Flows for simultaneous manifold learning and density estimation

Johann Brehmer
New York University

Kyle Cranmer
New York University

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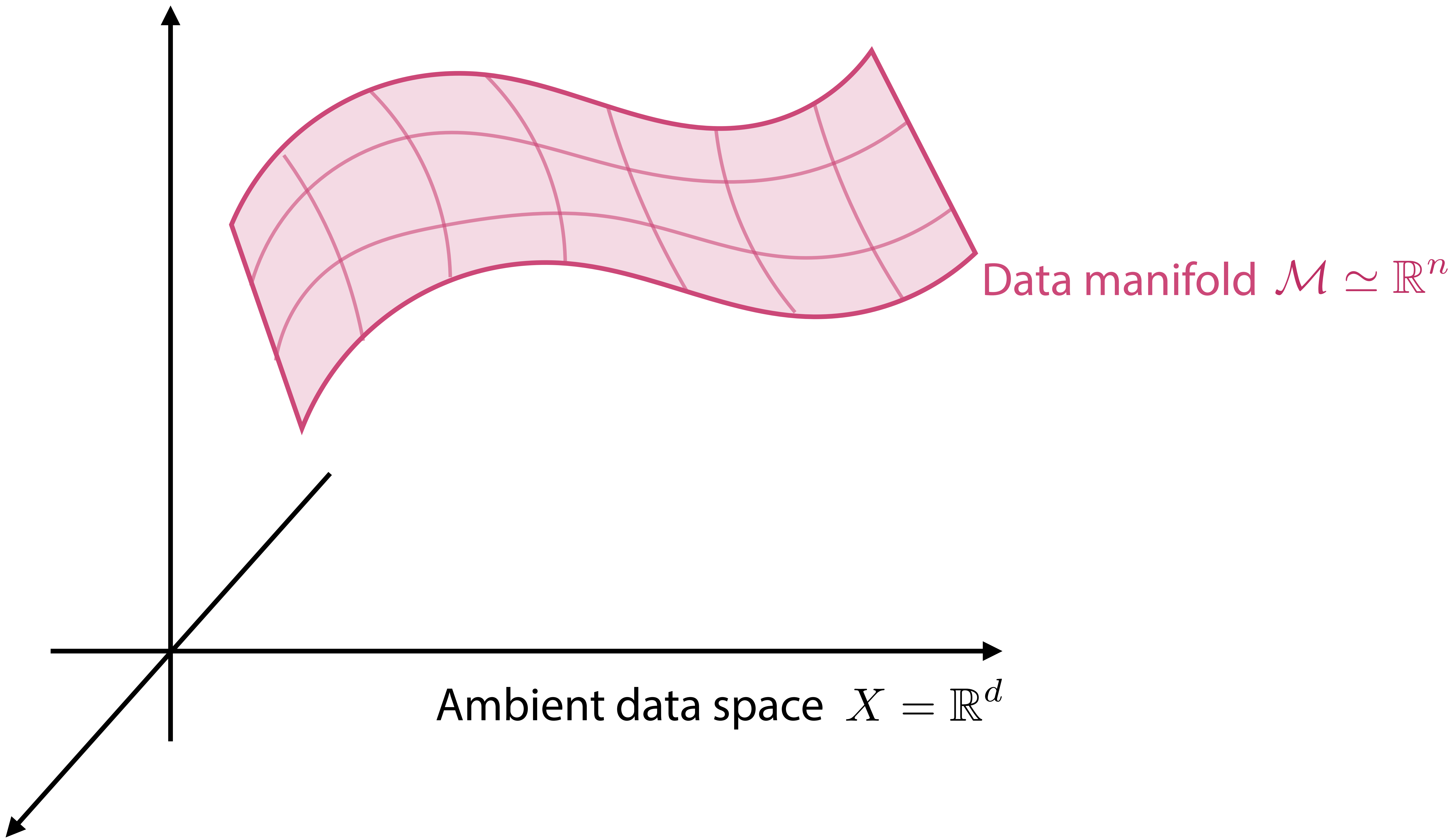
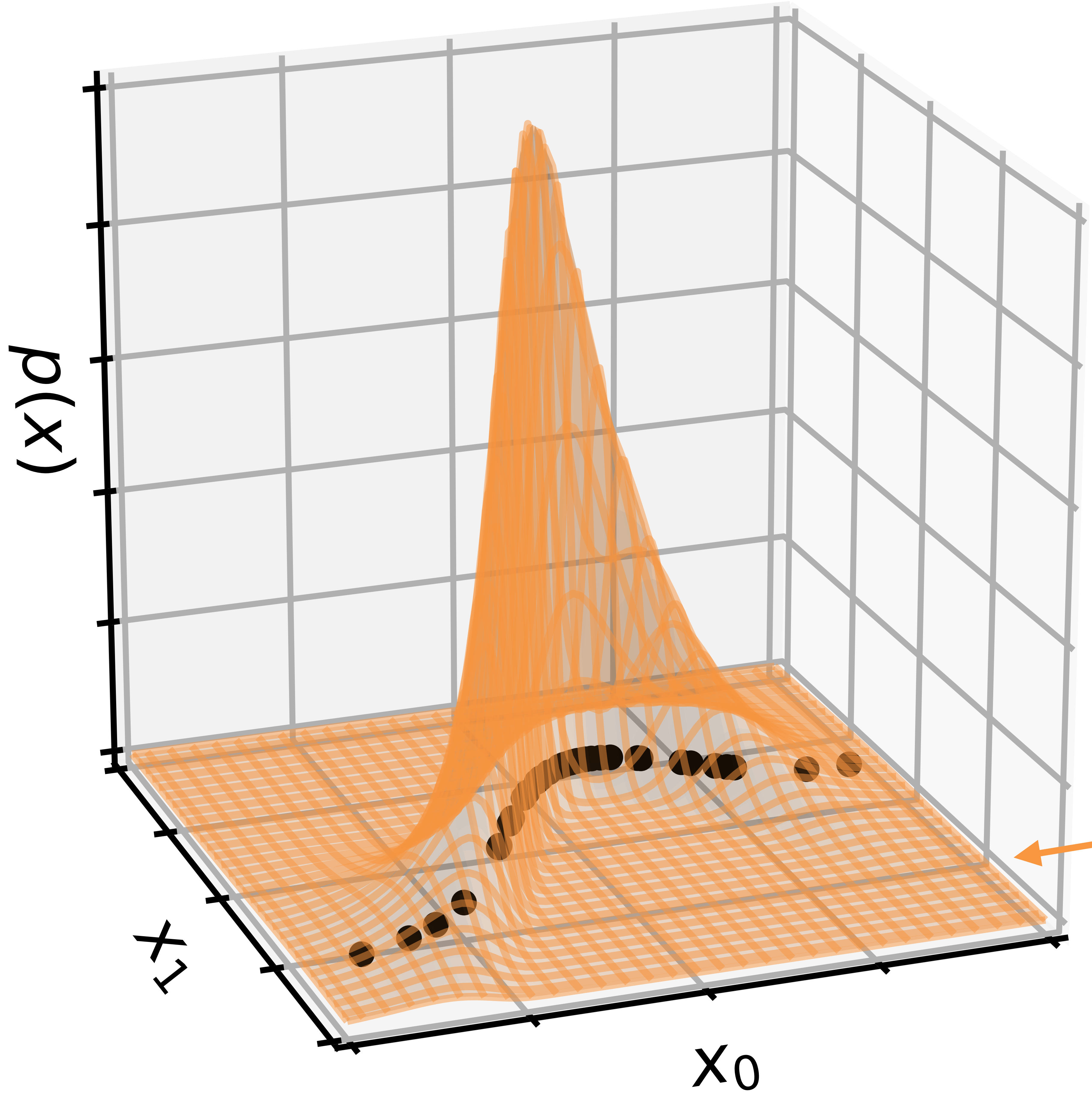


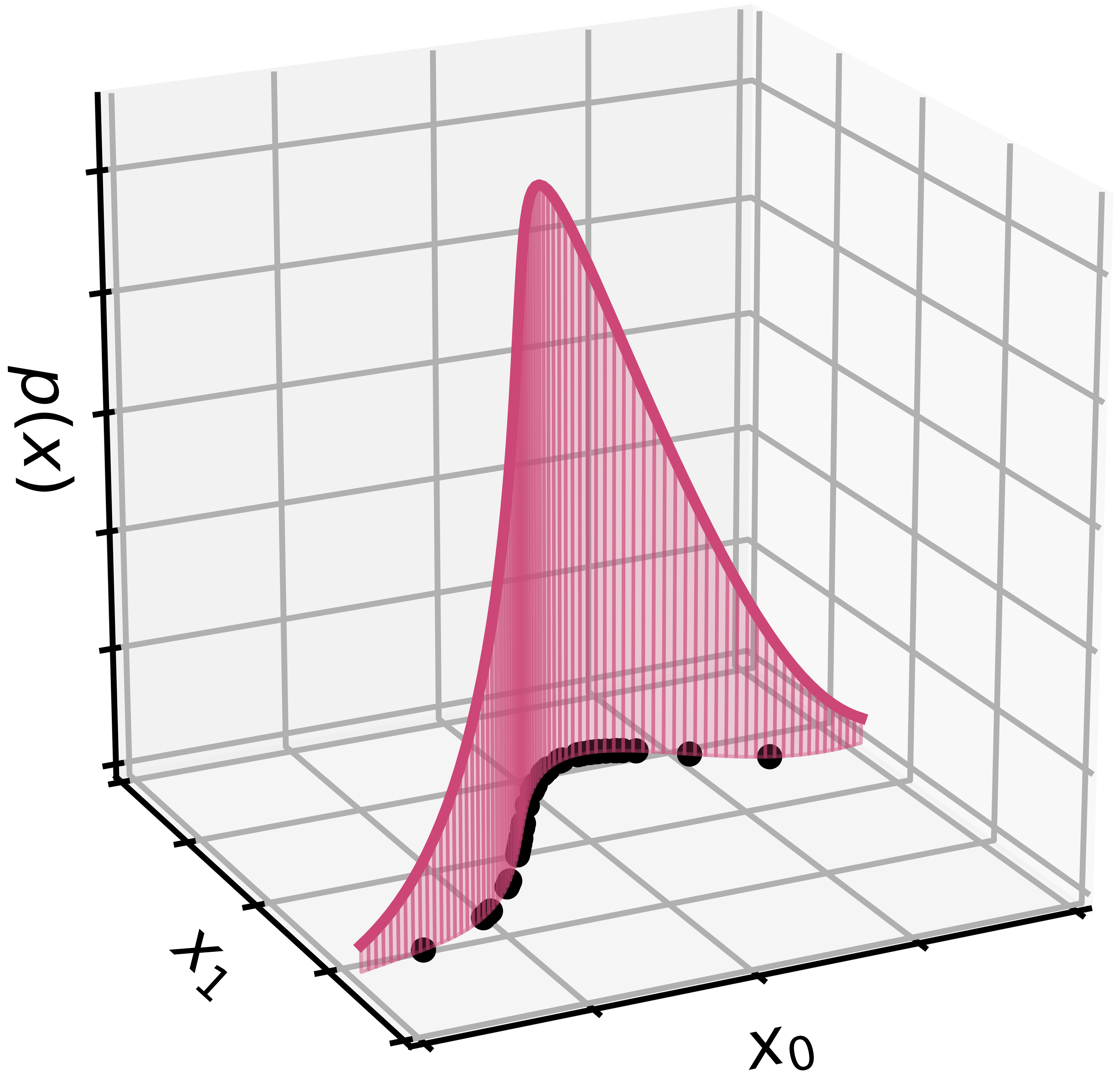
Data manifold $\mathcal{M} \simeq \mathbb{R}^n$
Ambient data space $X = \mathbb{R}^d$

Normalizing flow in ambient data space:

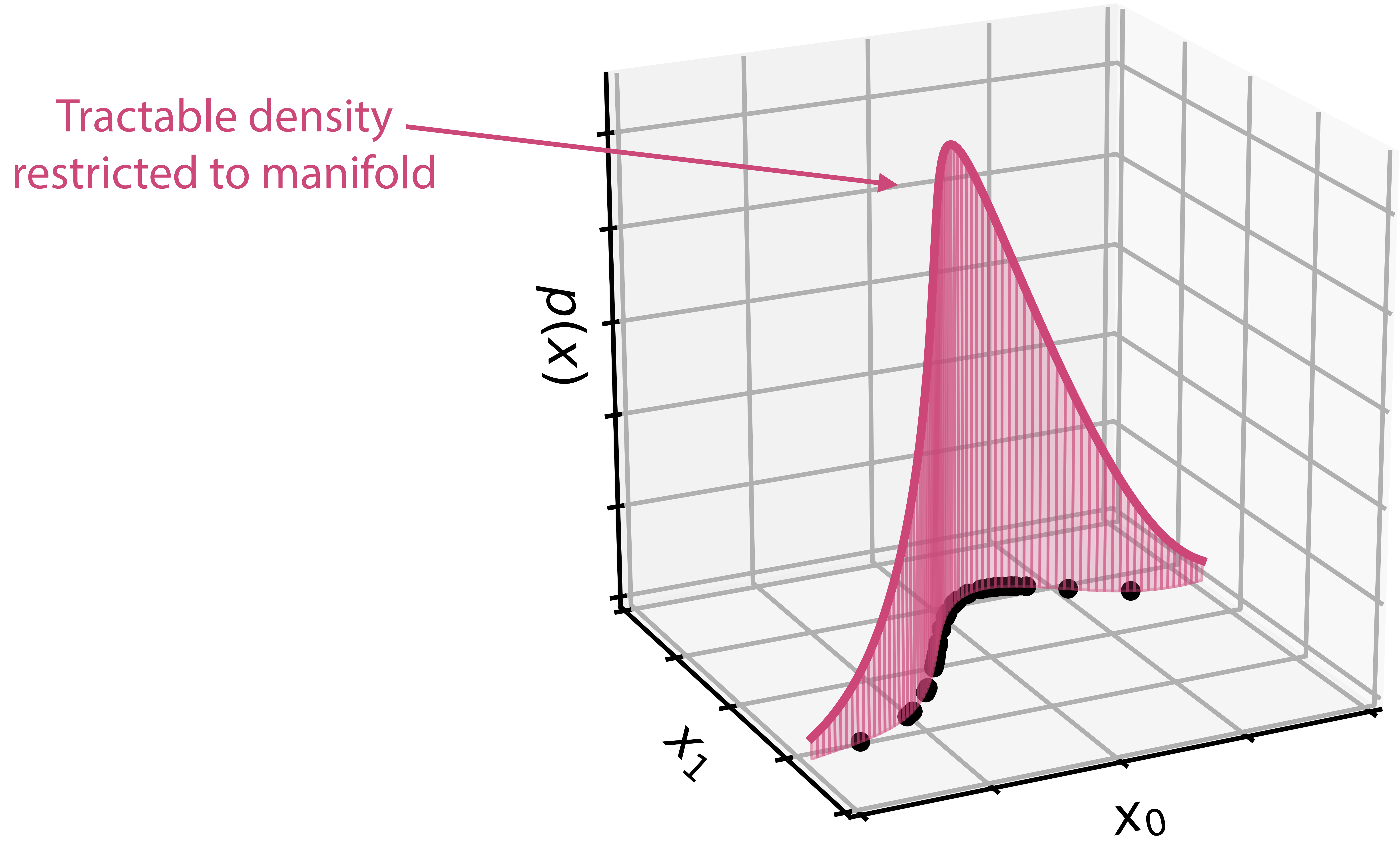


Density has support
off the data manifold

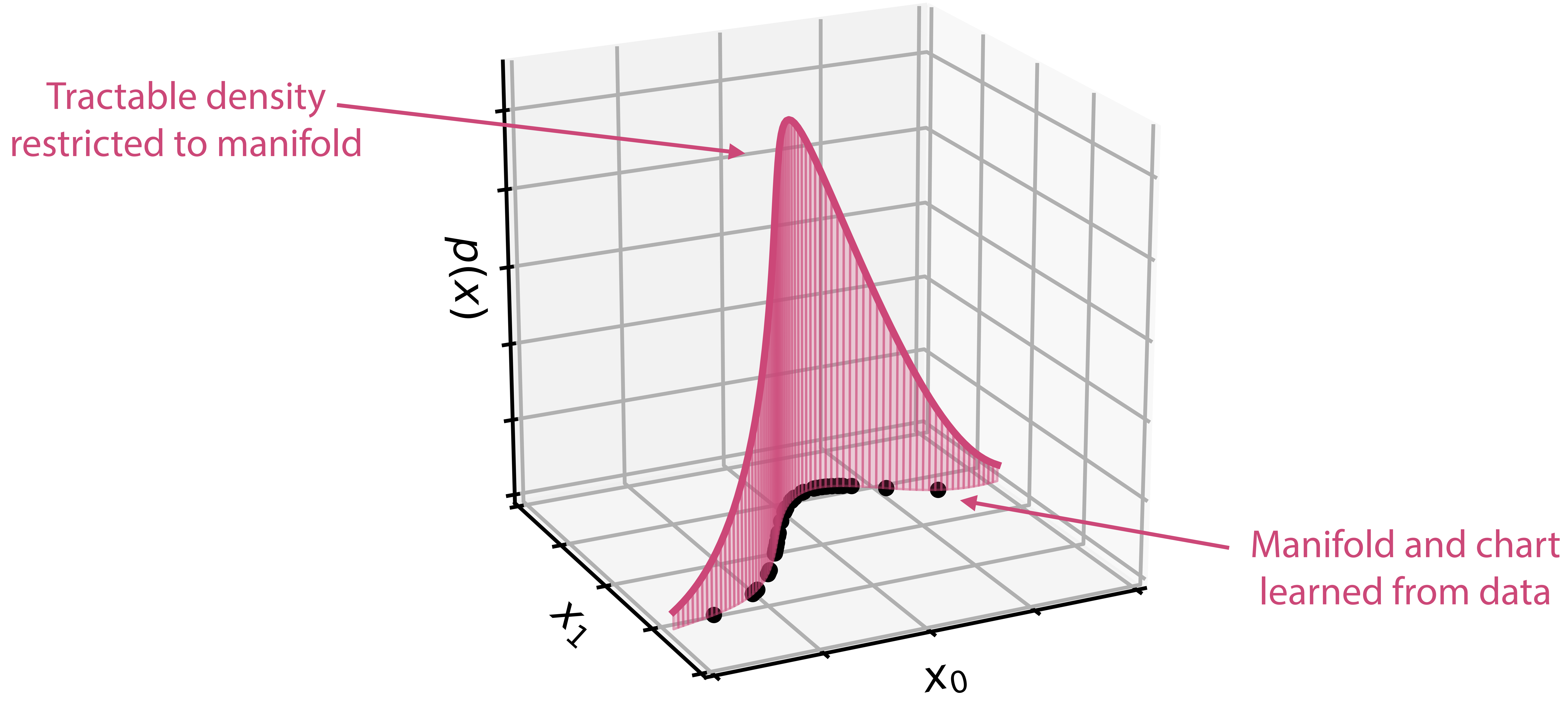
$\mathcal{M}$-flow:



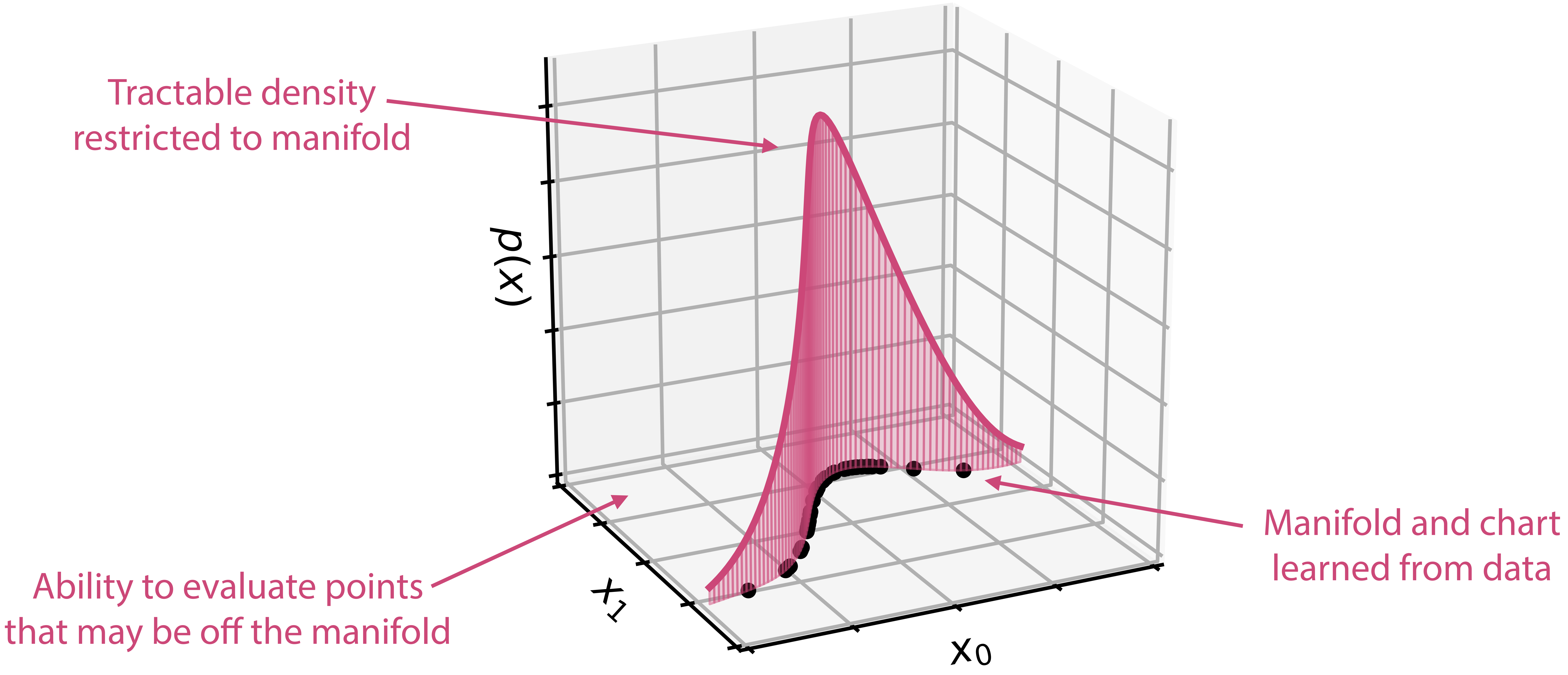
$\mathcal{M}$-flow:

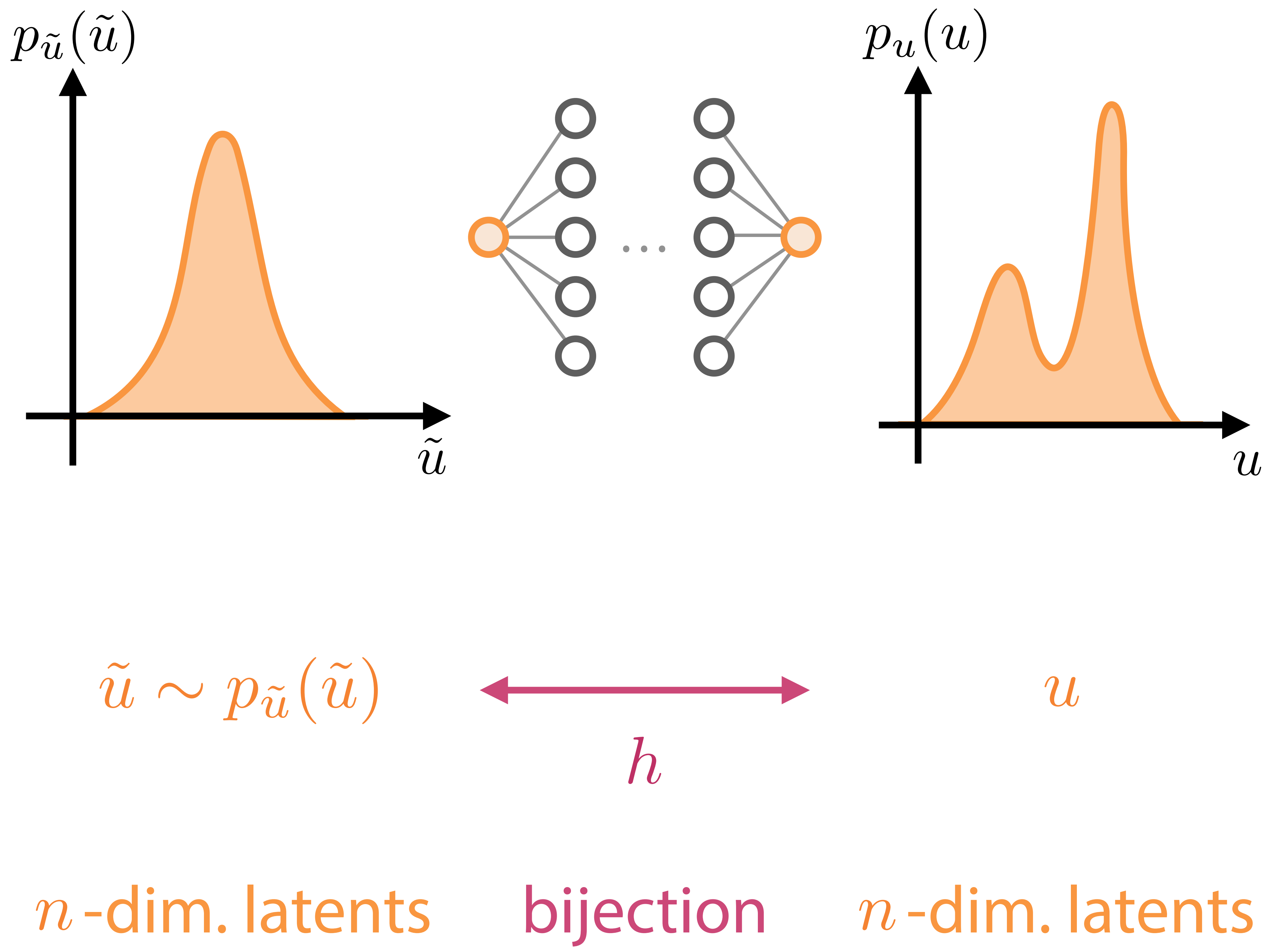


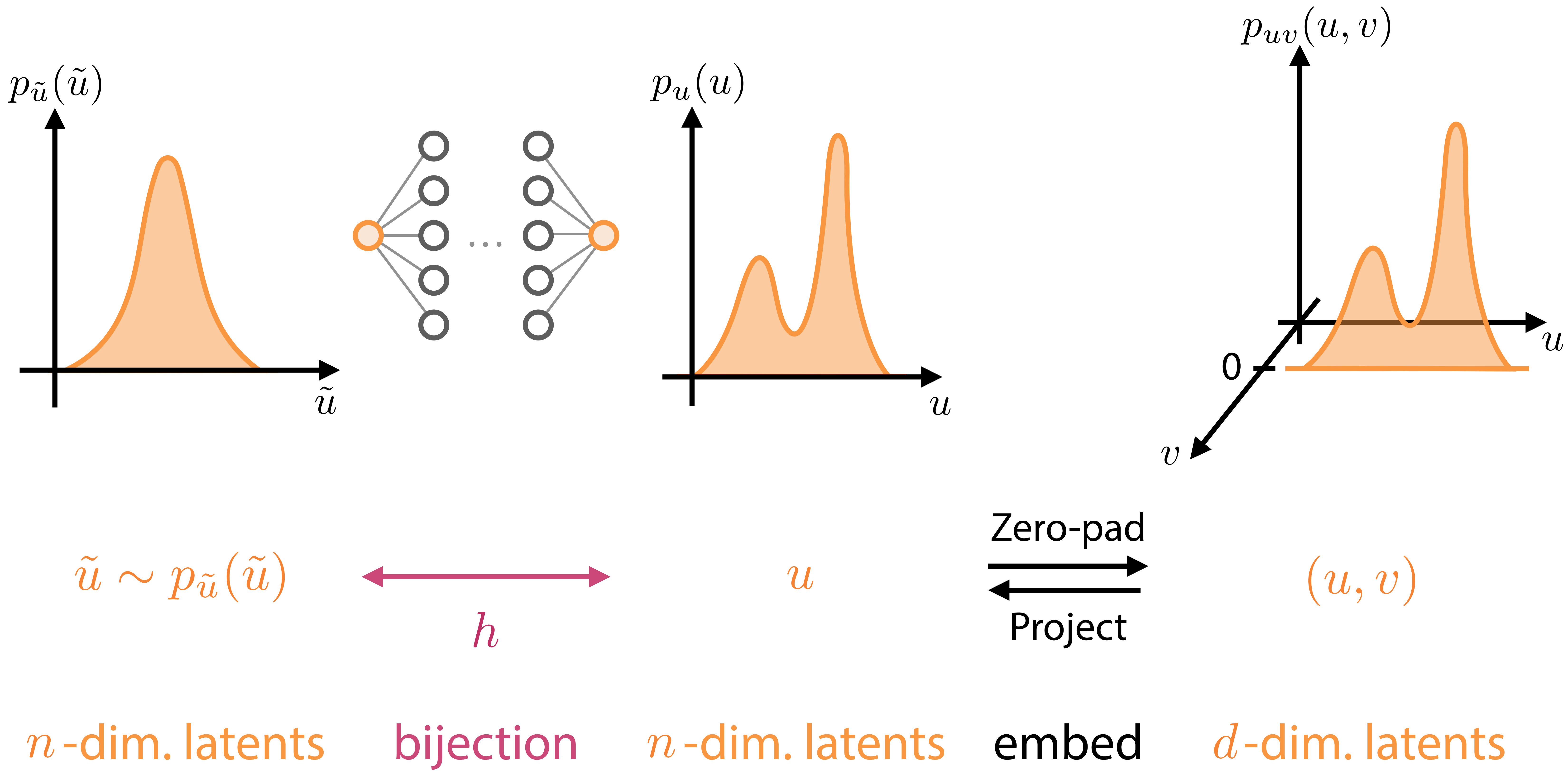
$\mathcal{M}$-flow:



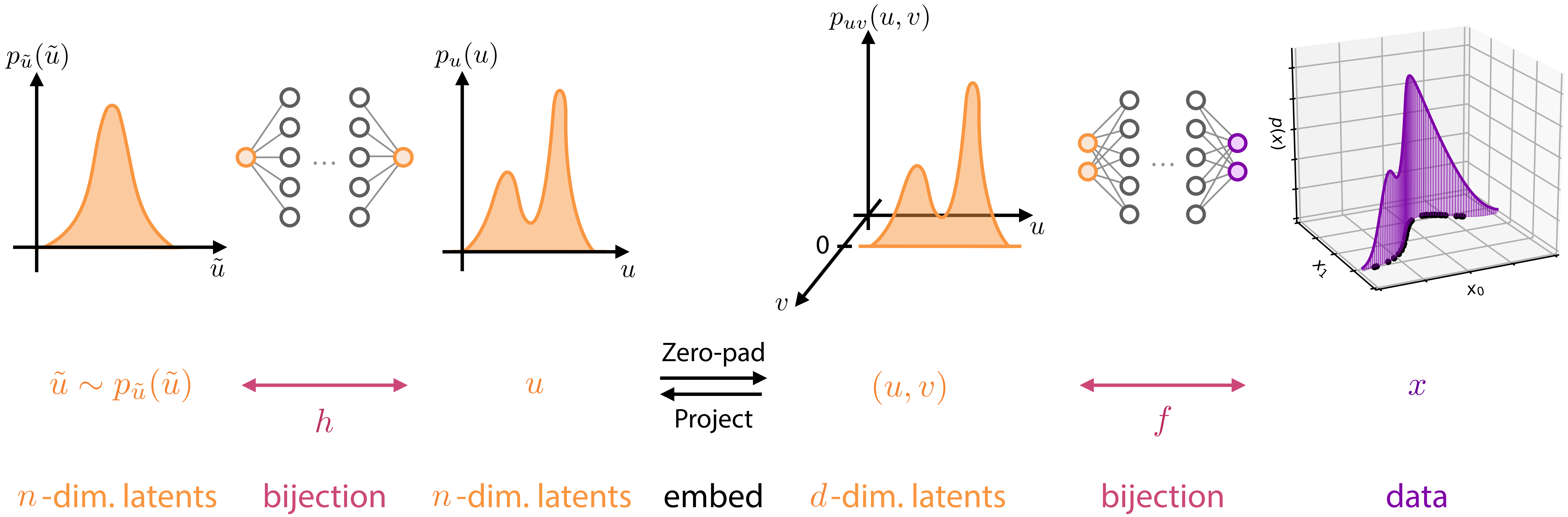
$\mathcal{M}$-flow:



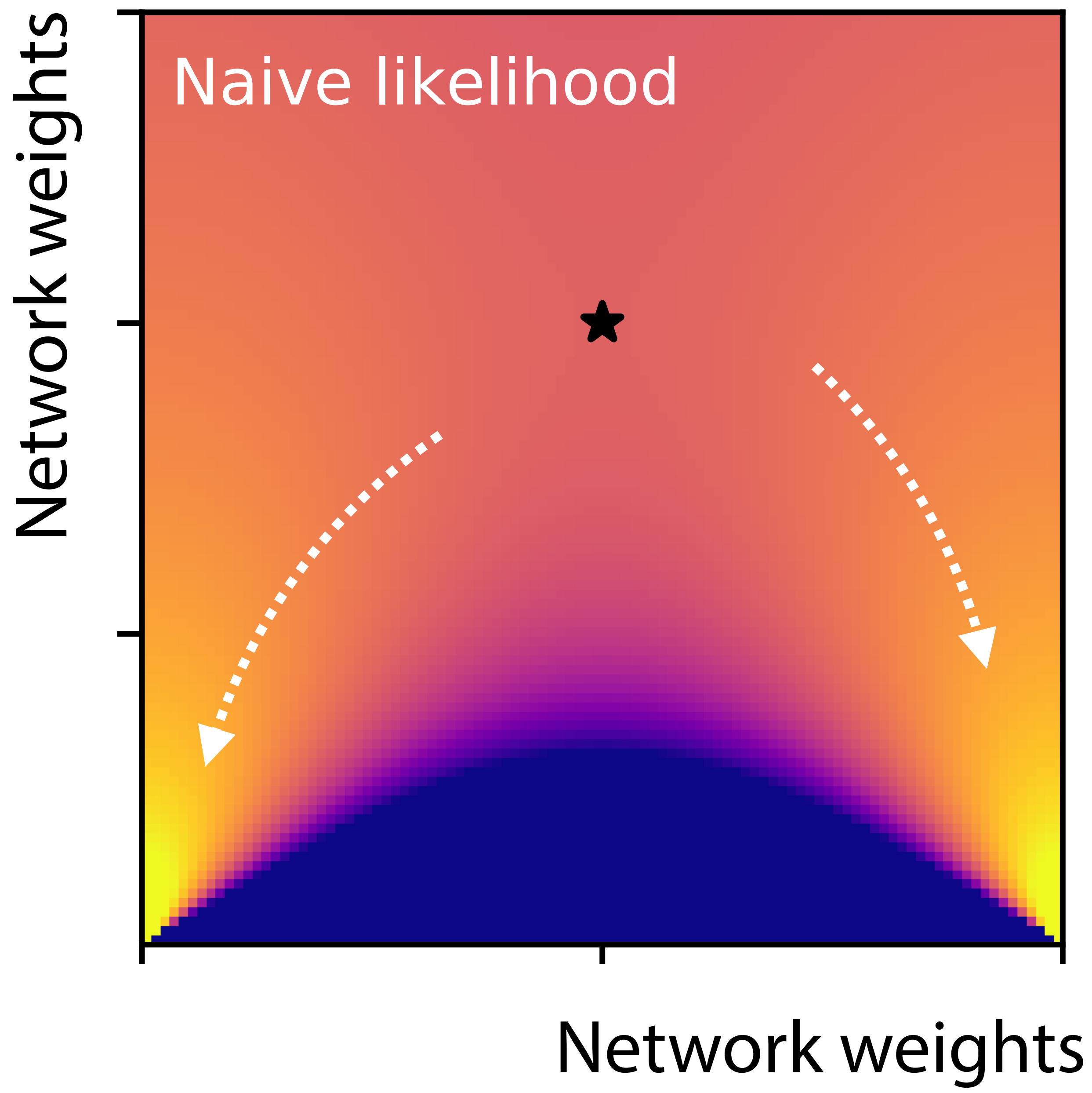

$p_{\tilde{u}}(\tilde{u})$
$\tilde{u}$
$p_u(u)$
u
$\tilde{u} \sim p_{\tilde{u}}(\tilde{u})$
h
u
n-dim. latents
bijection
n-dim. latents



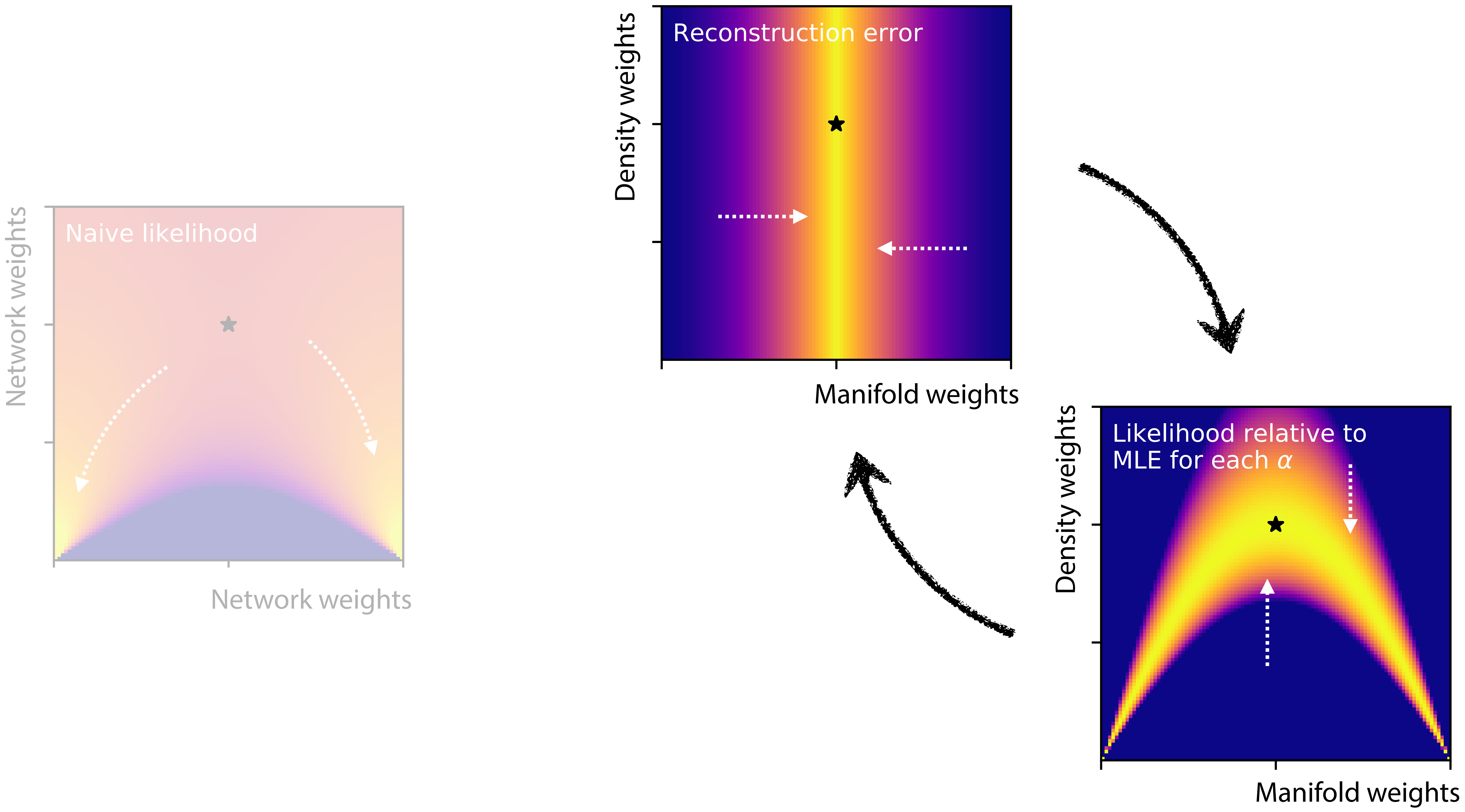
$p_{\tilde{u}}(\tilde{u})$
$\tilde{u}$
$p_u(u)$
u
$p_{uv}(u, v)$
u
0
v
$\tilde{u} \sim p_{\tilde{u}}(\tilde{u})$
h
u
Zero-pad
Project
(u, v)
n-dim. latents
bijection
n-dim. latents
embed
d-dim. latents



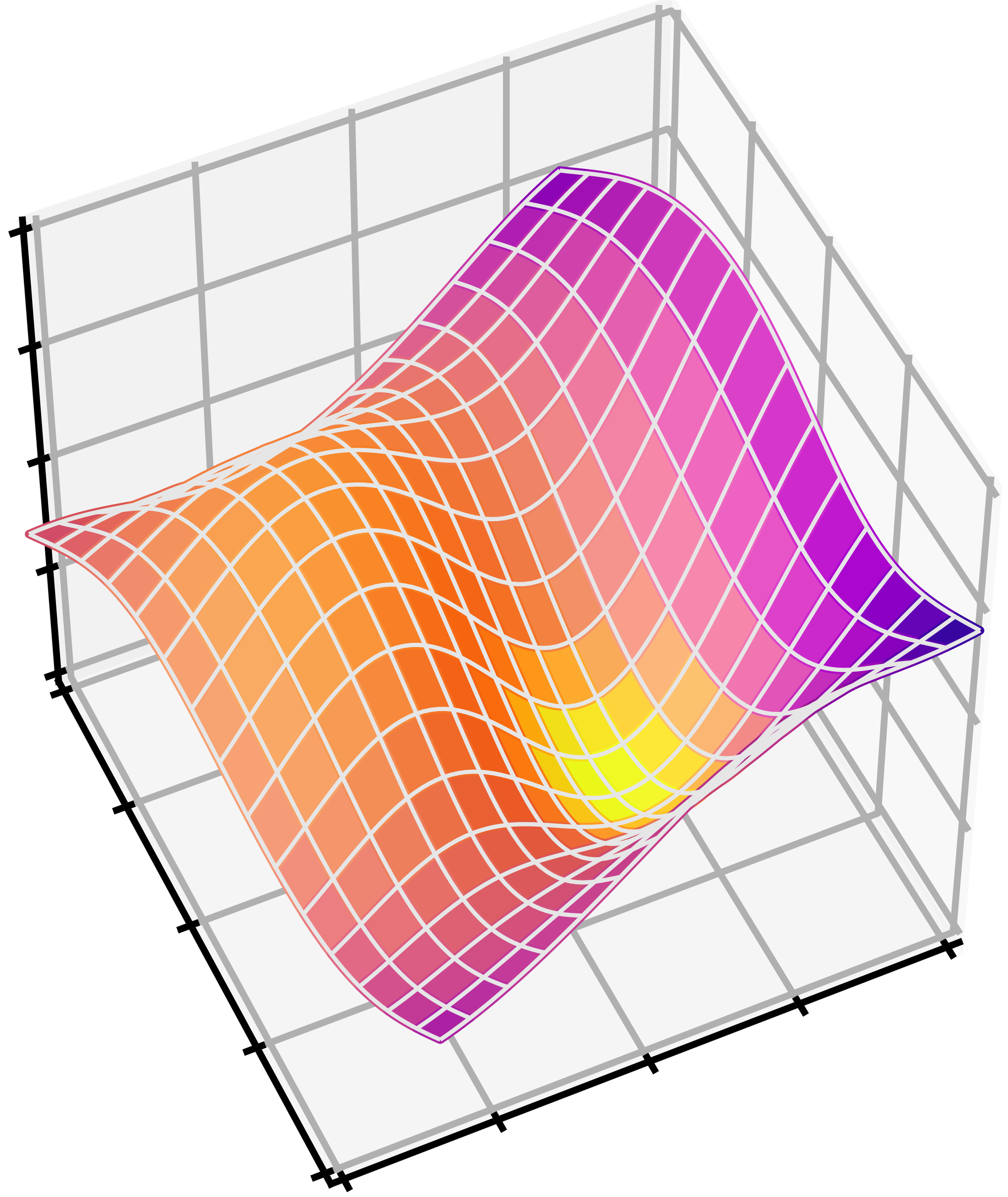
$p_{\tilde{u}}(\tilde{u})$
$\tilde{u}$
$p_u(u)$
u
$p_{uv}(u, v)$
u
0
v
p(x)
x_1
x_0
Zero-pad
Project
$\tilde{u} \sim p_{\tilde{u}}(\tilde{u})$
h
u
(u, v)
f
x
n-dim. latents
bijection
n-dim. latents
embed
d-dim. latents
bijection
data



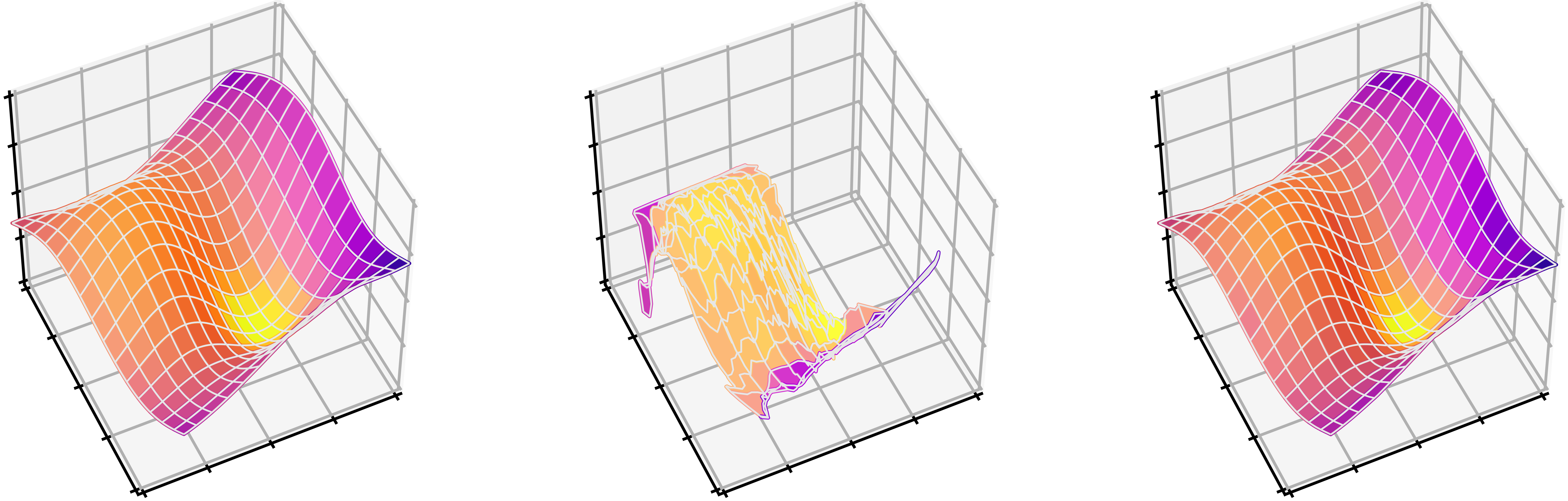
Naive likelihood
Network weights
Network weights

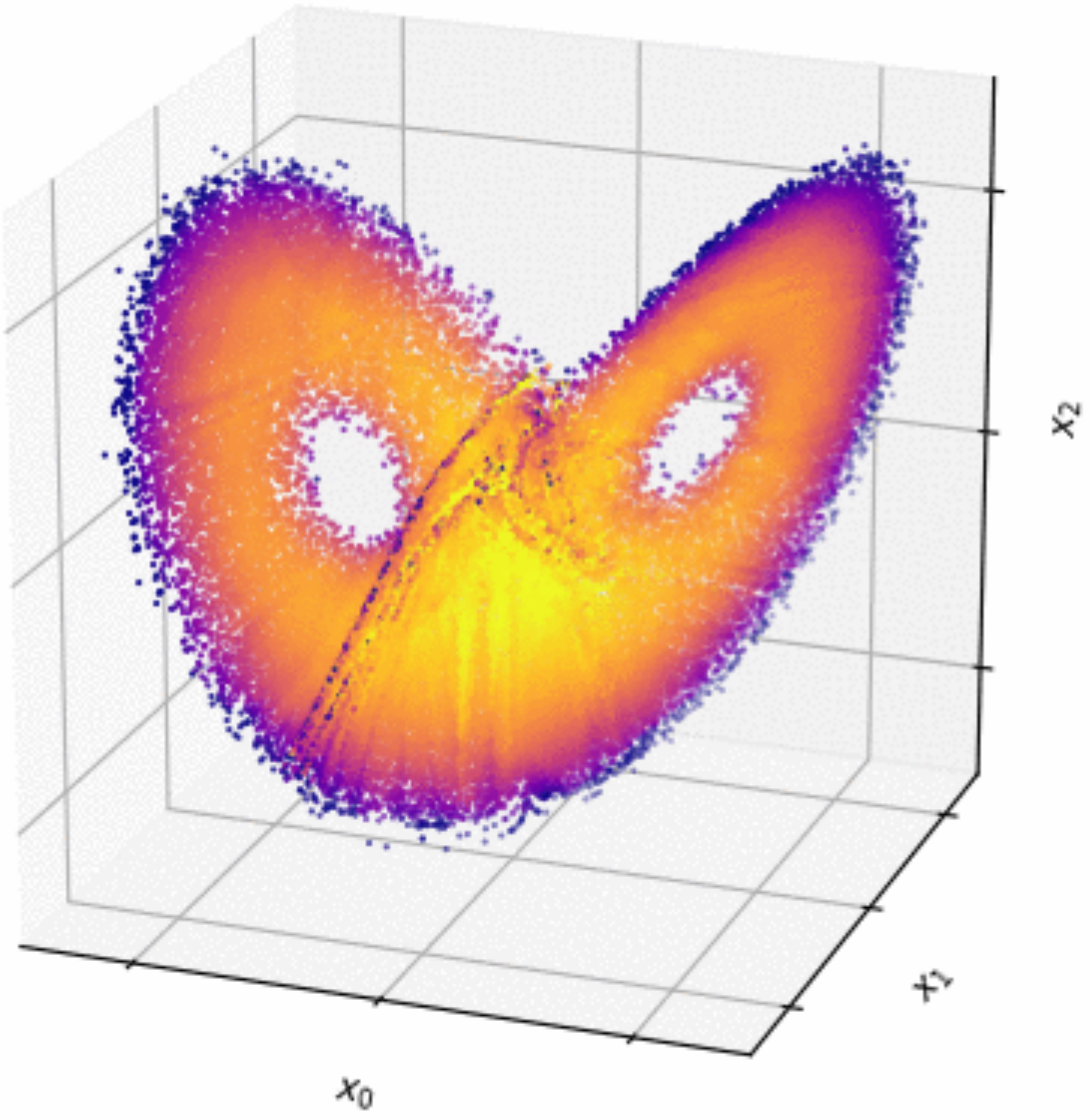

Naive likelihood
Network weights
Network weights
Reconstruction error
Density weights
Manifold weights
Likelihood relative to
MLE for each α
Density weights
Manifold weights

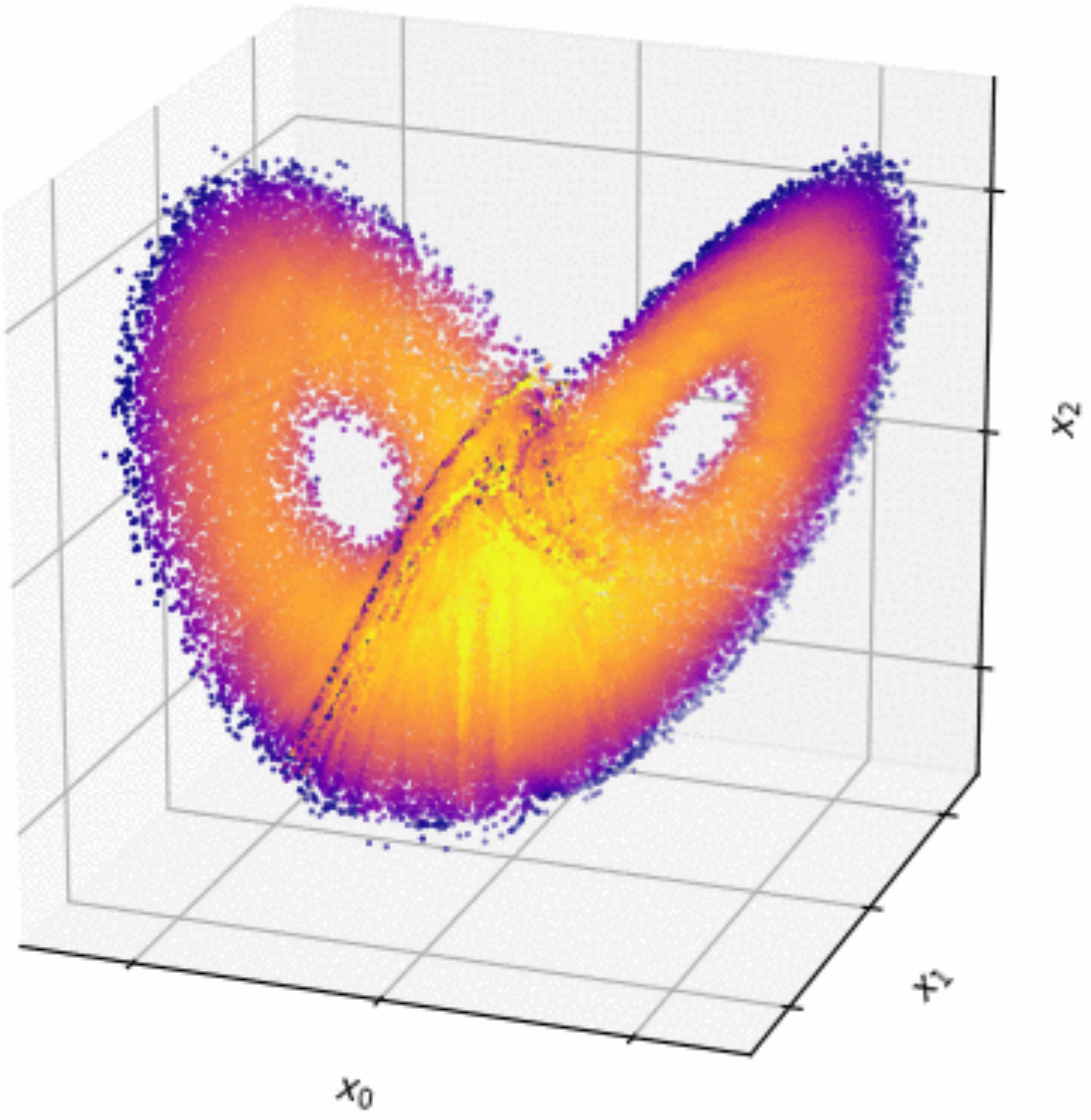
Ground truth, $\theta = 0$



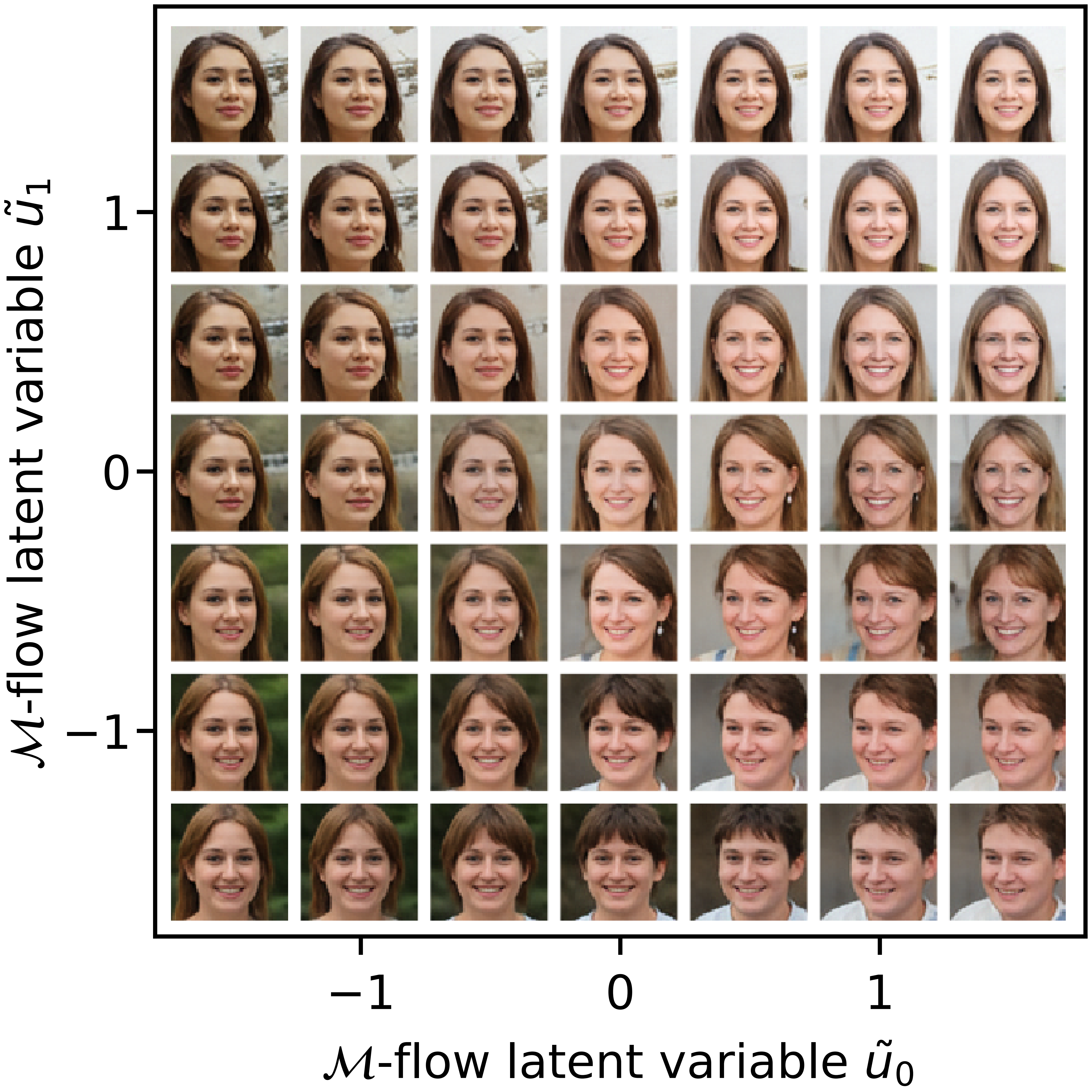
Ground truth, $\theta = 0$ PIE, $\theta = 0$ $\mathcal{M}$-flow (M/D), $\theta = 0$




x_0
x_1
x_2


x_0
x_1
x_2

[CMS collaboration]



1
0
−1
−1
0
1
$\mathcal{M}$-flow latent variable $\tilde{u}_1$
$\mathcal{M}$-flow latent variable $\tilde{u}_0$

Extended version on arXiv: 2003.13913

Flows for simultaneous manifold learning and density estimation

Johann Brehmer[a,b,1] **and Kyle Cranmer**[a,b]

[a]Center for Data Science, New York University, USA; [b]Center for Cosmology and Particle Physics, New York University, USA

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We introduce manifold-learning flows ($\mathcal{M}$-flows), a new class of generative models that simultaneously learn the data manifold as well as a tractable probability density on that manifold. Combining aspects of normalizing flows, GANs, autoencoders, and energy-based models, they have the potential to represent datasets with a manifold structure more faithfully and provide handles on dimensionality reduction, denoising, and out-of-distribution detection. We argue why such models should not be trained by maximum likelihood alone and present a new training algorithm that separates manifold and density updates. In a range of experiments we demonstrate how $\mathcal{M}$-flows learn the data manifold and allow for better inference than standard flows in the ambient data space.

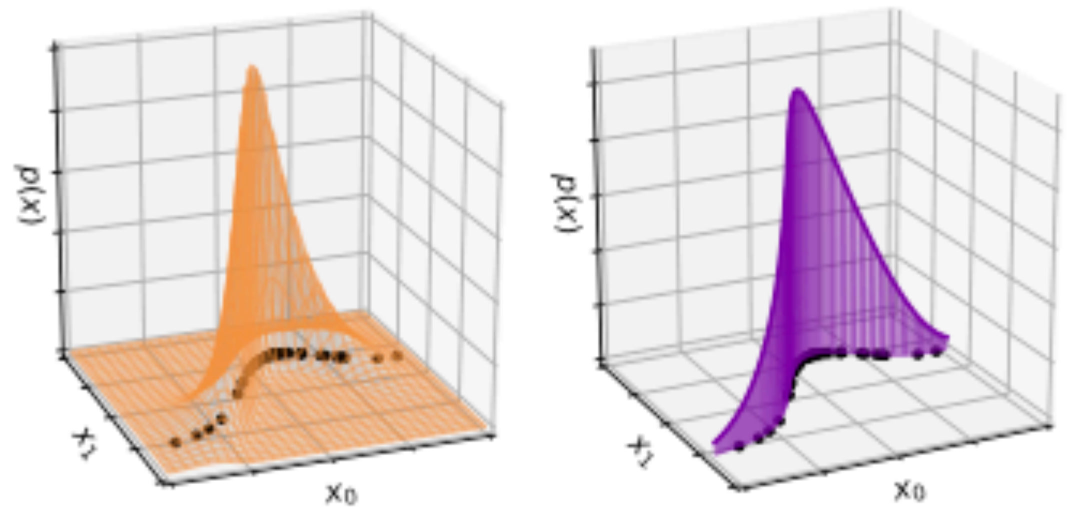

Fig. 1. Sketch of how a standard normalizing flow in the ambient data space (left, orange surface) and an $\mathcal{M}$-flow (right, purple) model data (black dots).

Contents

1. Introduction

Inferring a probability distribution from example data is a common problem that is increasingly tackled with deep generative models. Generative adversarial networks (GANs) (1) and variational autoencoders (VAEs) (2) are both based on a lower-dimensional latent space and a learnable mapping from