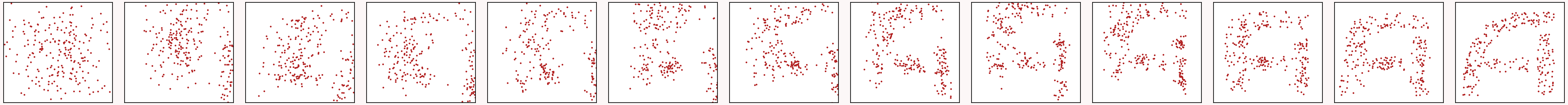
Target density

$$p(\theta) = p_z\left(f^{-1}(\theta)\right) |\det \nabla f|^{-1}$$

Efficient density estimation: $\log \hat{p}(\theta)$



Efficient sampling: $\theta \sim \hat{p}(\theta)$



Normalizing flows

The distribution $p(z)$ should

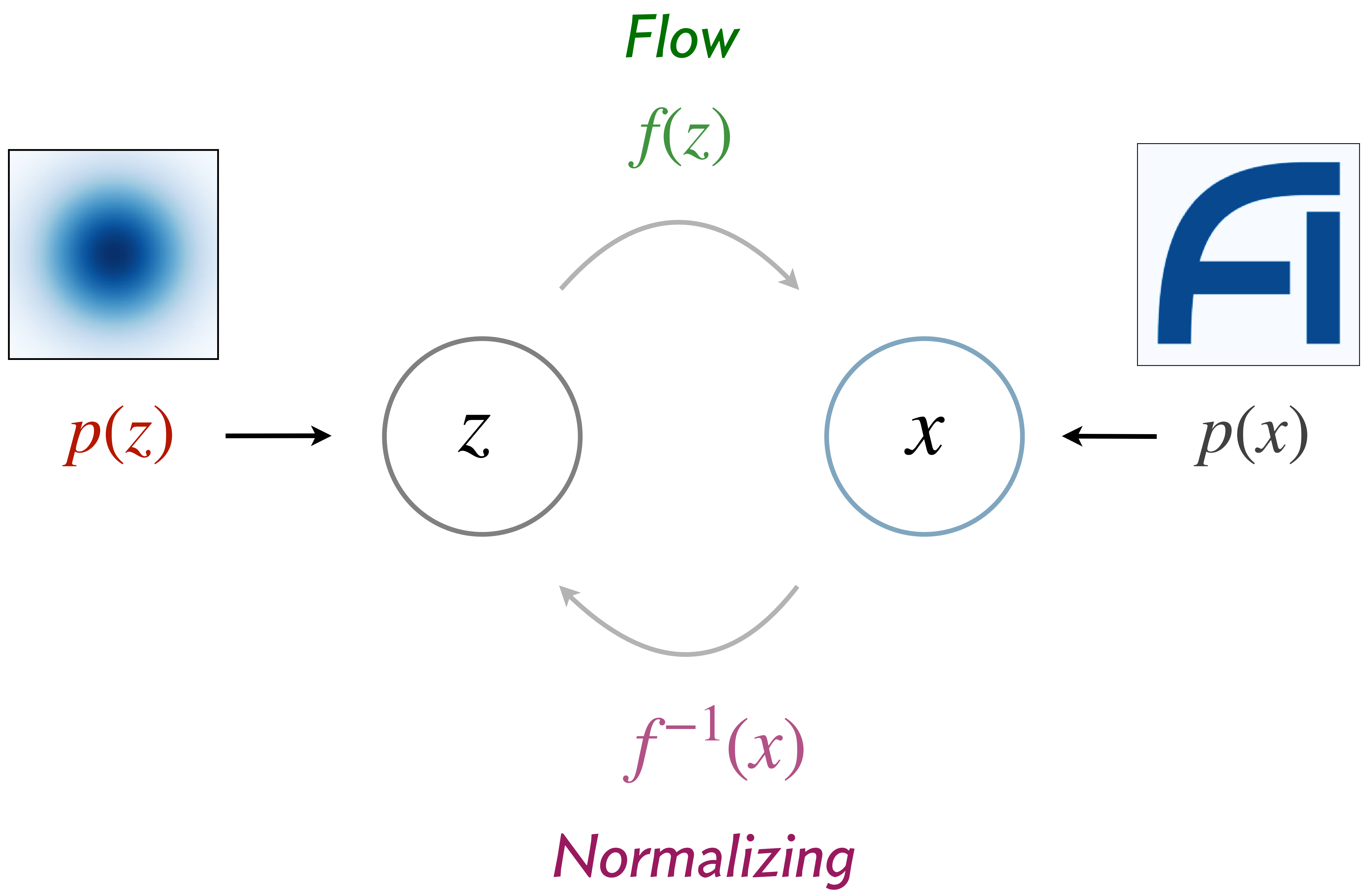
- *Have an easy-to-evaluate density*
- *Be easy to sample from* $z \sim p(z)$

Typically
$$p(z) = \mathcal{N}(0, \mathbb{1})$$

The function f should be

- *One-to-one*
- *Differentiable*
- *Invertible*
- *Tractable* f^{-1} and $\det \nabla f$

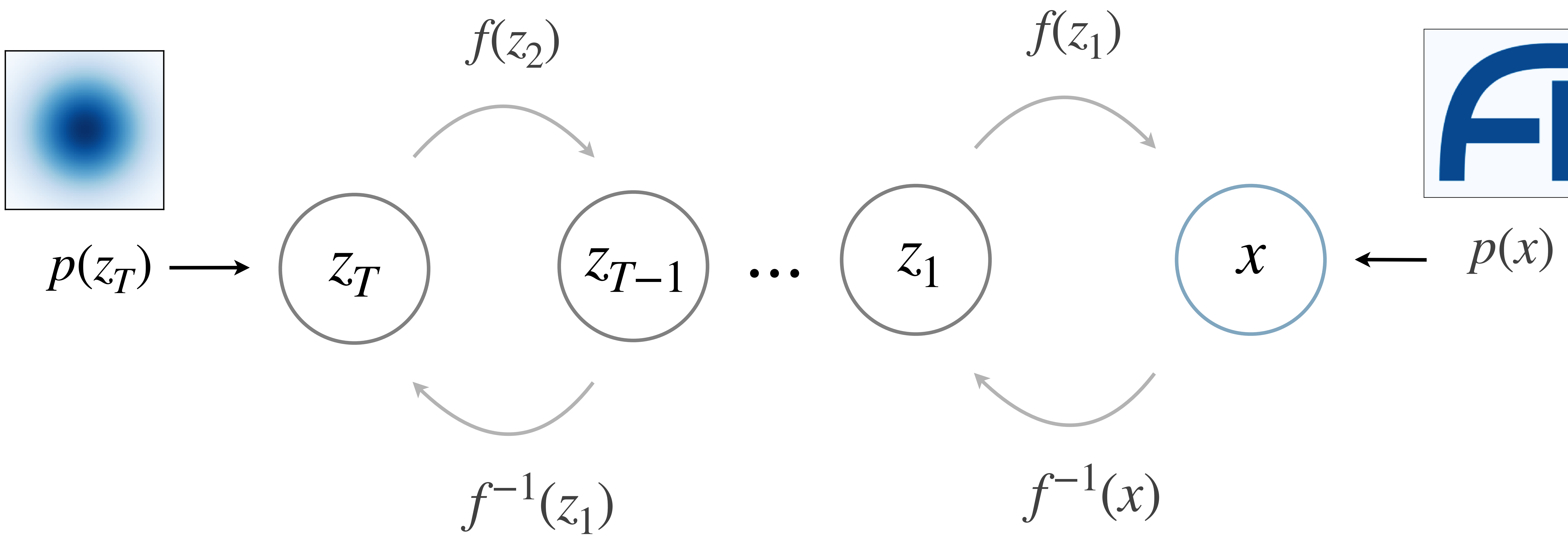
$\left.\begin{array}{l}\textit{One-to-one}\\ \textit{Differentiable}\\ \textit{Invertible}\end{array}\right\}$ Diffeomorphism



- Constrained form of the transformation can limit the expressivity of flows compared to e.g. diffusion models.
- However, for certain physics applications the transformation can be restricted in a specific, desired way; *see Miranda Cheng's lectures on Wednesday!*

Normalizing flows

Multiple flow transformation can be easily composed for e.g. expressivity



Computing $p(x)$: *change-of-variables formula*

$$\int p(x)dx = \int p(z)dz = 1$$

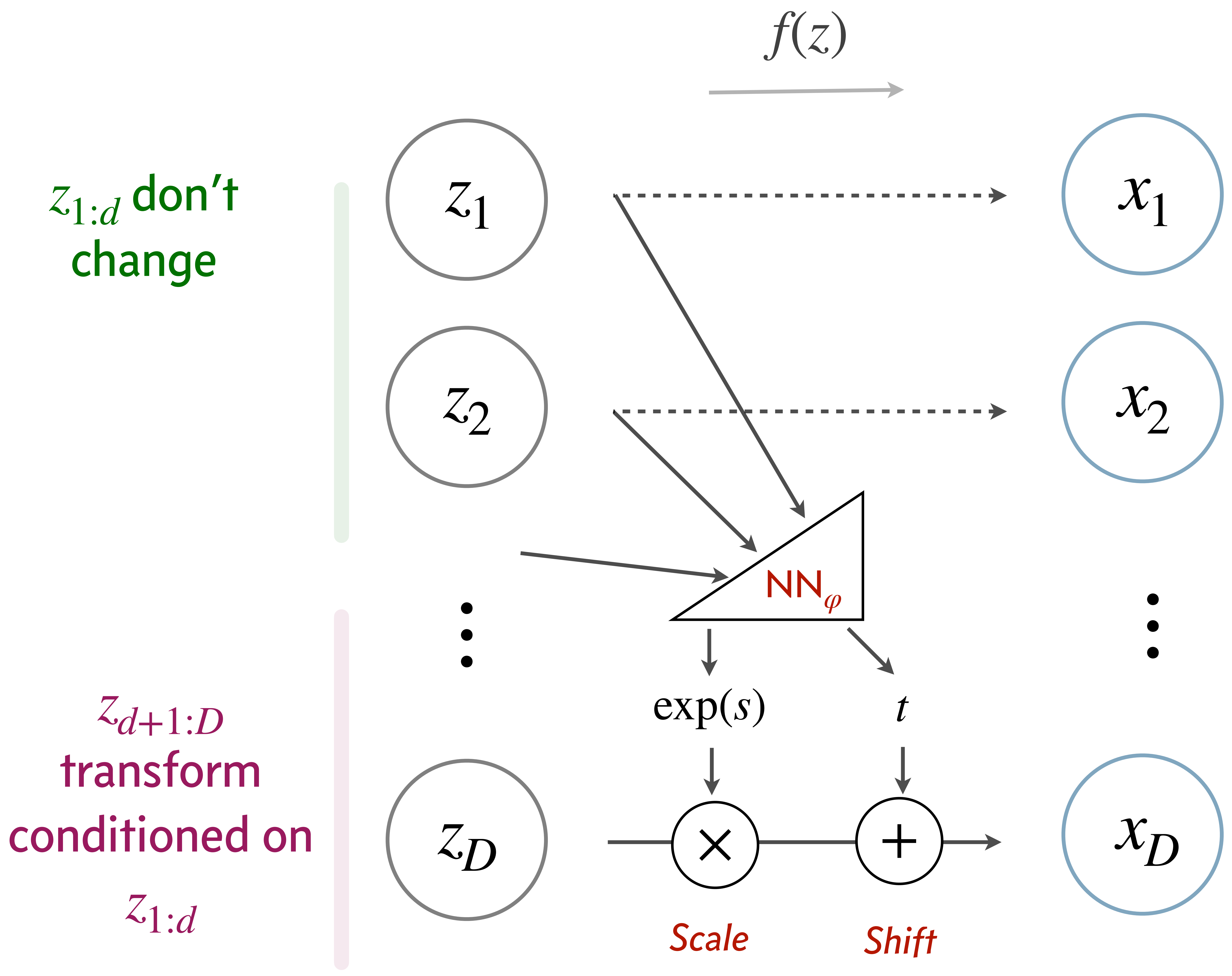
$$p(x) = p(z)\left|\frac{dz}{dx}\right| = p\left(f^{-1}(x)\right)\left|\frac{df^{-1}}{dx}\right| = p\left(f^{-1}(x)\right)|\det \nabla f|^{-1}$$

Train using maximum-likelihood objective

$$\varphi^* = \left\langle \arg\max_{\varphi} p\left(f_{\varphi}^{-1}(x)\right)|\det \nabla f_{\varphi}|^{-1} \right\rangle_{x\sim p(x)}$$

Simple flow transformations

Example: *Affine coupling flow* [RealNVP; Dinh et al 2016]



Transformation ✅

$$x_{d+1:D} = z_{d+1:D} \odot \exp\left(s\left(x_{1:d}\right)\right) + t\left(x_{1:d}\right)$$

$\Updownarrow$

Inverse ✅

$$z_{d+1:D} = \left(x_{d+1:D} - t\left(x_{1:d}\right)\right) \odot \exp\left(-s\left(x_{1:d}\right)\right)$$

Jacobian determinant ✅

$$\det(\nabla f) = \prod_{j=1}^{D-d} \exp\left(s\left(z_{1:d}\right)\right)_j = \exp\left(\sum_{j=1}^{D-d} s\left(z_{1:d}\right)_j\right)$$

+ Switch up order of transformed variables at every transformation

Continuous-time normalizing flows

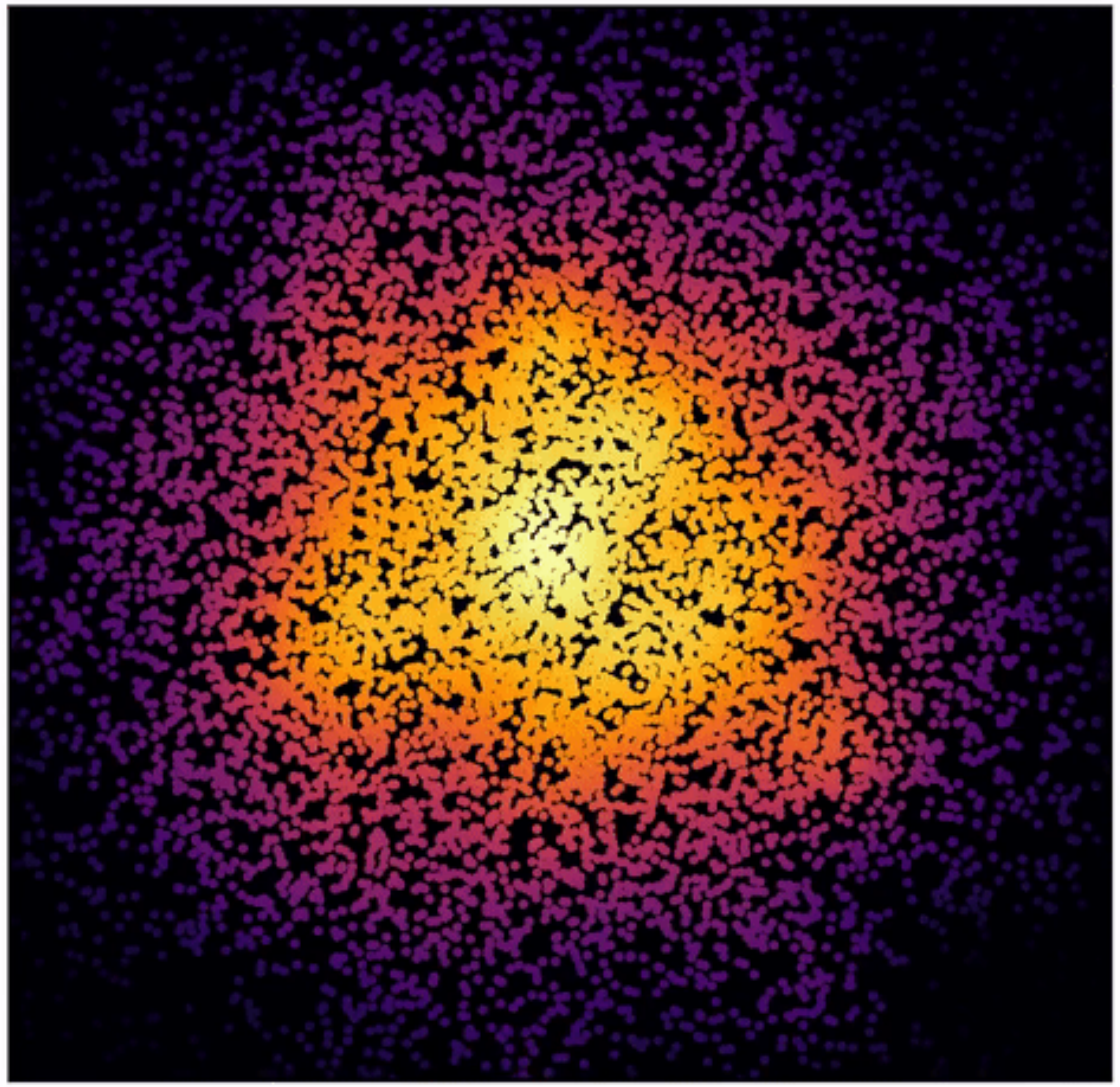
Parameterize the transformation by a neural ODE

ODE with reversible dynamics

$$\frac{\mathrm{d}x}{\mathrm{d}t} = f\left(x(t)\right)$$

Instantaneous change-of-variable formula

$$\frac{\mathrm{d}\log p(x(t))}{\mathrm{d}t} = -\operatorname{Tr}\left(\frac{\mathrm{d}f}{\mathrm{d}x(t)}\right)$$



Pro ✅

Unrestricted form of transformation $f(x)$!

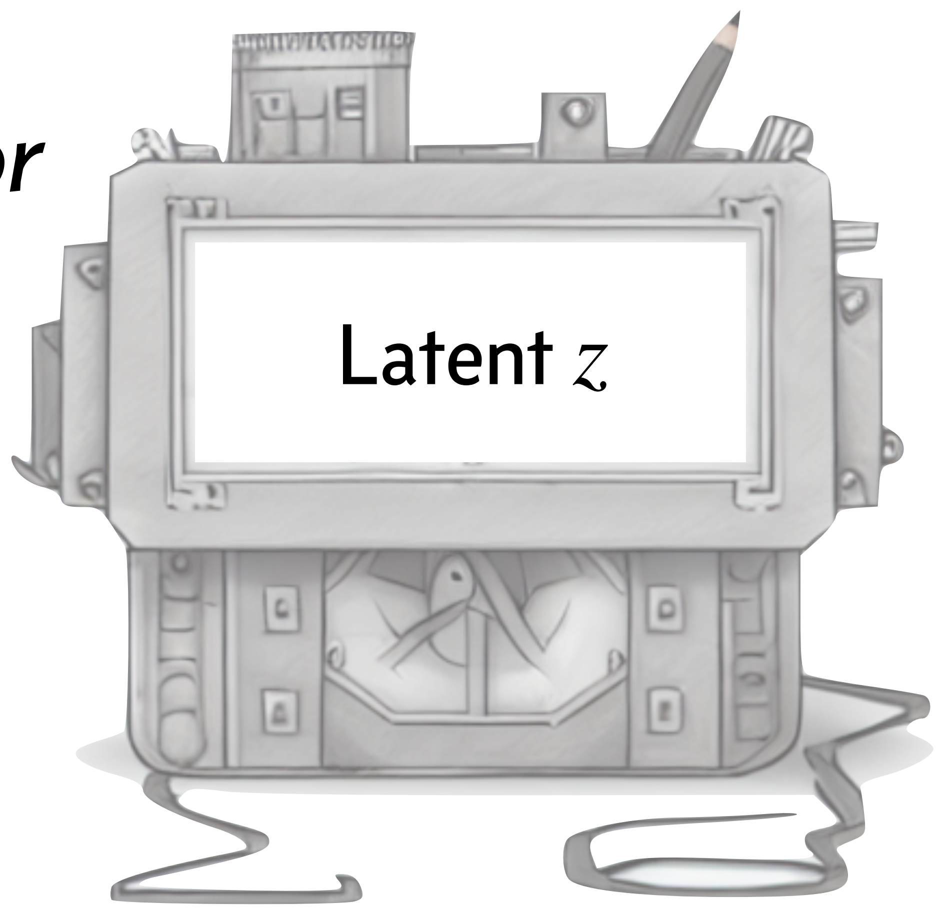
Cons 😵‍💫

- Need for efficient trace calculation
- Solving an ODE and backpropping through the solution can make for cumbersome training

Simulation-based inference (SBI)

Simulator

Parameters
θ



Observations
x

Prediction:

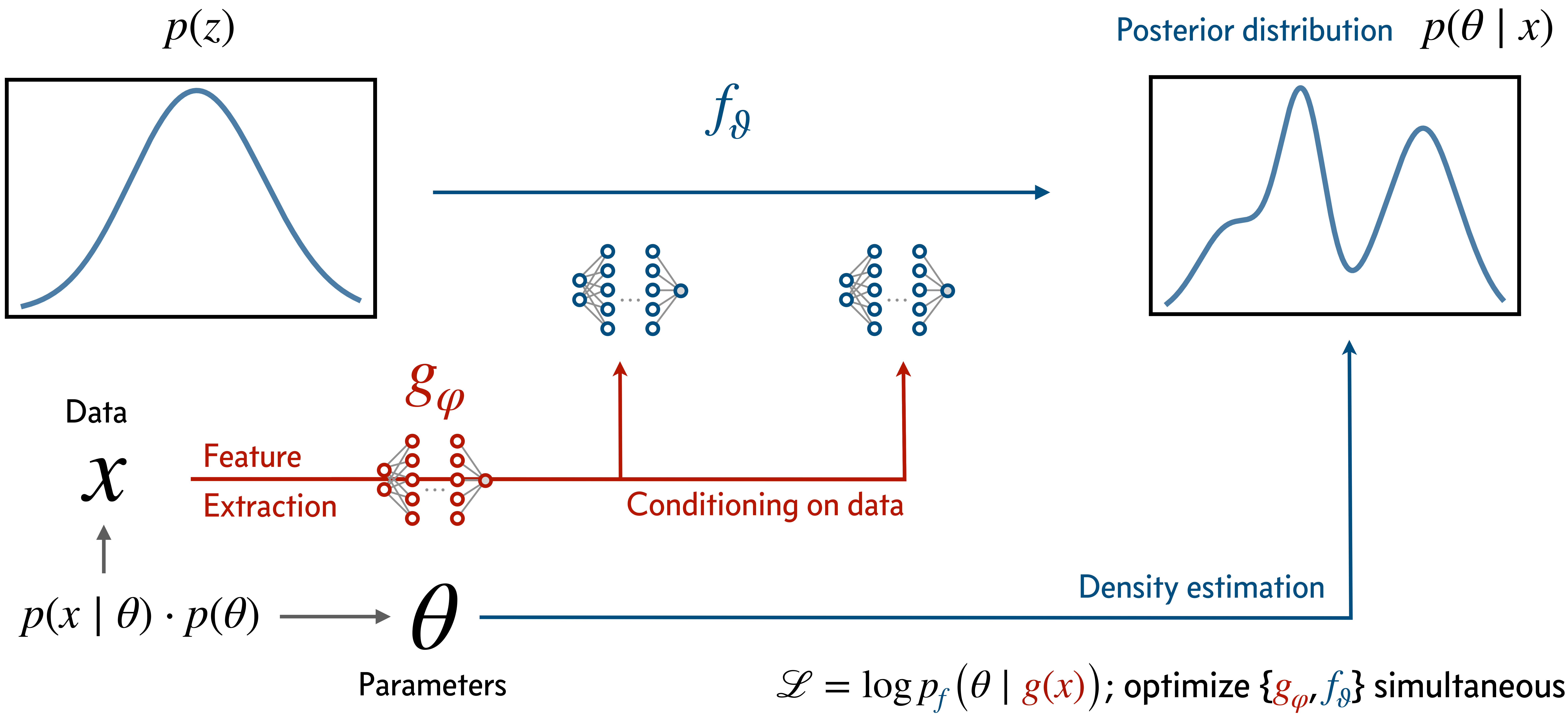
- Well-motivated mechanistic, causal model
- Simulator can generate samples $x \sim p(x \mid \theta)$

Inference:

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

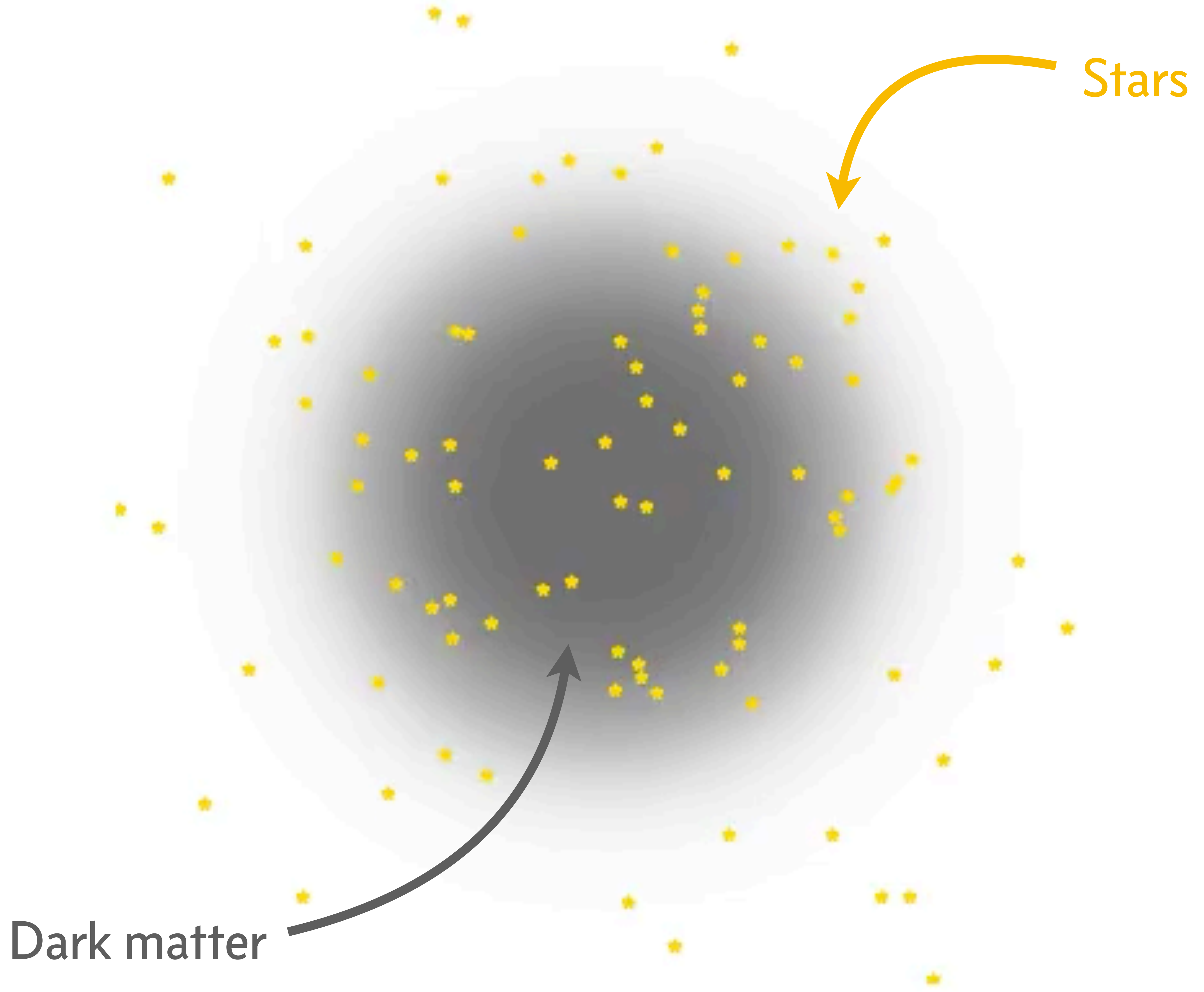
Flows in *simulation-based inference*

Flows are commonly employed as *conditional posterior density estimators* in simulation-based inference



$\mathscr{L} = \log p_f\left(\theta \mid g(x)\right)$; optimize $\{g_\varphi, f_\vartheta\}$ simultaneously

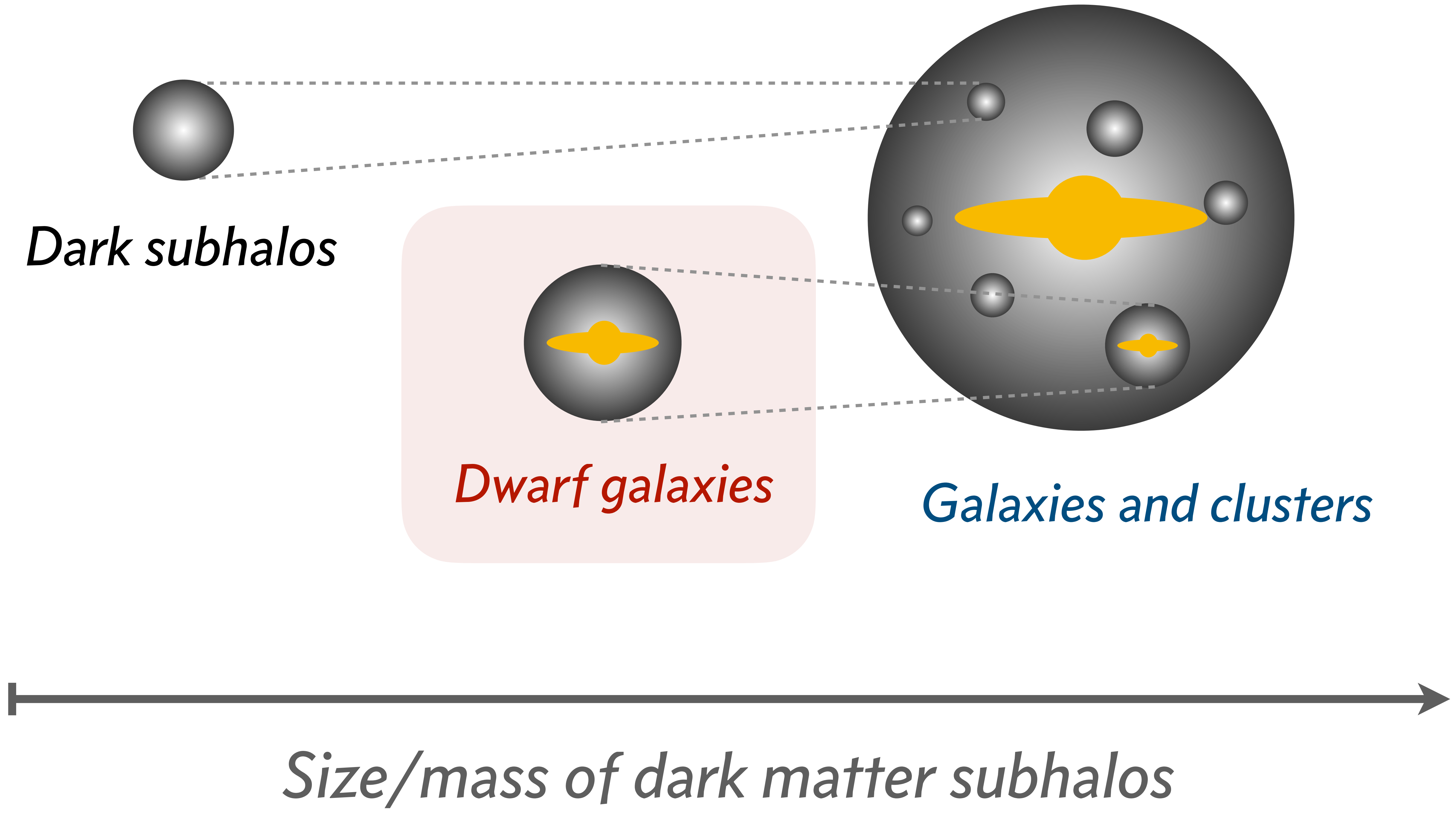
An application to *dwarf galaxies*



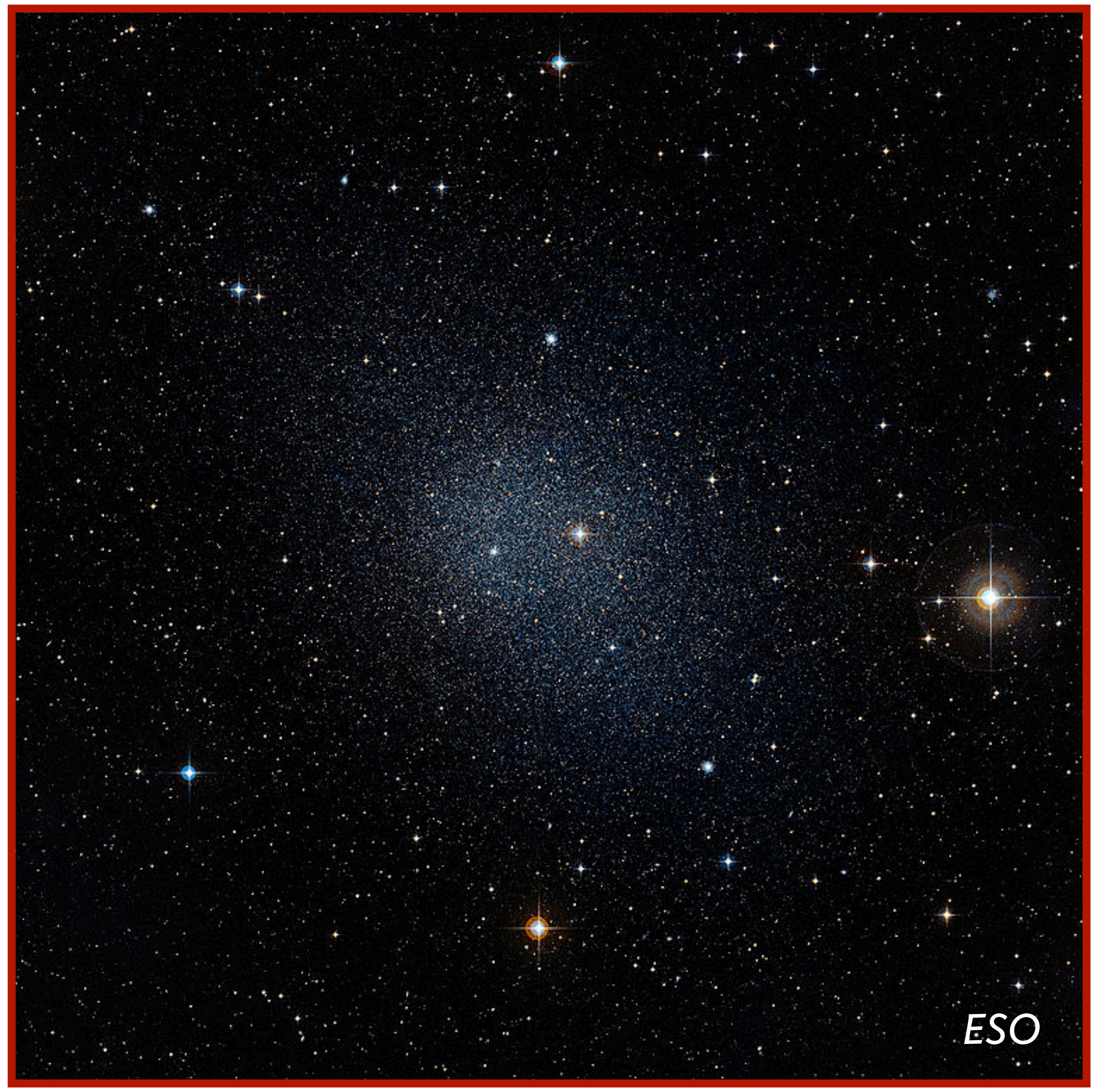
Another application: extracting the dark matter distribution from dwarf galaxies

Dwarf galaxies are intermediate-sized galaxies well-suited for studying dark matter

[Nguyen, SM et al 2022]

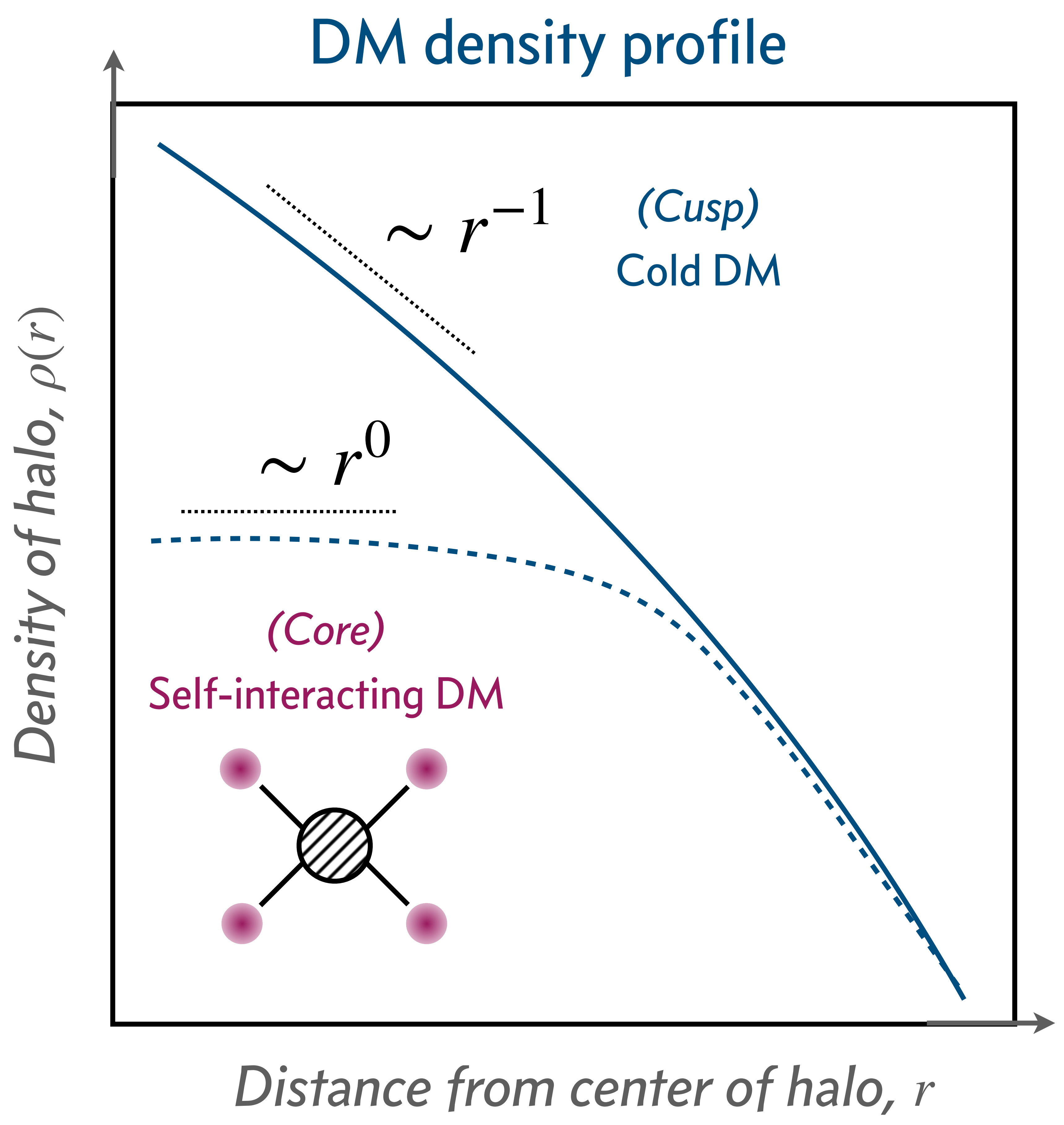


Fornax dwarf galaxy



Extracting the dark matter distribution from dwarf galaxies

[Nguyen, SM et al 2022]

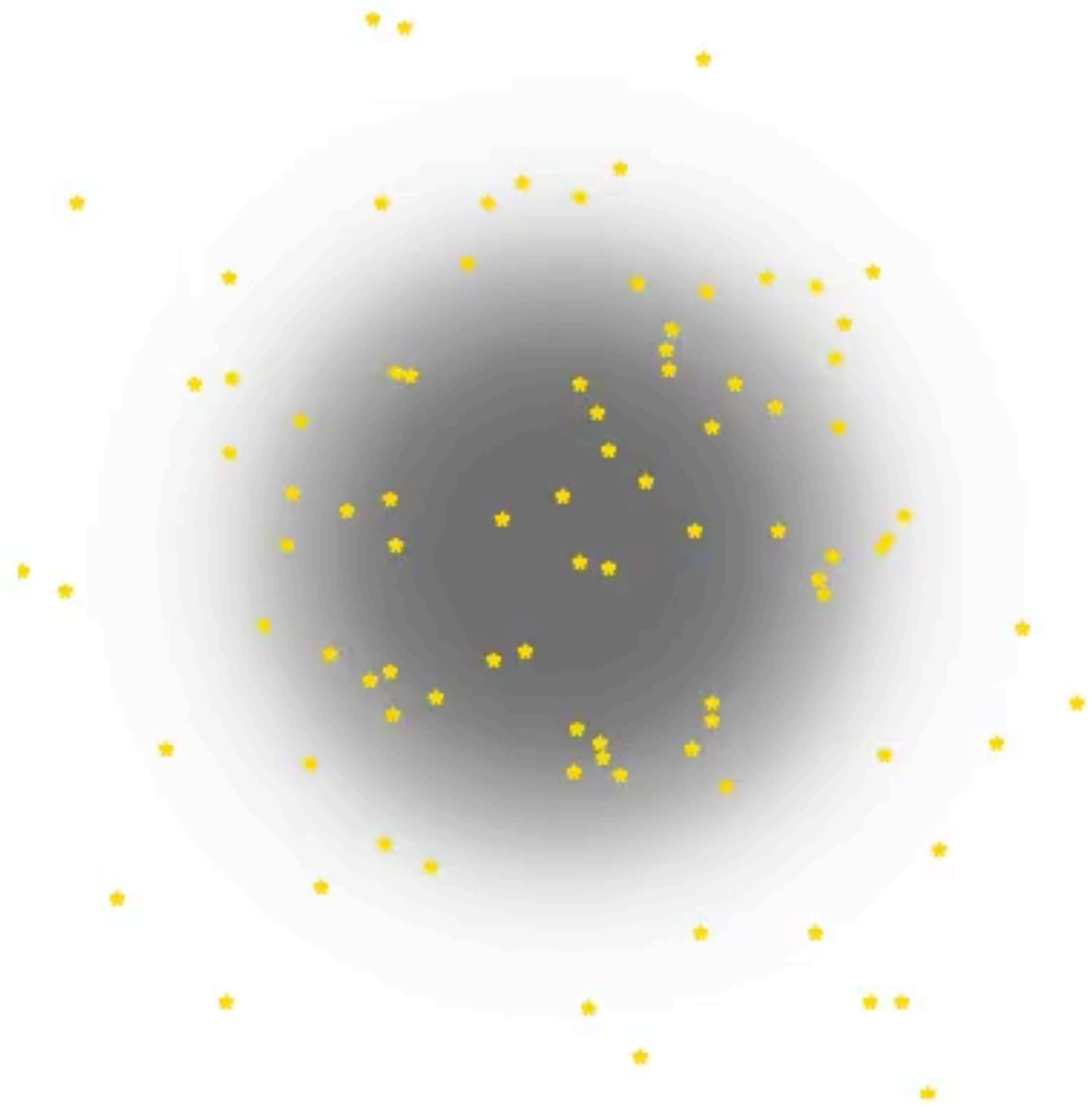


Prediction

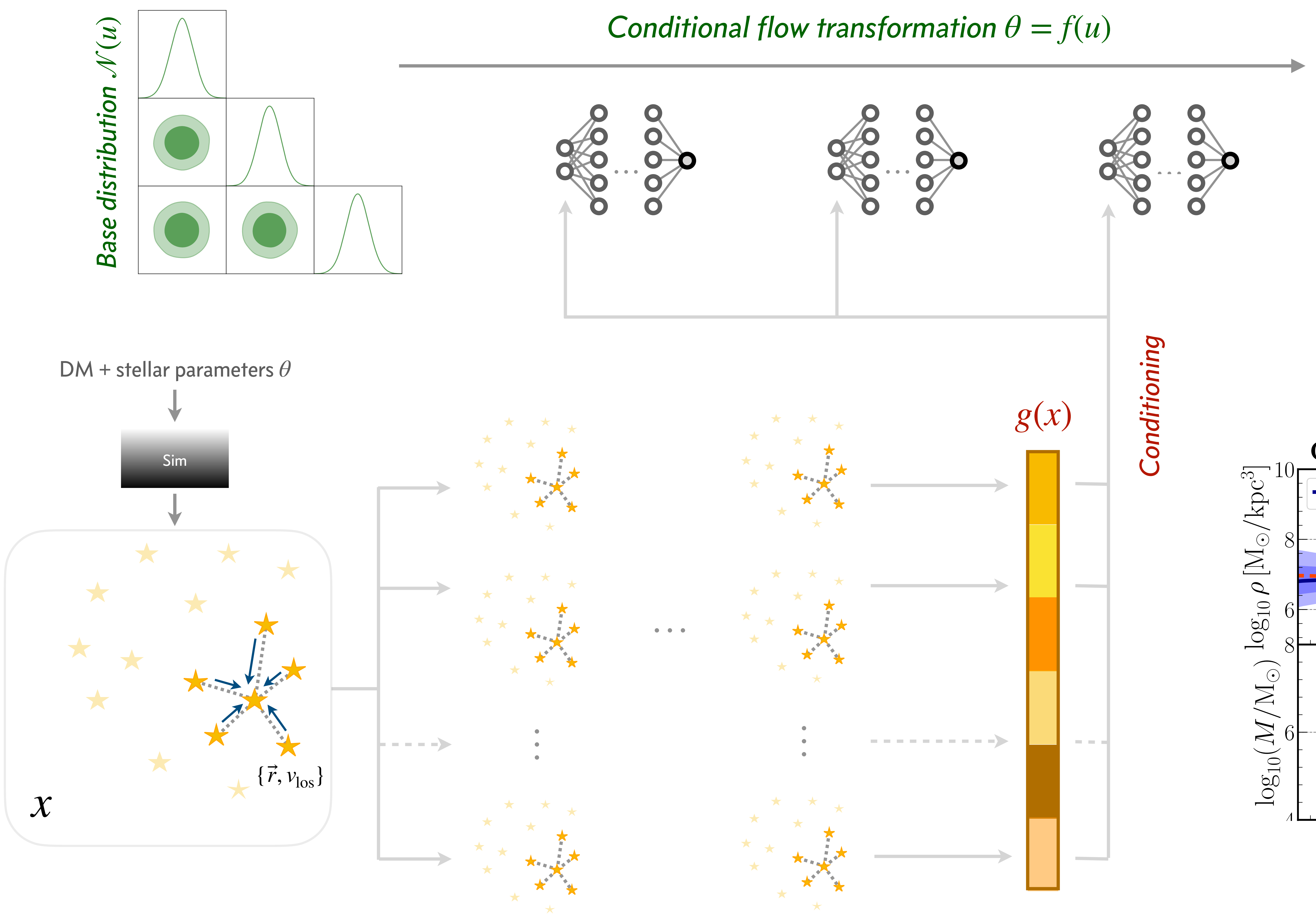
(🤗 with a simulator!)

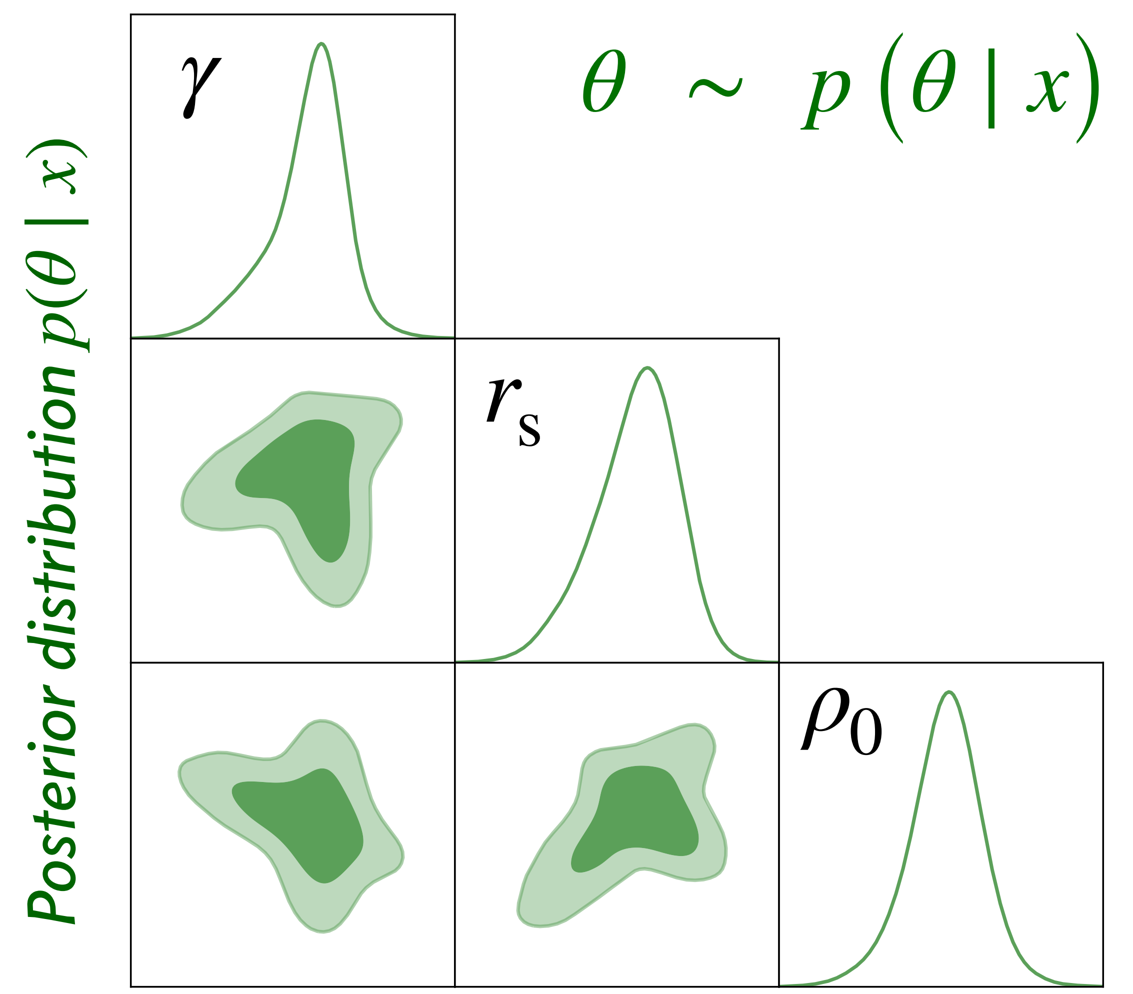
Inference

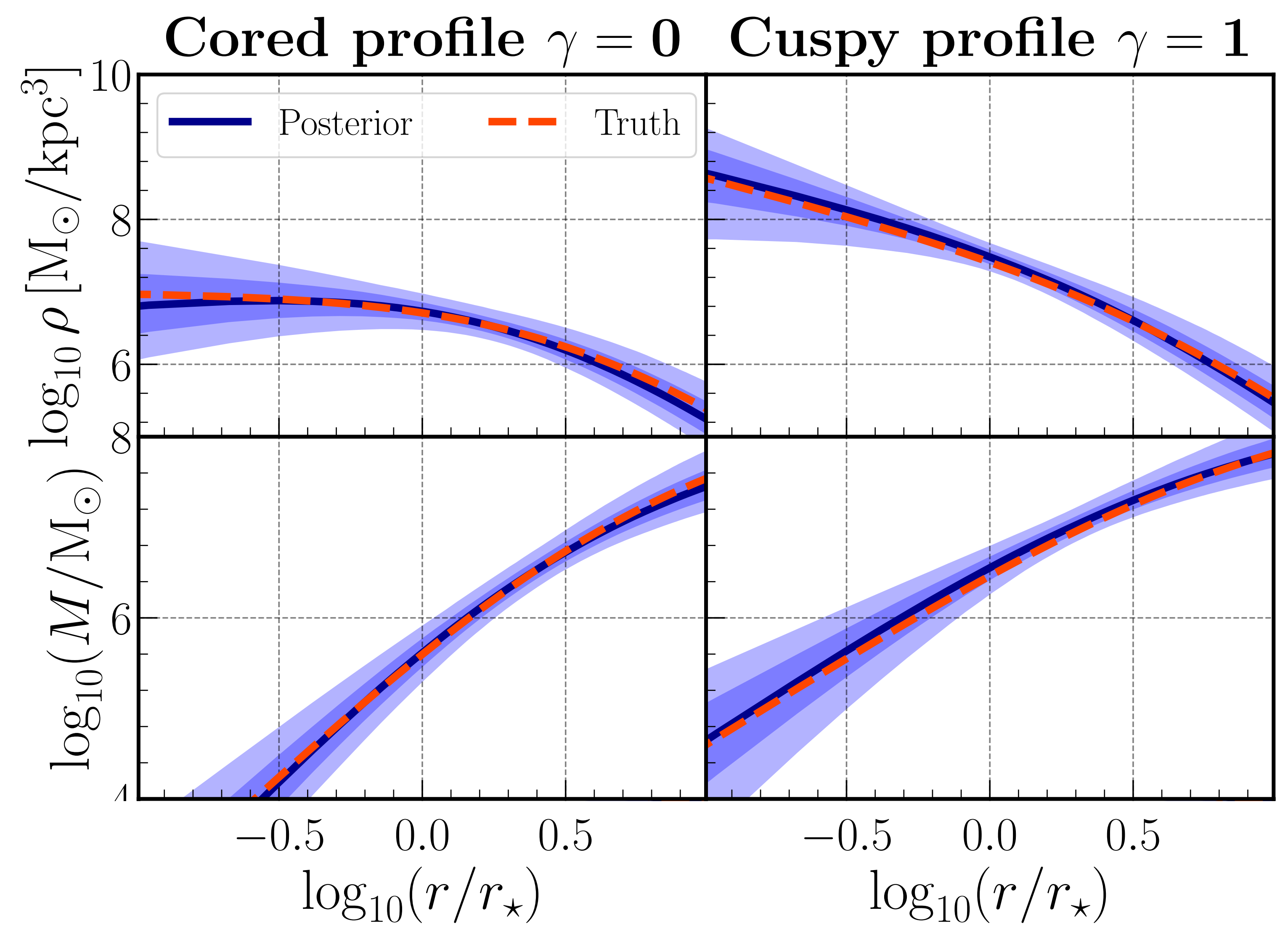
(💀)



Extracting the dark matter distribution [Nguyen, SM et al 2022]

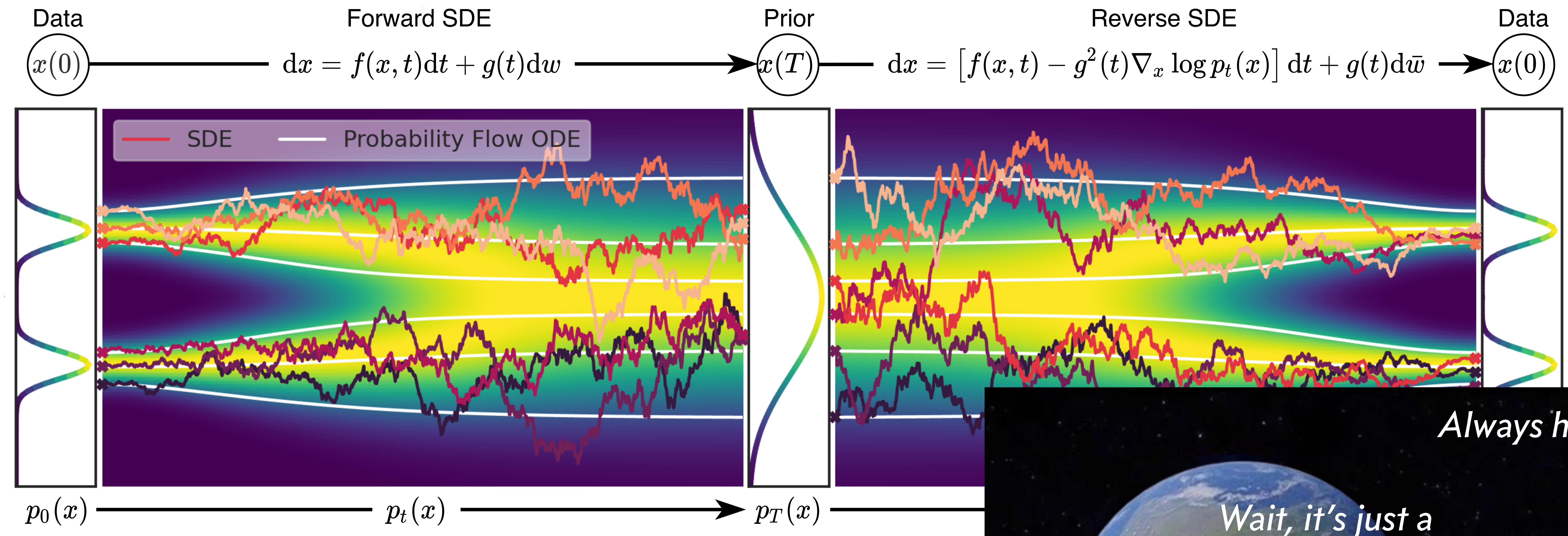






Back to diffusion: the *probability flow ODE*

For any diffusion process, there exists a corresponding deterministic process whose trajectories share the same marginal probability densities $p(x_t)$ as the SDE [Song et al 2021]



Probability flow ODE

$$\mathrm{d}x = \left[f(x,t) - \frac{1}{2}g^2(t)\nabla_x \log p_t(x)\right]\mathrm{d}t$$

Diffusion mo

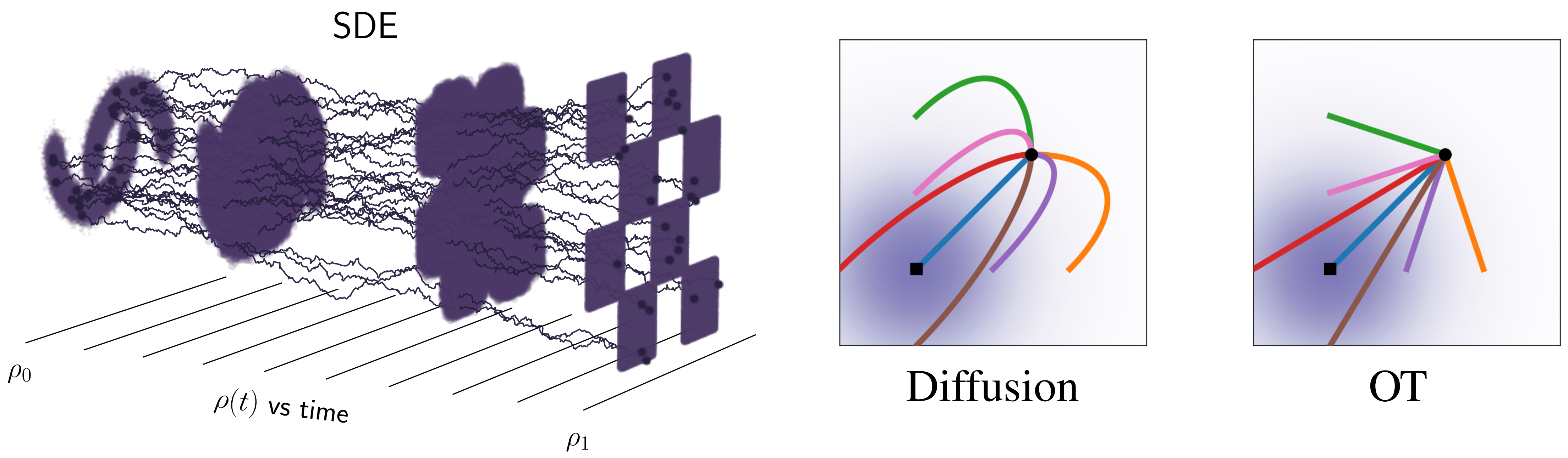
“simulation-f

Iterative refinement, interpolants, consistency, …

Empirical success of diffusion models has led to many new formulations and methods of training

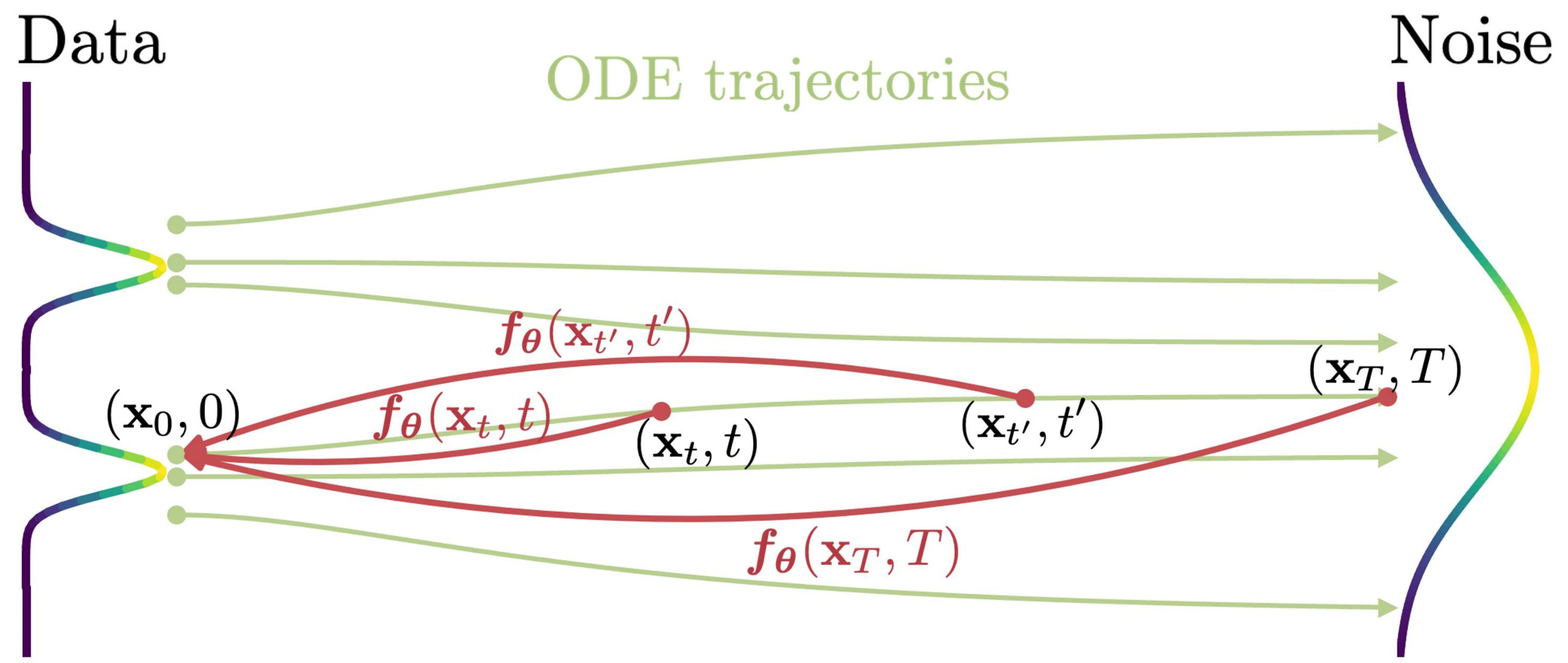
Stochastic interpolants and flow matching

[Albergo et al 2023, Lipman et al 2022, …]



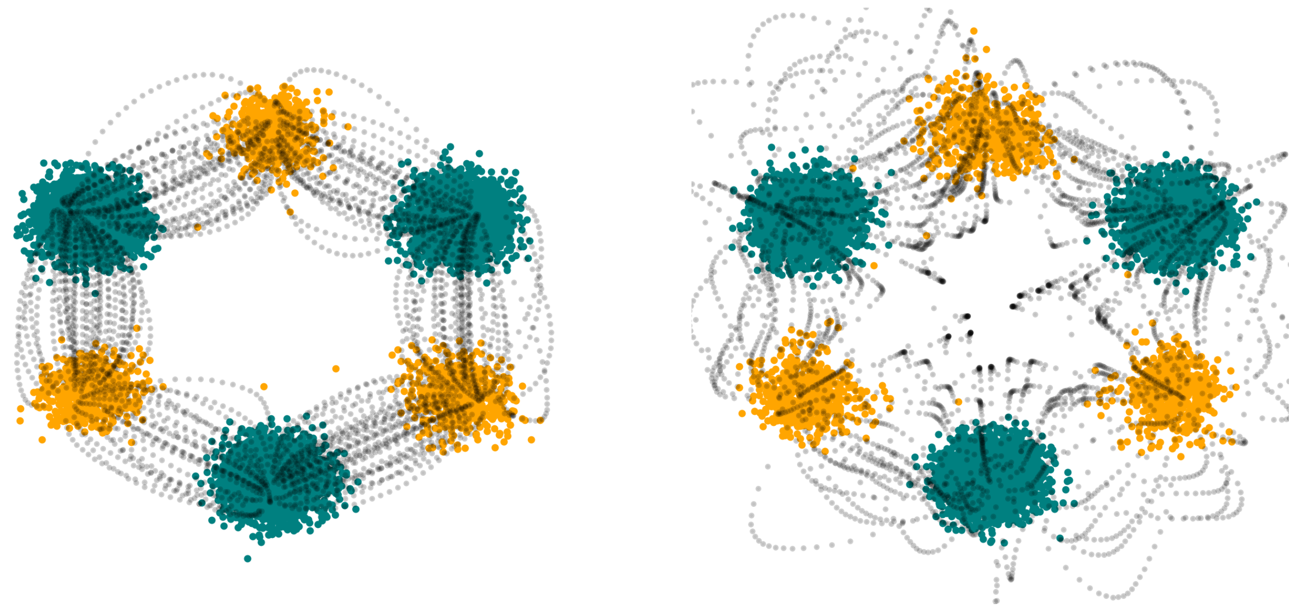
ODE trajectory consistency, Fokker-Planck regularization, …

[Song et al 2023, Lai et al 2023, …]



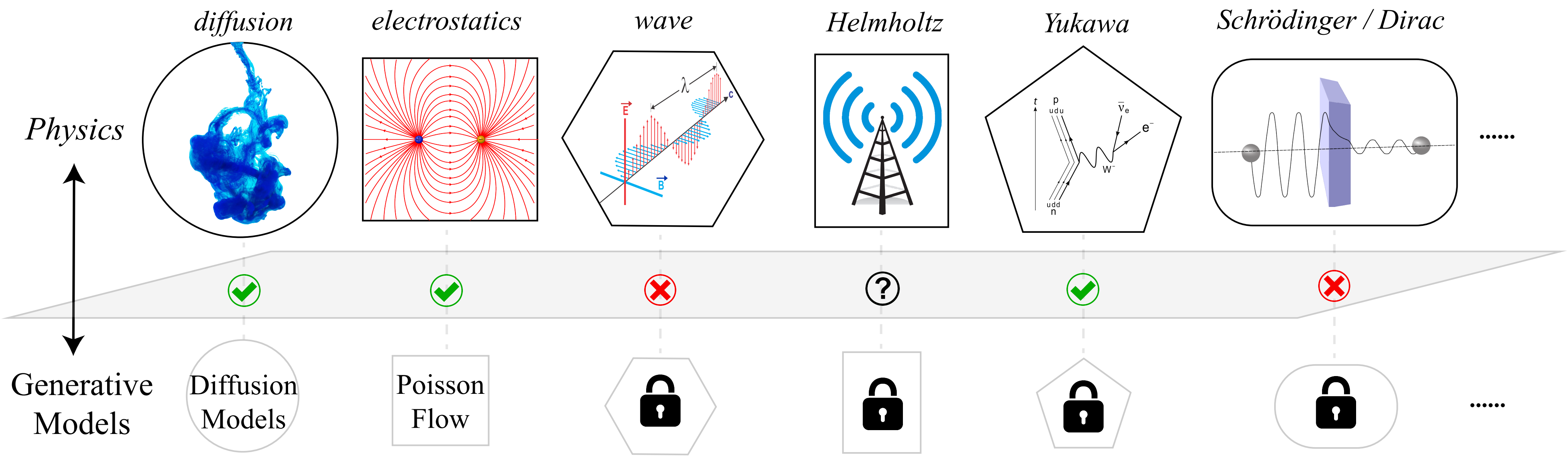
Diffusion Schrödinger's bridges

[Shi et al 2023, …]



Generative models inspired by other physical processes

[Xu et al 2022, Liu et al 2023, …]



End.