NOTAGAN

Normalizing flows for simul**t**aneous m**a**nifold learnin**g** **a**nd density estimatio**n**

Johann Brehmer
New York University

Physics x ML meeting, NYU
June 26, 2020

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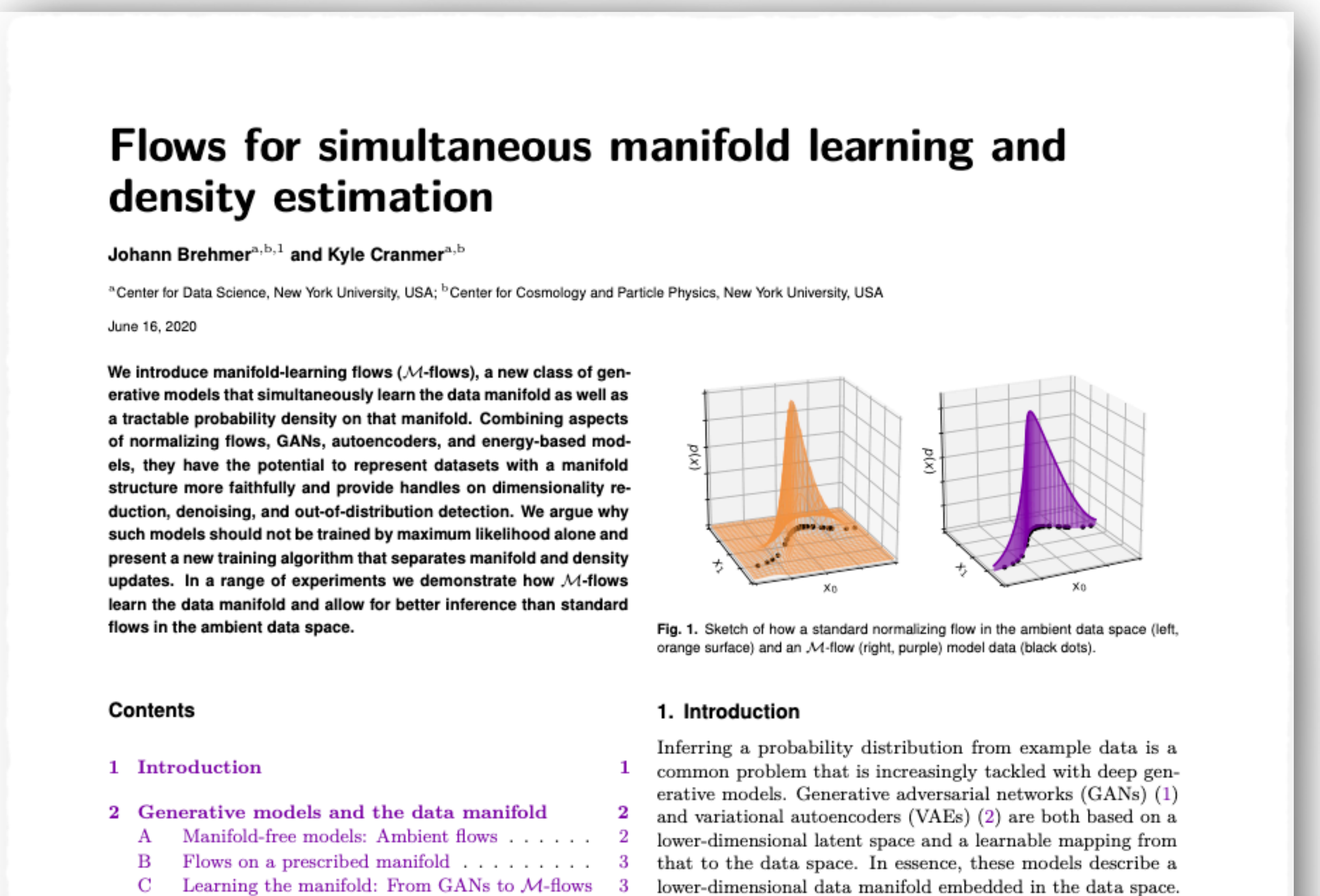
NYU MSDSE Moore - Sloan Data Science Environments dianahep iris hep Institute for Research and Innovation in Software for High Energy Physics The SCAILFIN Project scailfin.github.io BROOKHAVEN NATIONAL LABORATORY Scientific Data and Computing Center

$\mathcal{M}$-flow: [JB, Kyle Cranmer 2003.13913]

A new generative model that

- describes data with a probability density on a lower-dimensional manifold
- learns manifold and density from data
- has a tractable density and performs well on inference tasks
- provides handles for dimensionality reduction, denoising, OOD detection



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

June 16, 2020

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).

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2 Generative models and the data manifold 2
  A Manifold-free models: Ambient flows 2
  B Flows on a prescribed manifold 3
  C Learning the manifold: From GANs to $\mathcal{M}$-flows 3

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 that to the data space. In essence, these models describe a lower-dimensional data manifold embedded in the data space.

$\mathcal{M}$-flow: [JB, Kyle Cranmer 2003.13913]

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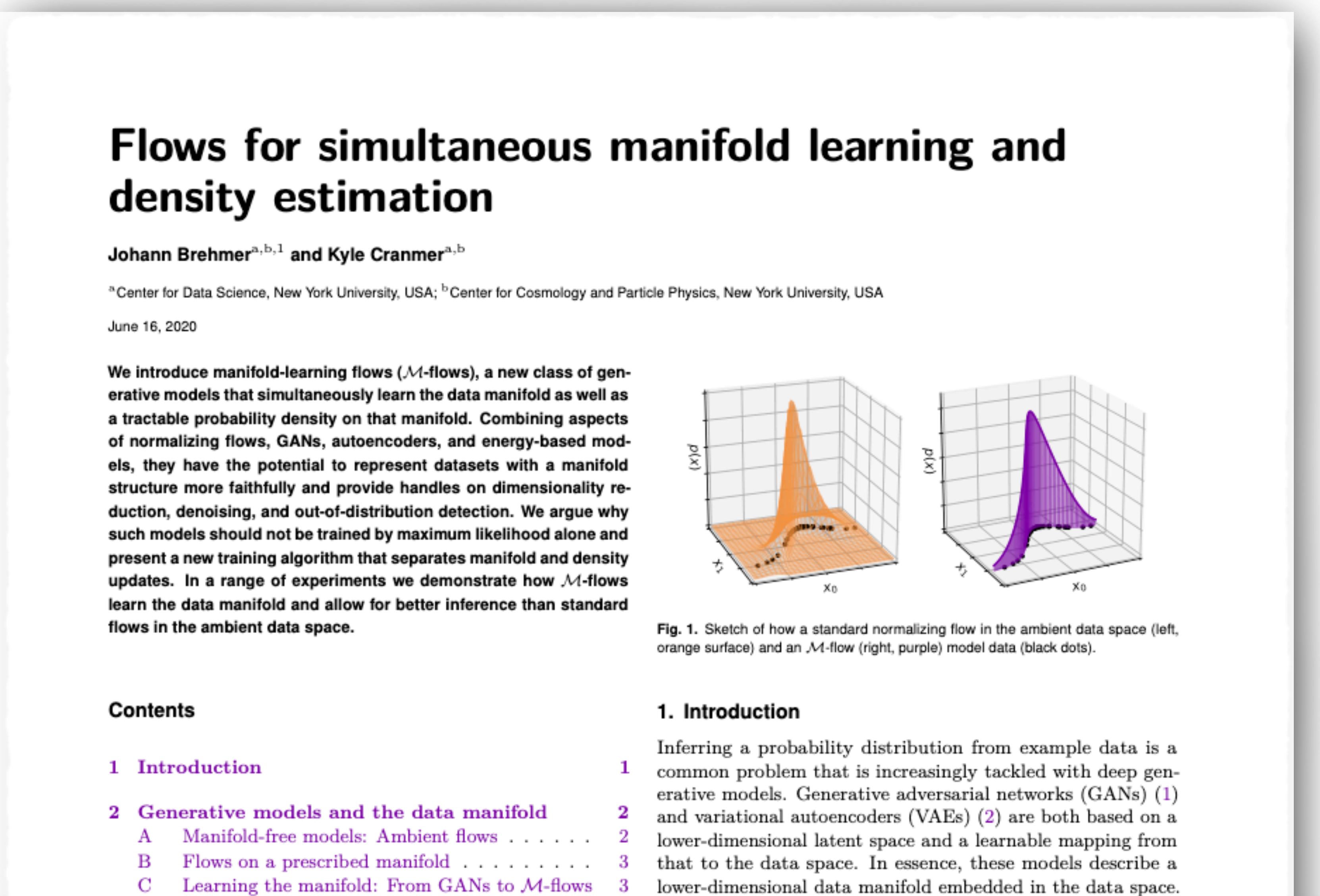

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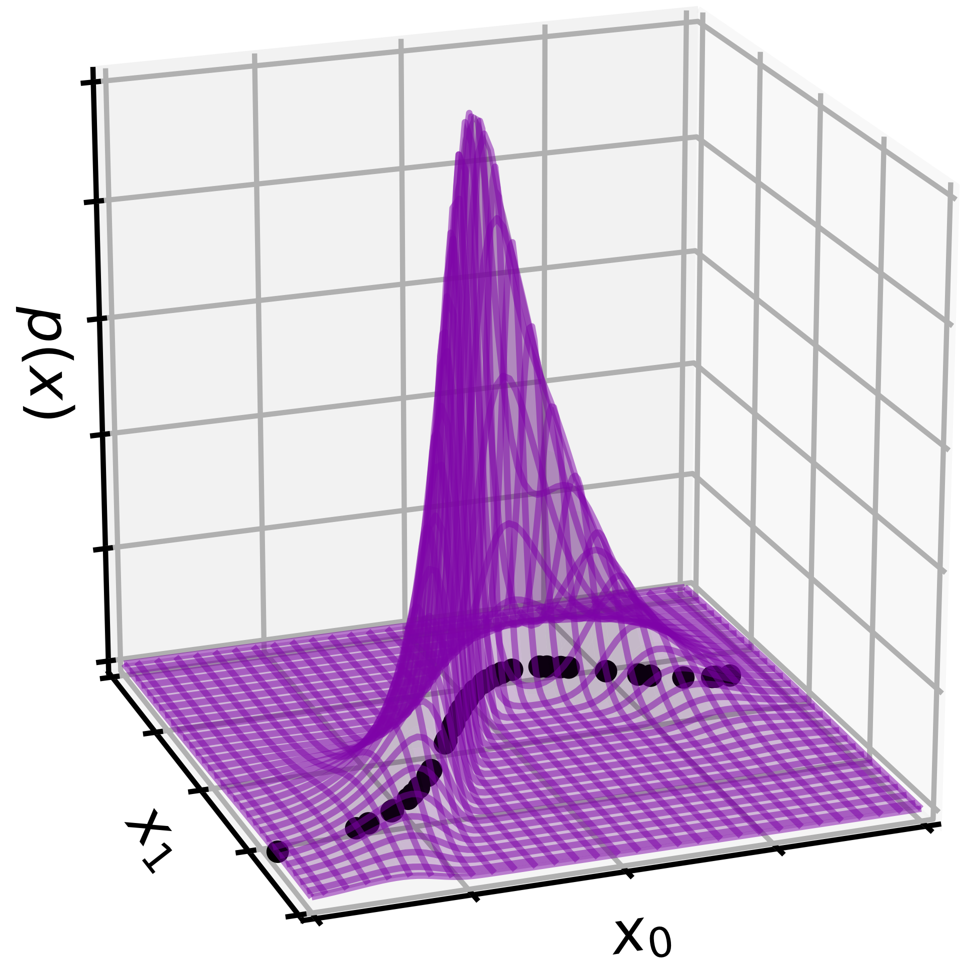
m-flo:

Japanese hip hop group known for

- Love me after 12 am
- The love bug
- Love song
- Love don't cry
- Stuck in your love
- The other side of love
- Lotta Love
- and many more

[m-flo / Rhythm Zone]



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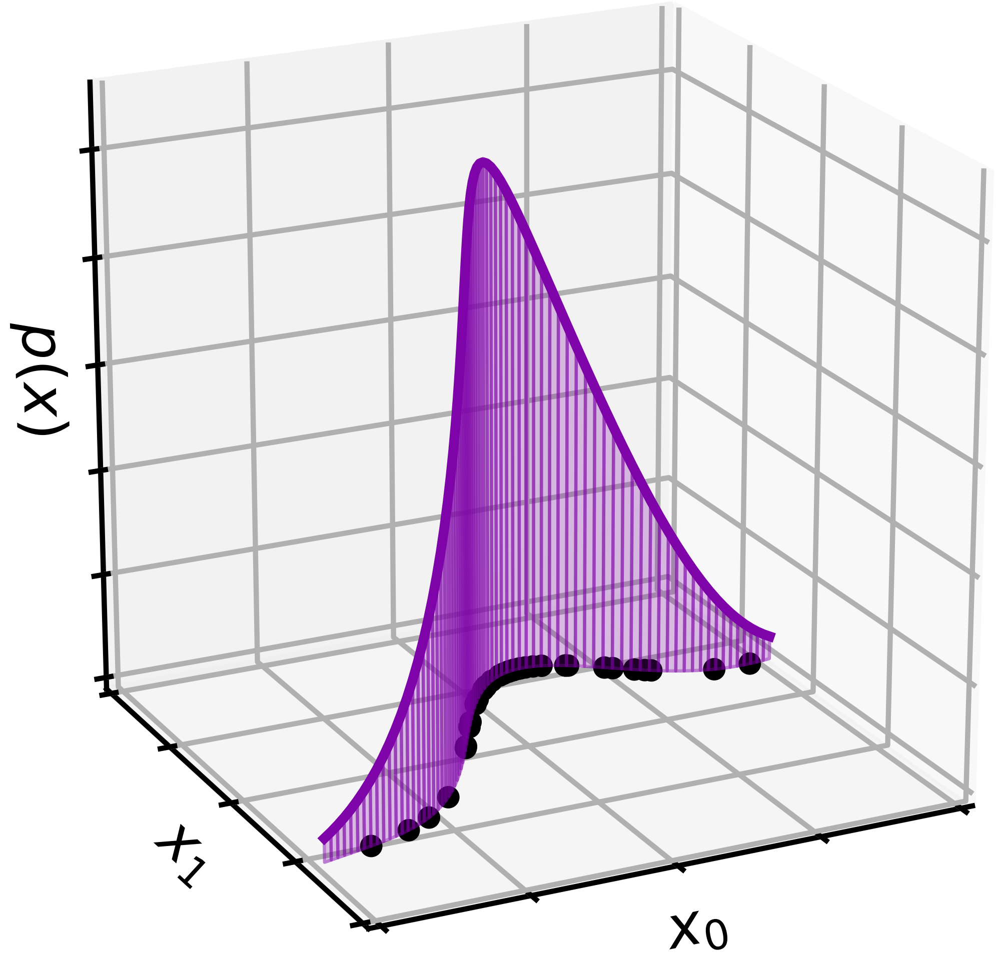
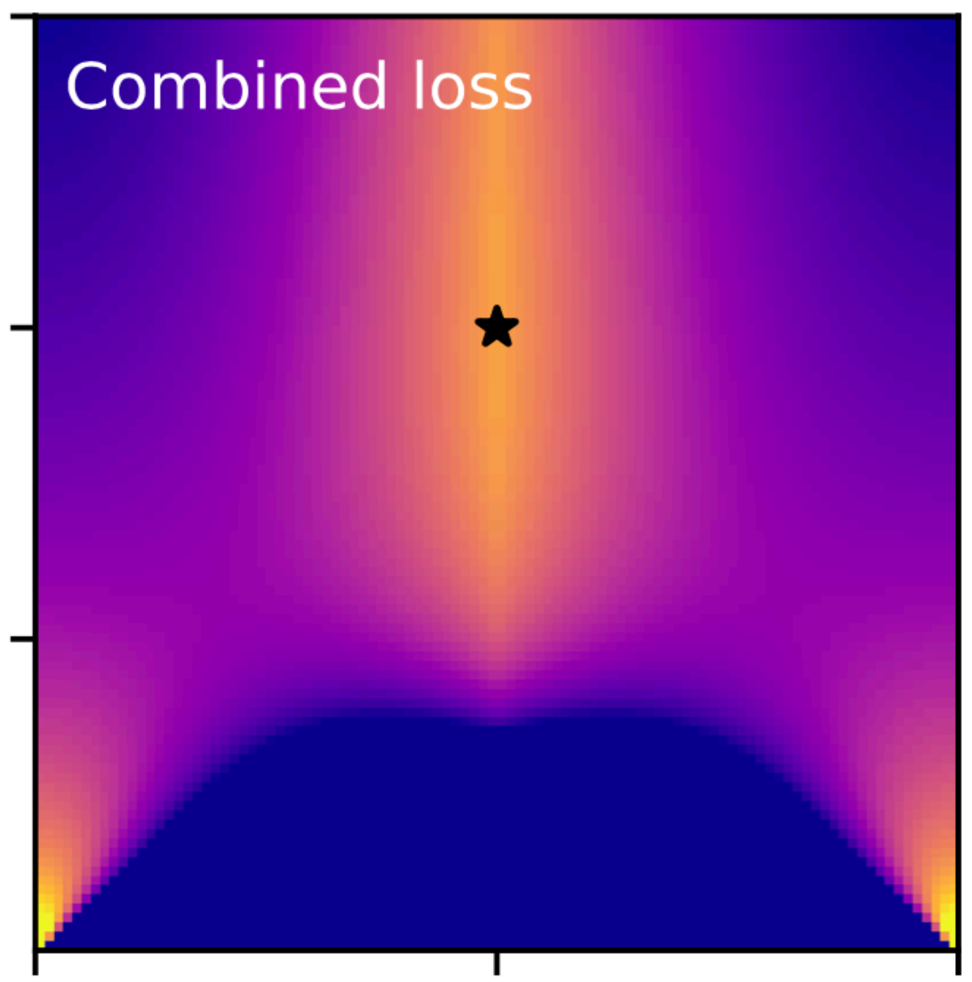
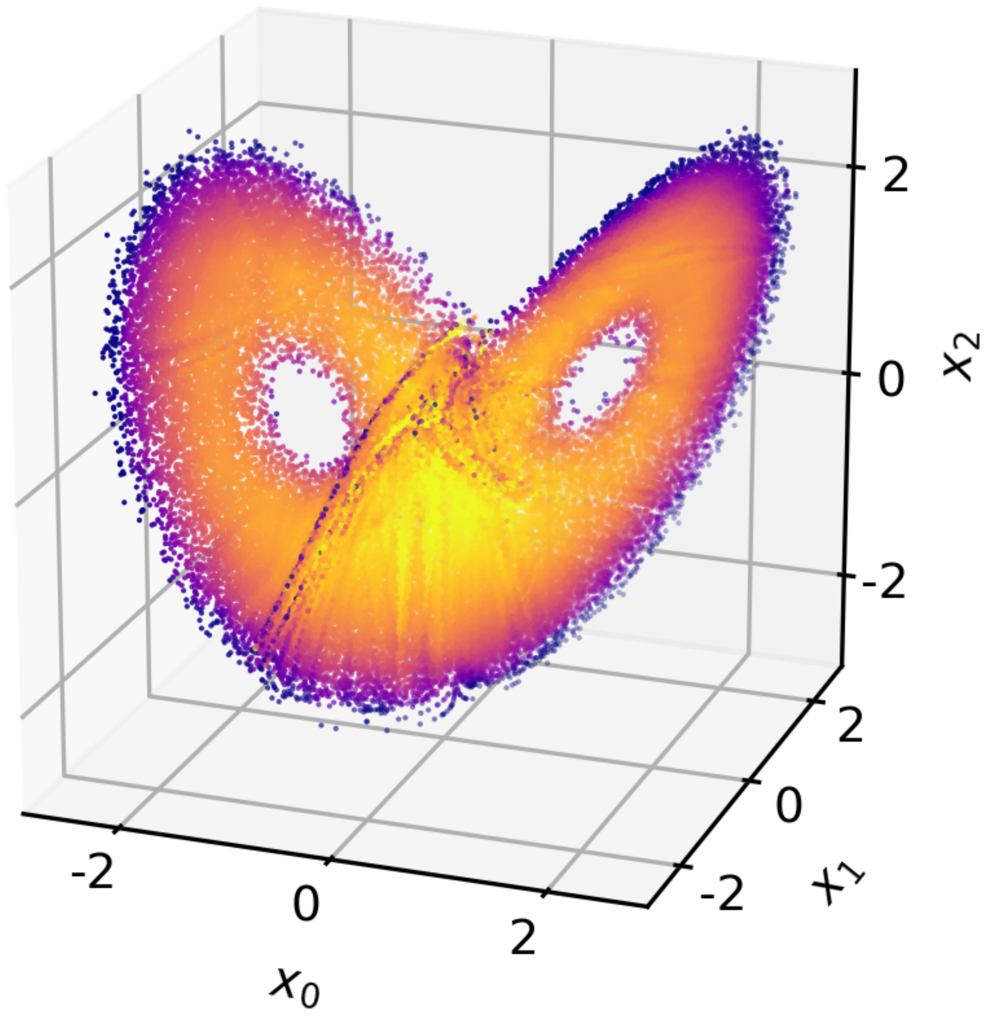


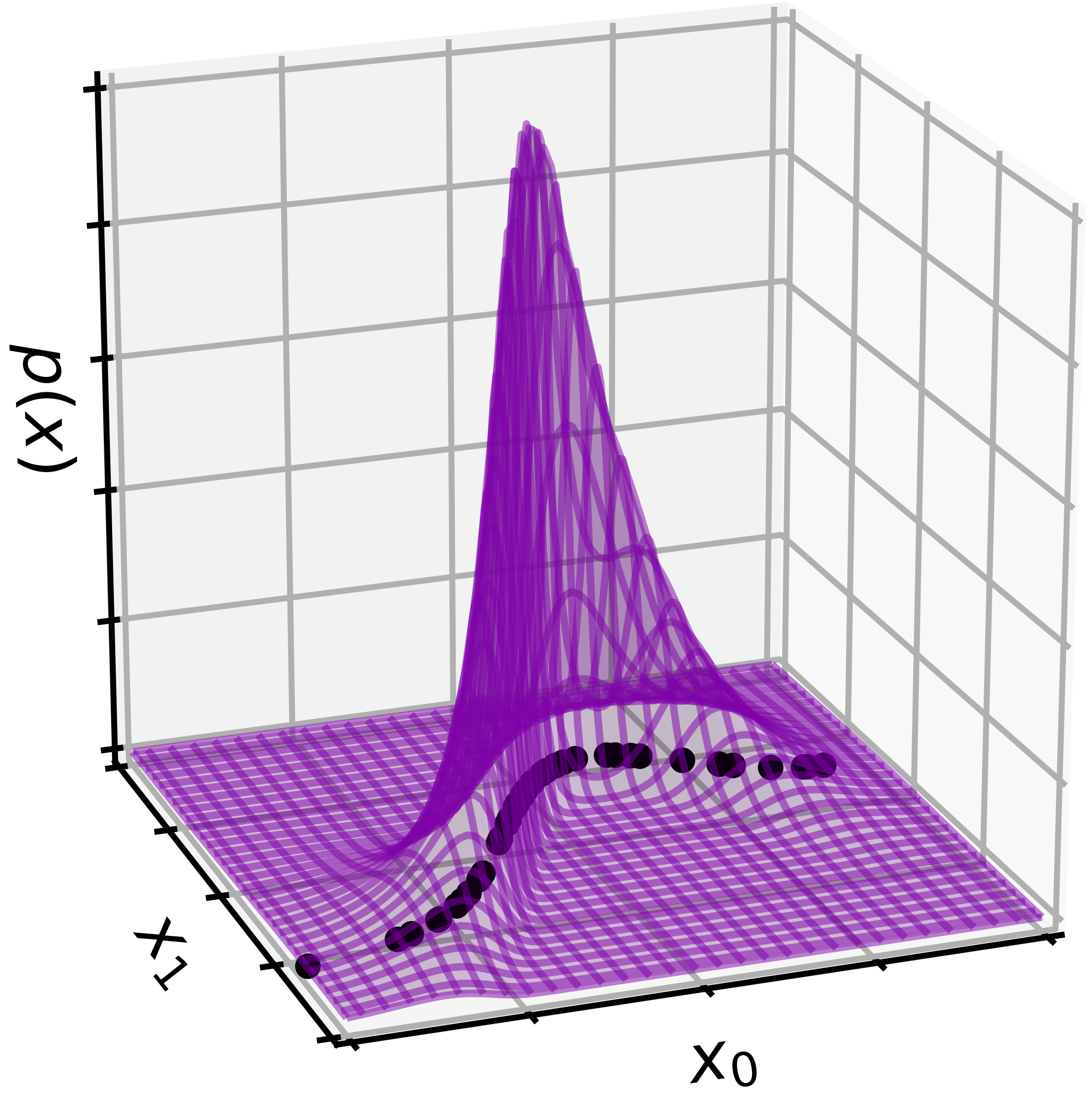
2. $\mathcal{M}$-flows



3. Training $\mathcal{M}$-flows



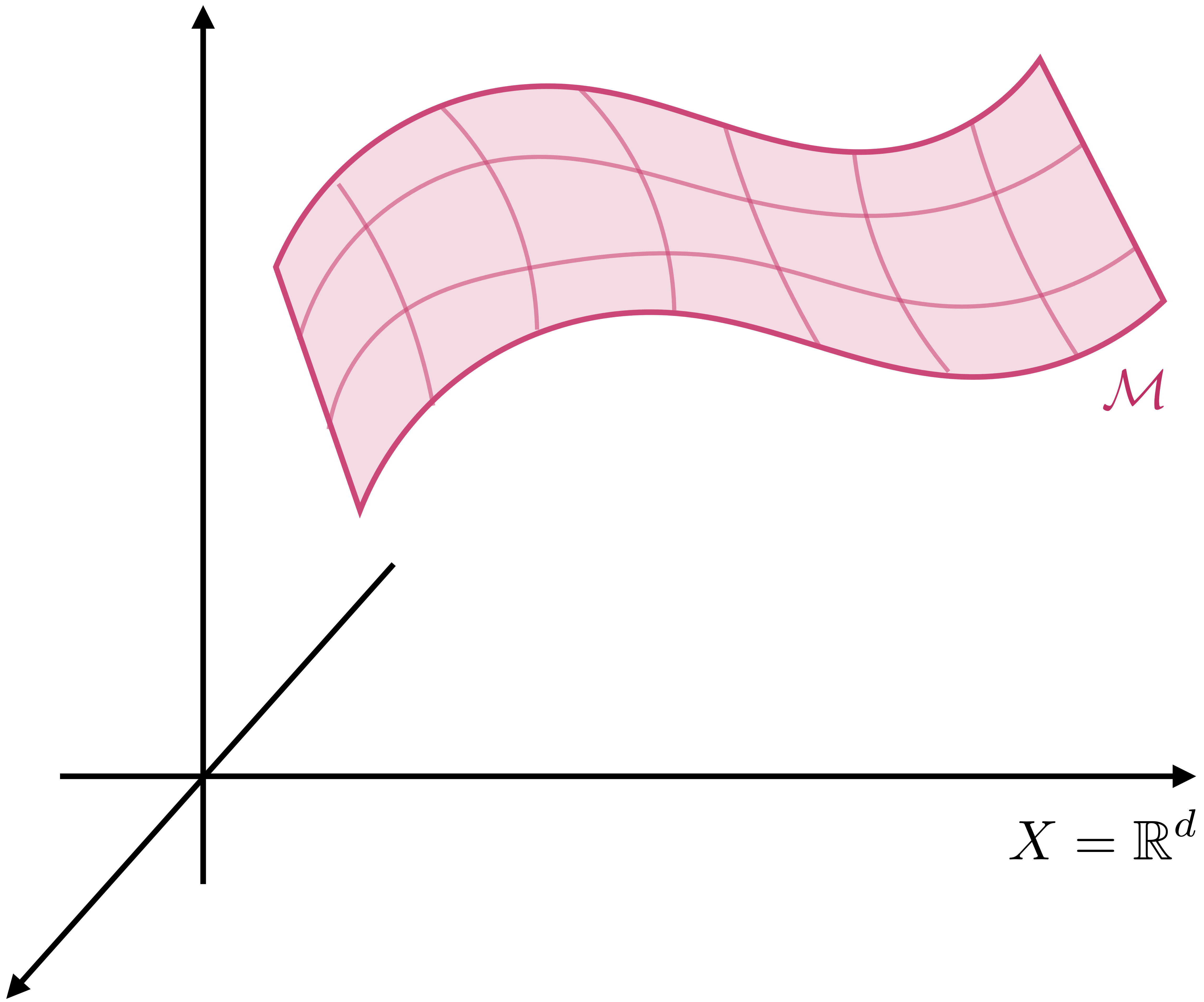
4. Experiments



Generative models and the data manifold

The data manifold

Data often live on a n-dimensional manifold embedded in the d-dimensional ambient space



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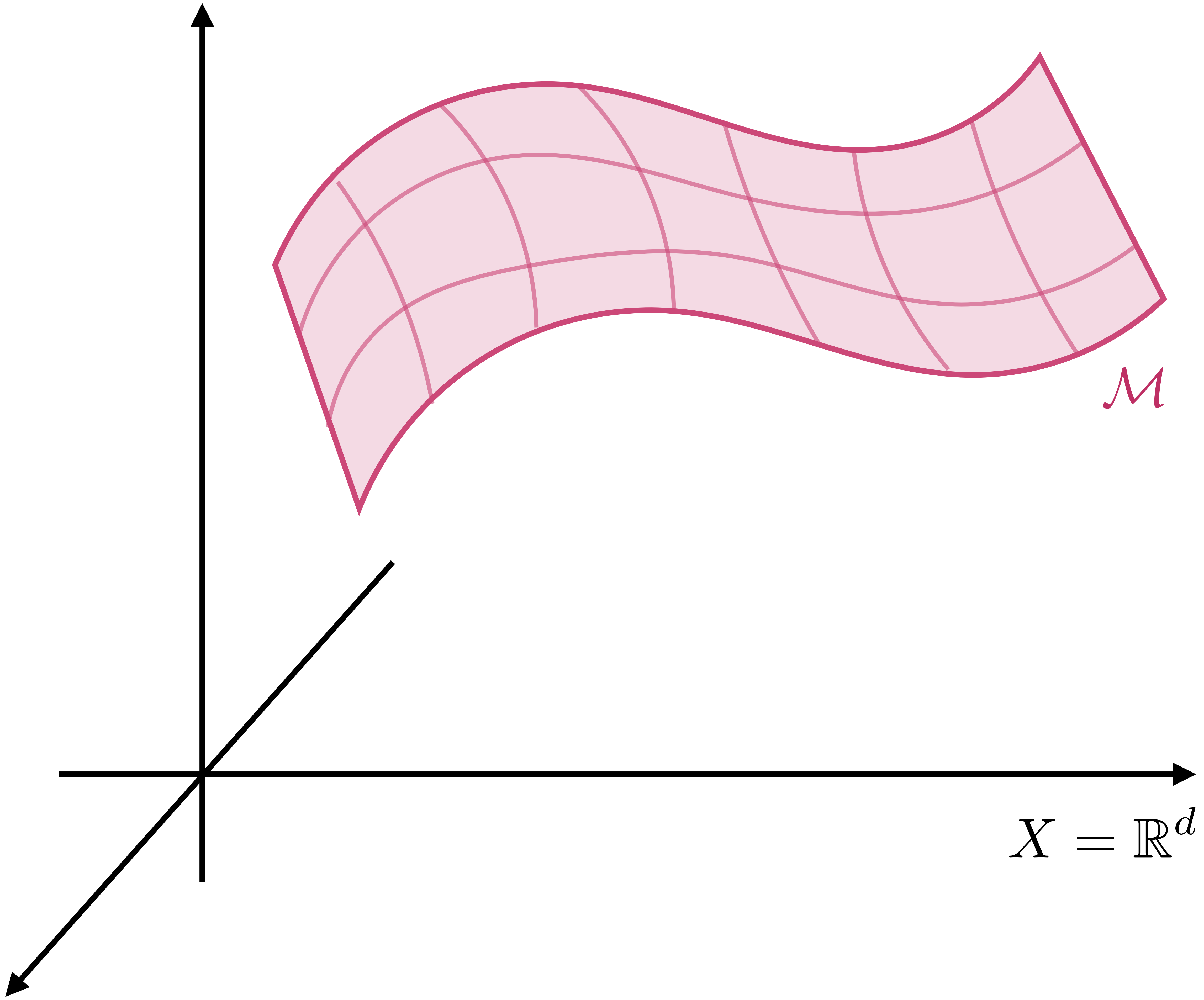

- Robot arms: limited degrees of freedom
- Particle physics: energy-momentum conservation, on-shell conditions, redundant observables
- Many other high-dimensional datasets (e.g. images): empirical evidence for (approximate) data manifold
  [L. Cayton 2005; …]

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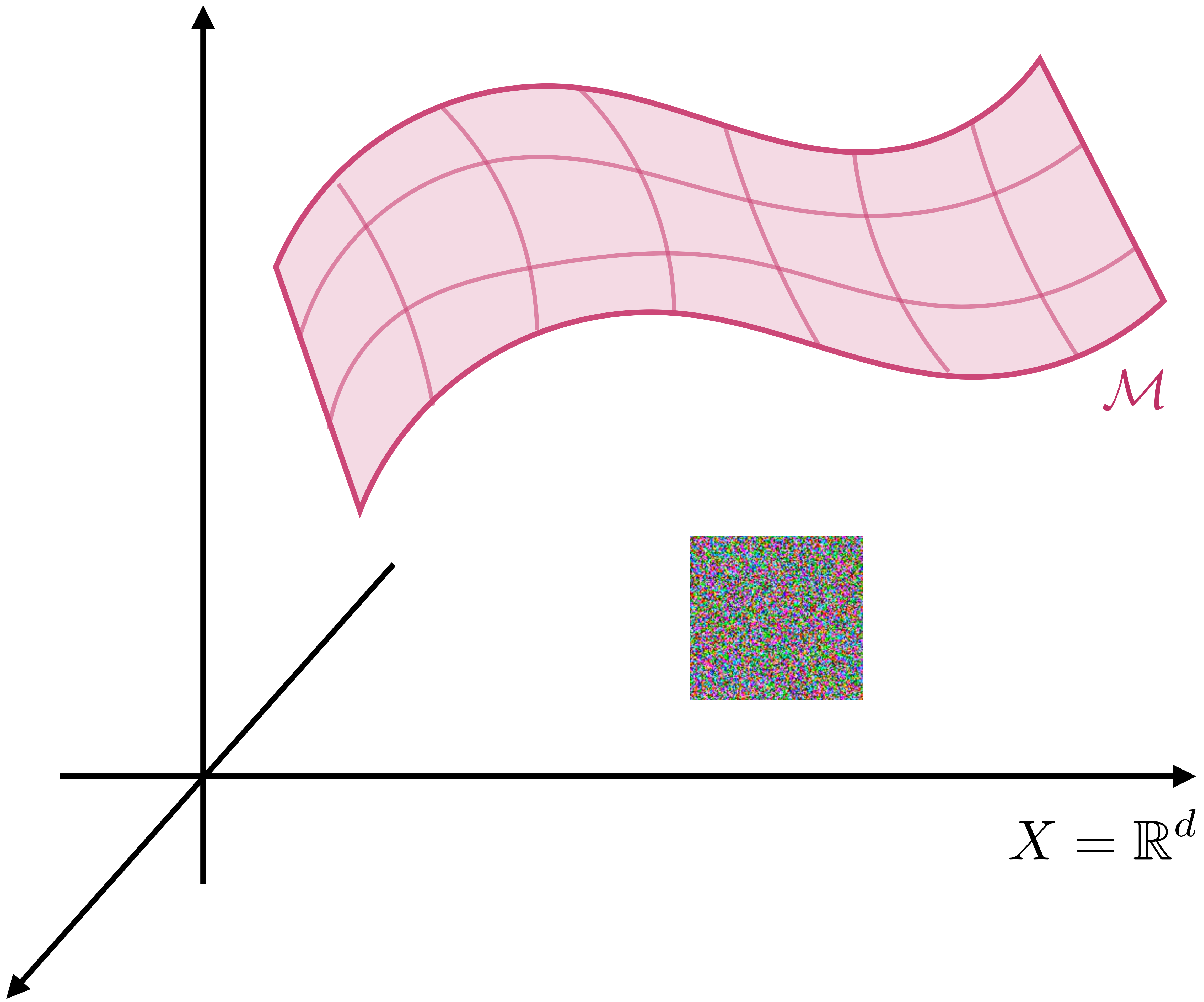

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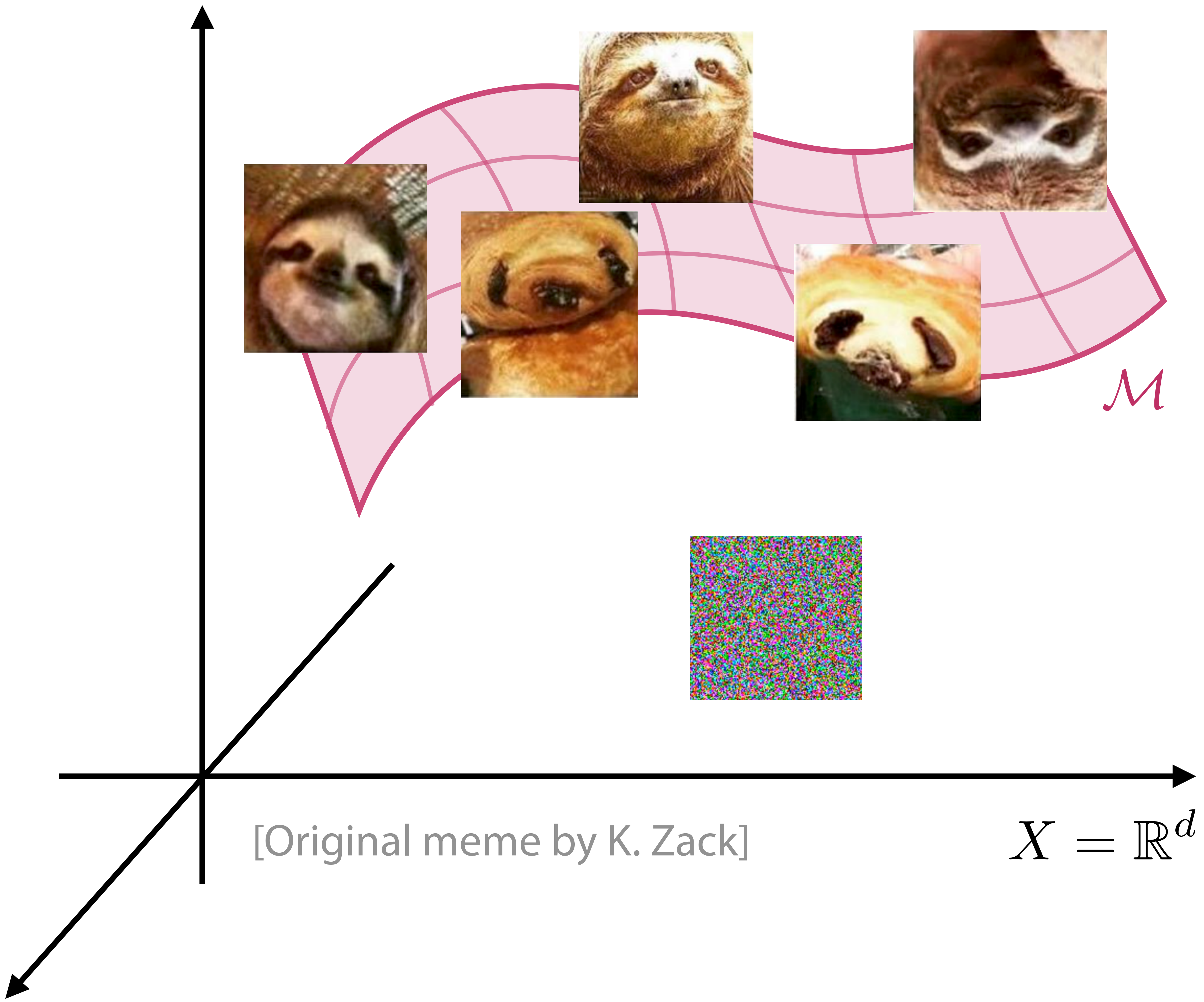

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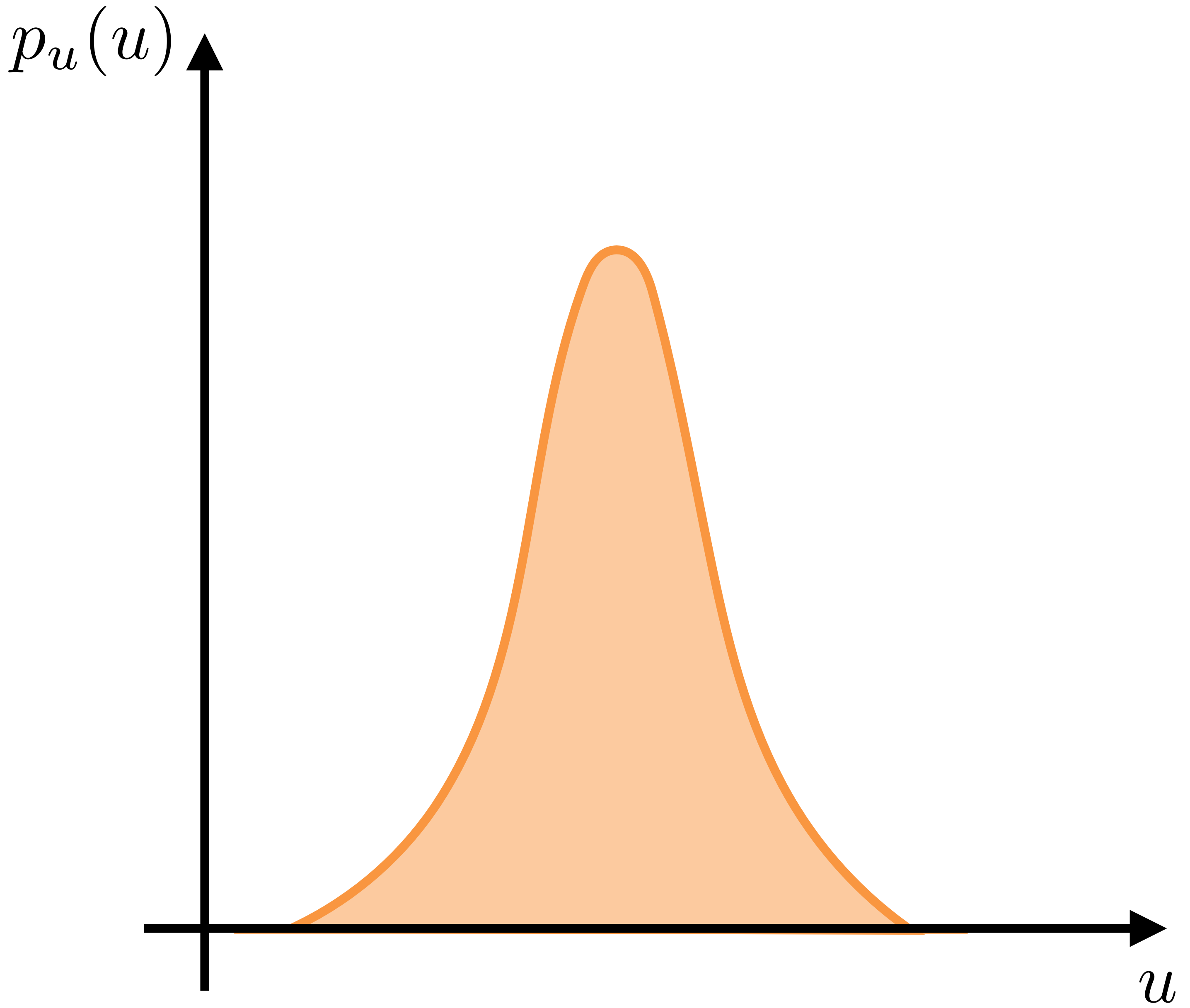
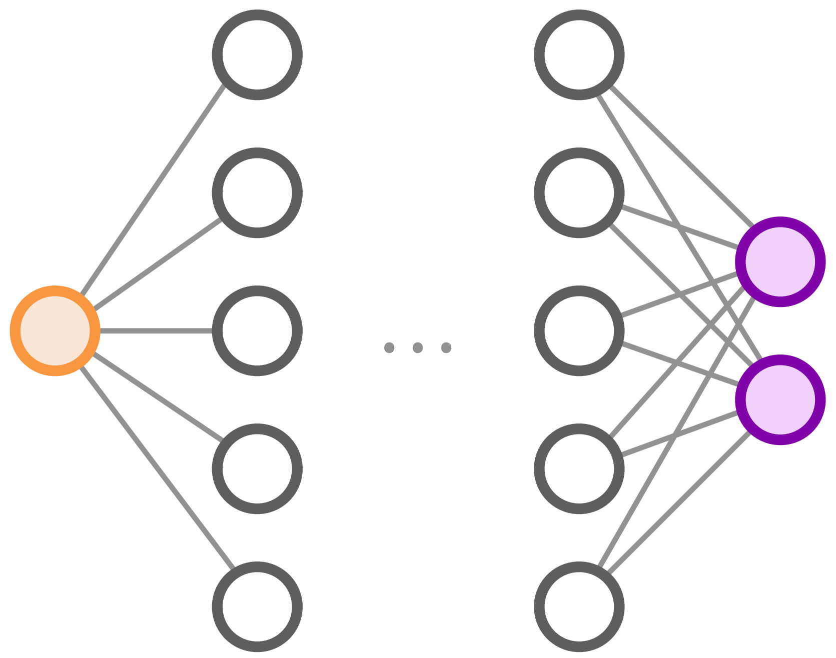
Generative adversarial networks (GANs)

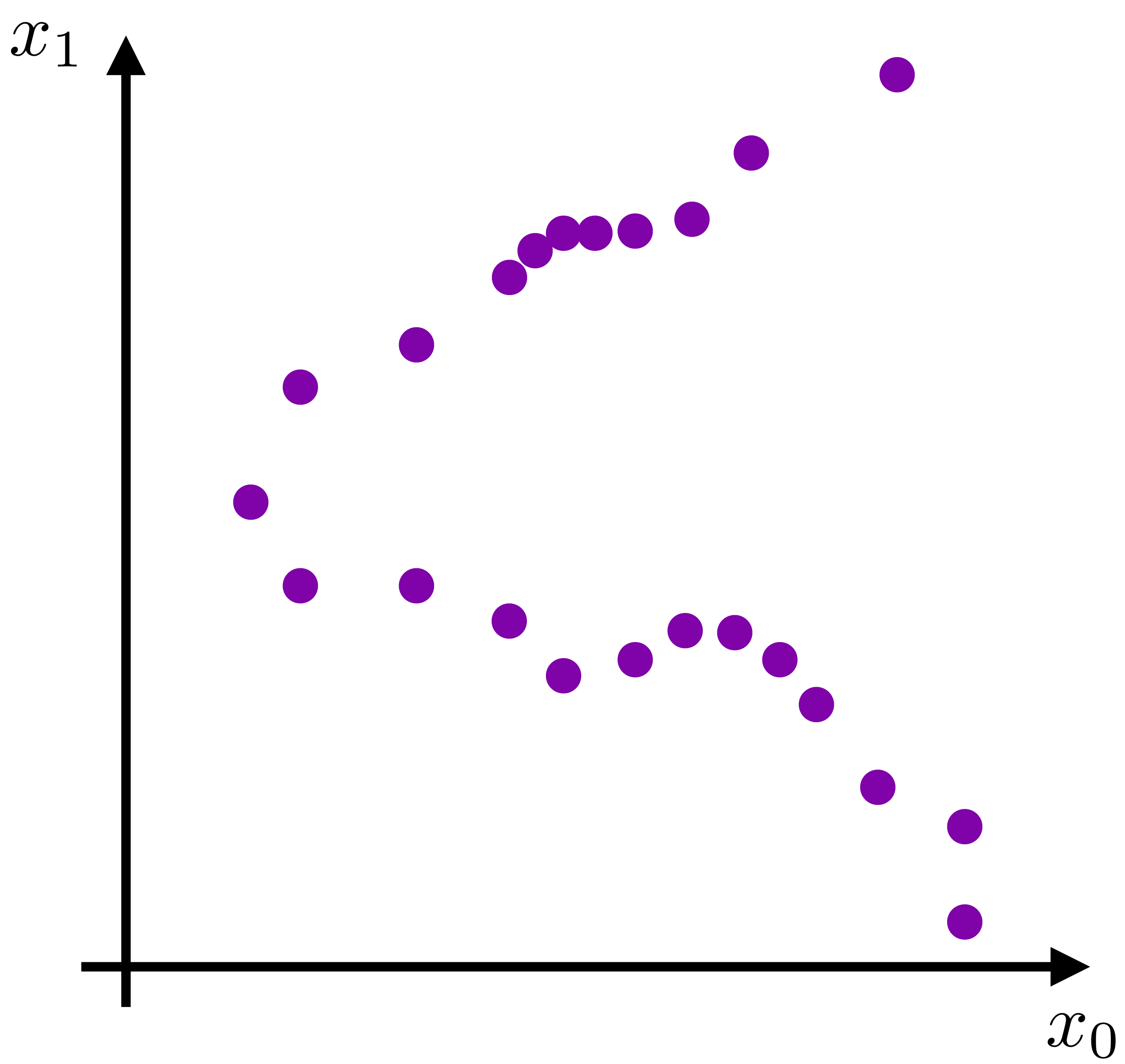
[I. Goodfellow et al 1406.2661]



$u \sim p_u(u)$



$\xrightarrow{g}$



x

n-dim. latent variables

unconstrained NN

implicit density over $\mathcal{M}$

$p_{\mathcal{M}}(x)$ intractable

Generative adversarial networks (GANs)

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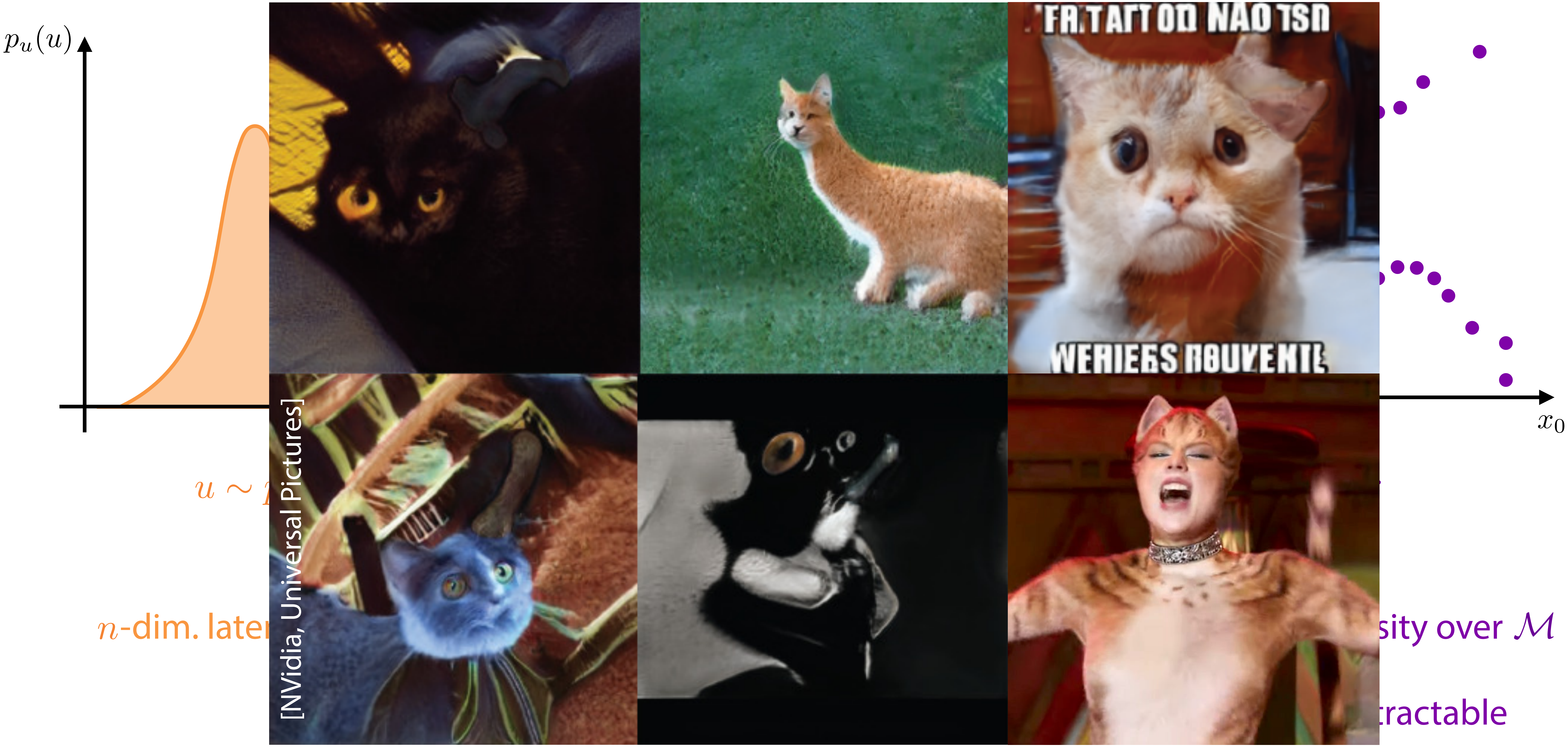
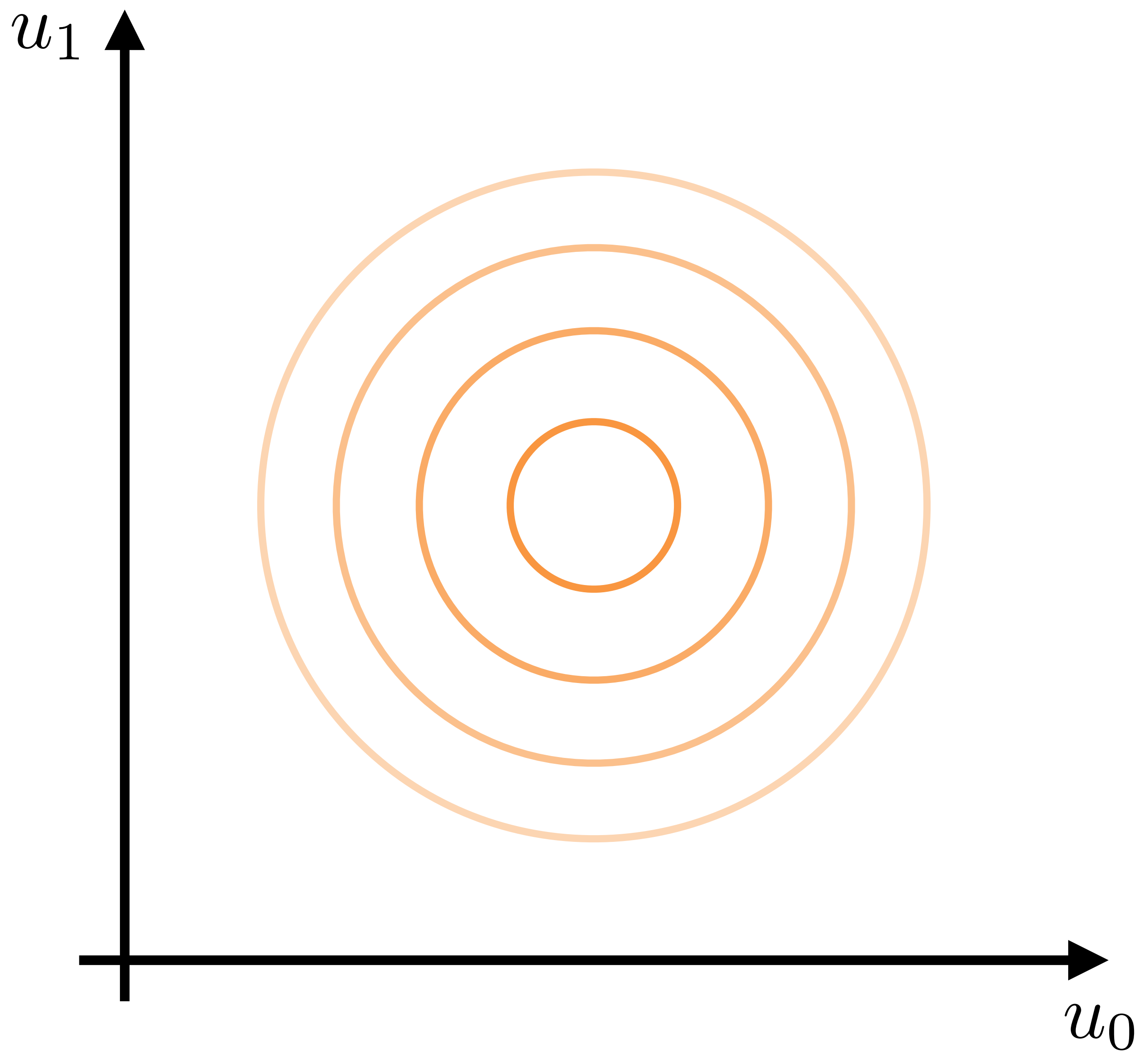
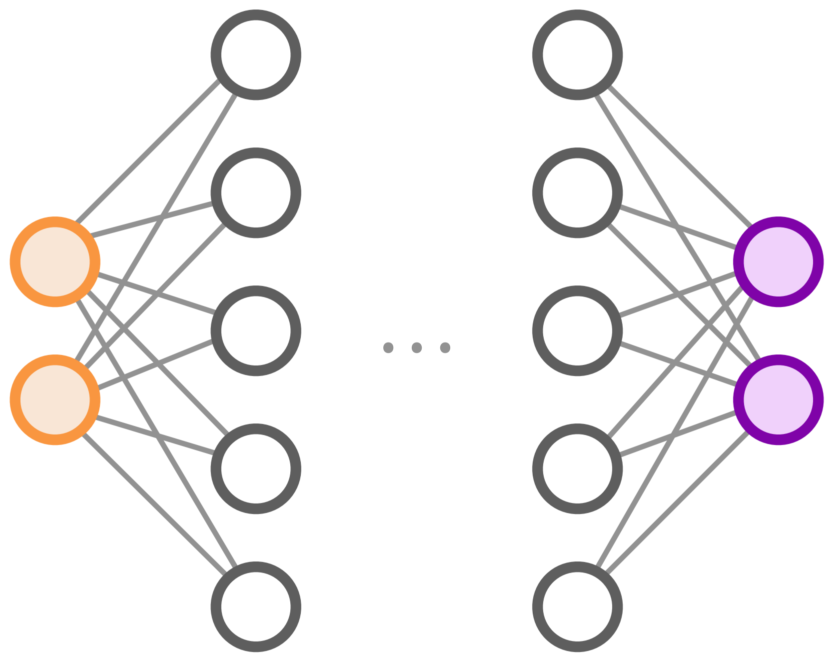
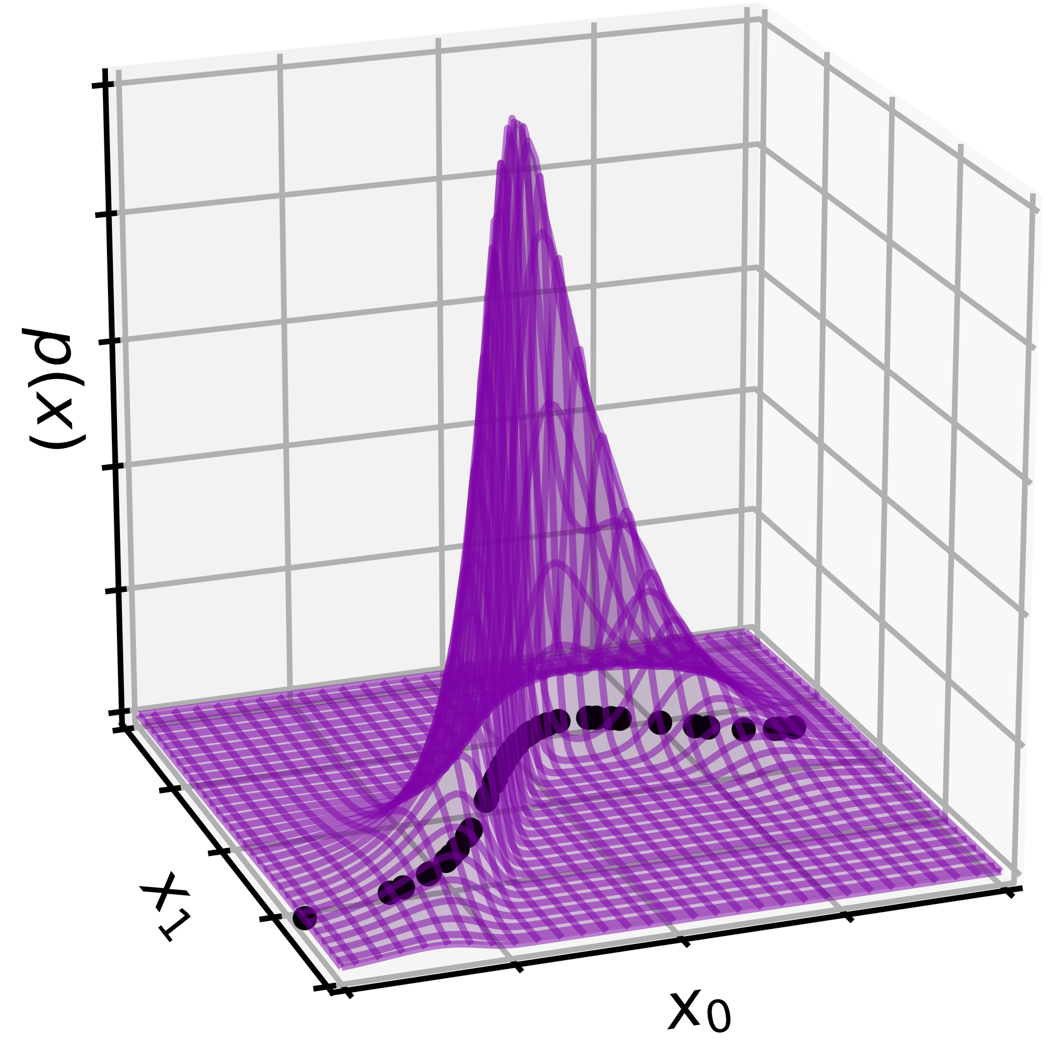


Normalizing flows in the ambient data space

[G. Papamakarios et al 1912.02762]







$u \sim p_u(u)$

f

x

d-dim. latent variables

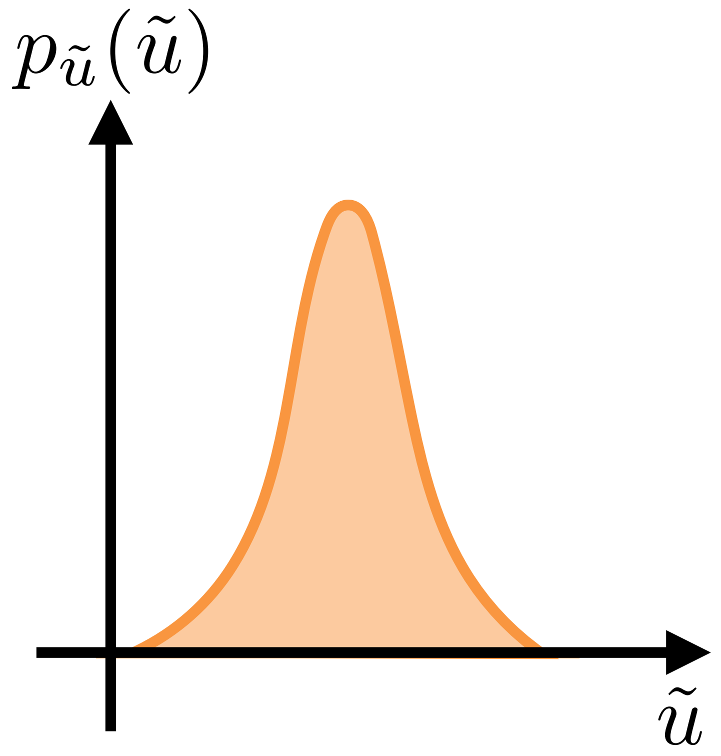
invertible NN

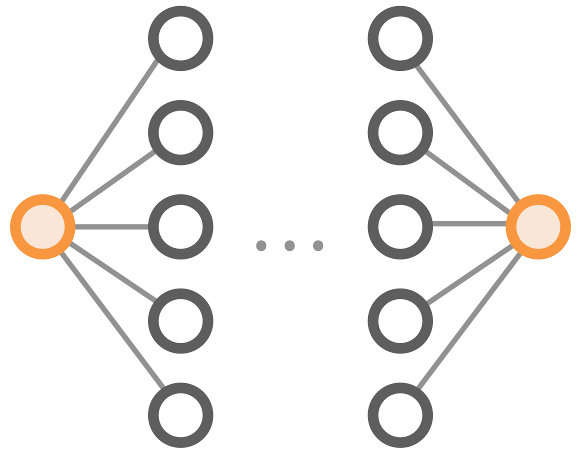
tractable density over ambient data space

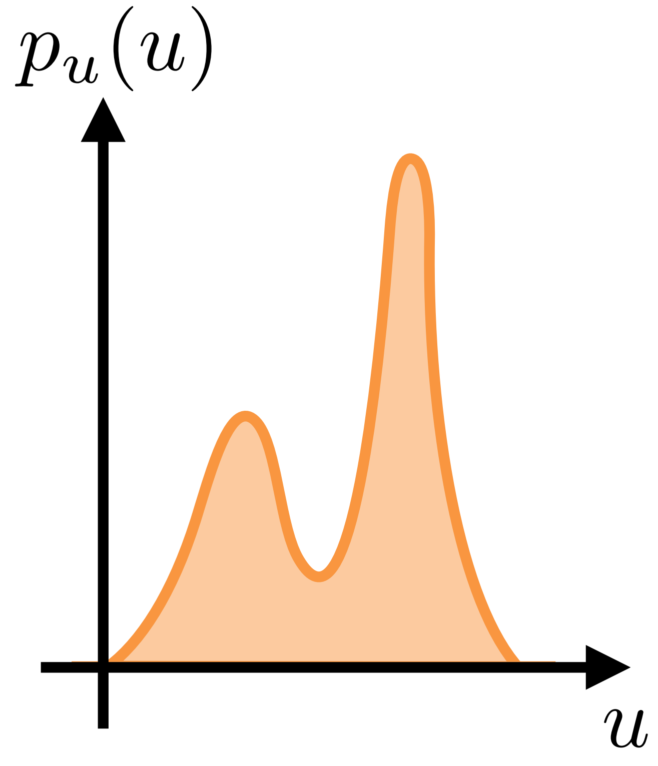
$$p_x(x) = p_u(f^{-1}(x))\ |\det J_f(f^{-1}(x))|^{-1}$$

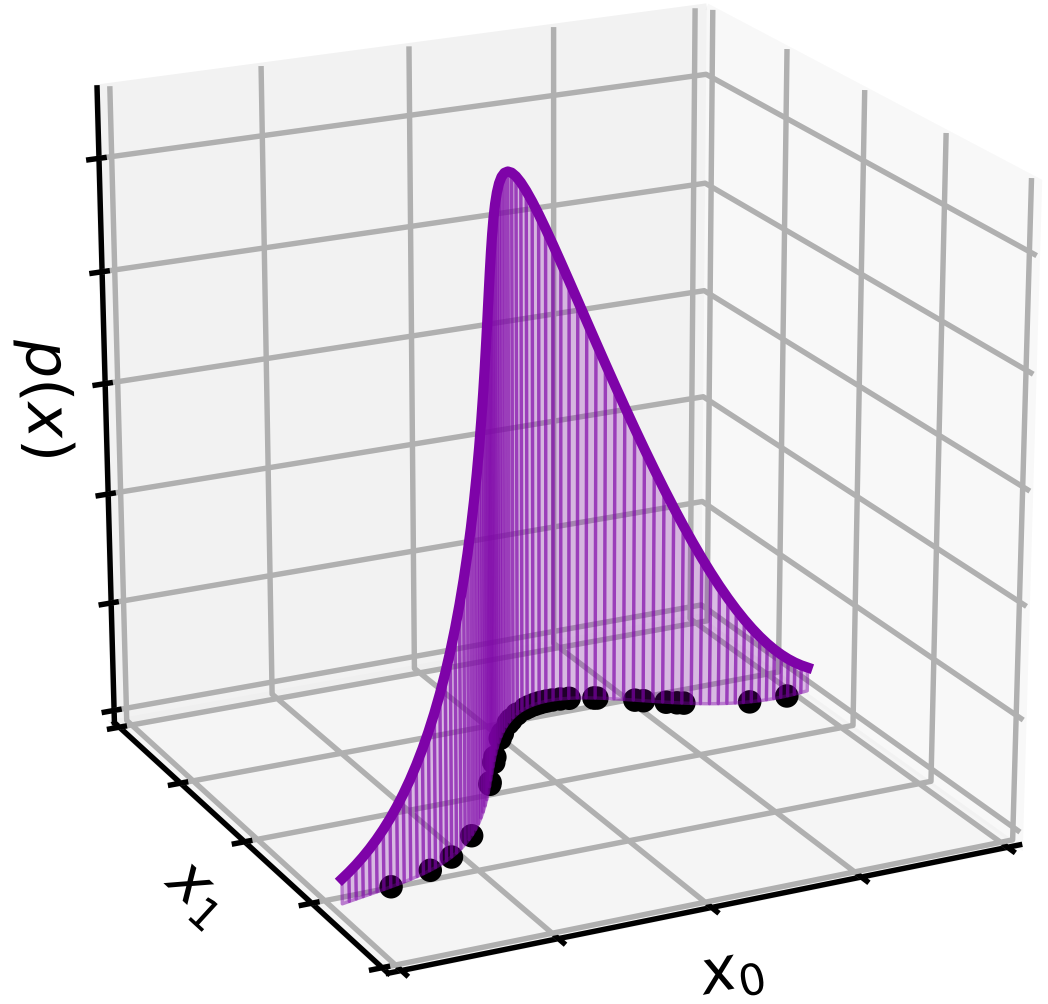
Flows on a prescribed manifold

[M. Gemici et al 1611.02304;
D. Rezende, …, M. Albergo, …, K. Cranmer 2002.02428]



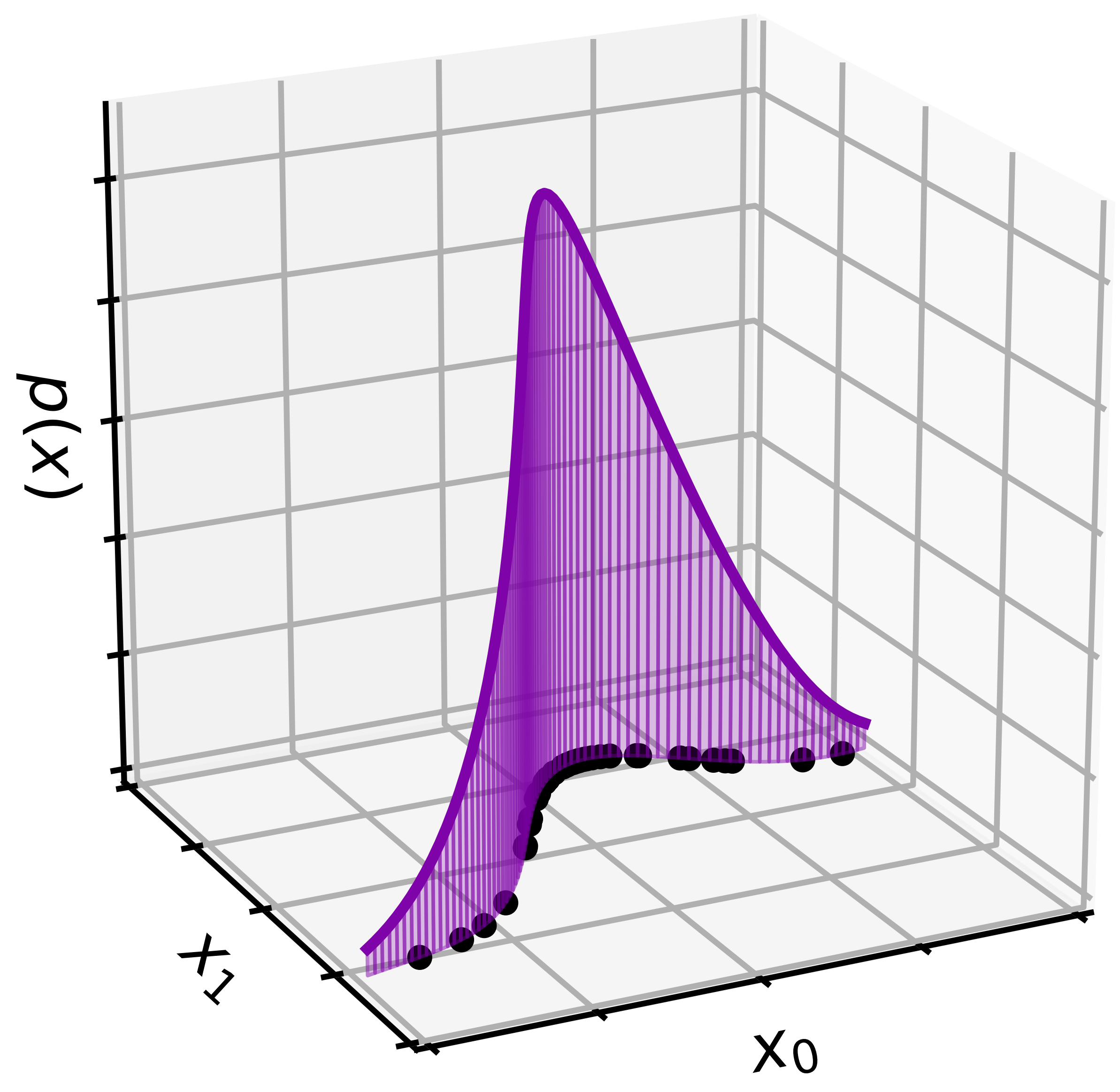






$\tilde{u} \sim p_{\tilde{u}}(\tilde{u})$	$\overset{}{\longleftrightarrow}$ h	u	$\longleftrightarrow$ g^*	x
n-dim. latents	invertible NN	n-dim. latents	prescribed chart	tractable density over $\mathcal{M}^*$

$$p_{\mathcal{M}^*}(x) = p_{\tilde{u}}(\tilde{u}) \; |\det J_h(\tilde{u})|^{-1} \cdot \left|\det[J_{g^*}^T(u) J_{g^*}(u)]\right|^{-\frac{1}{2}}$$



$\mathcal{M}$-flows

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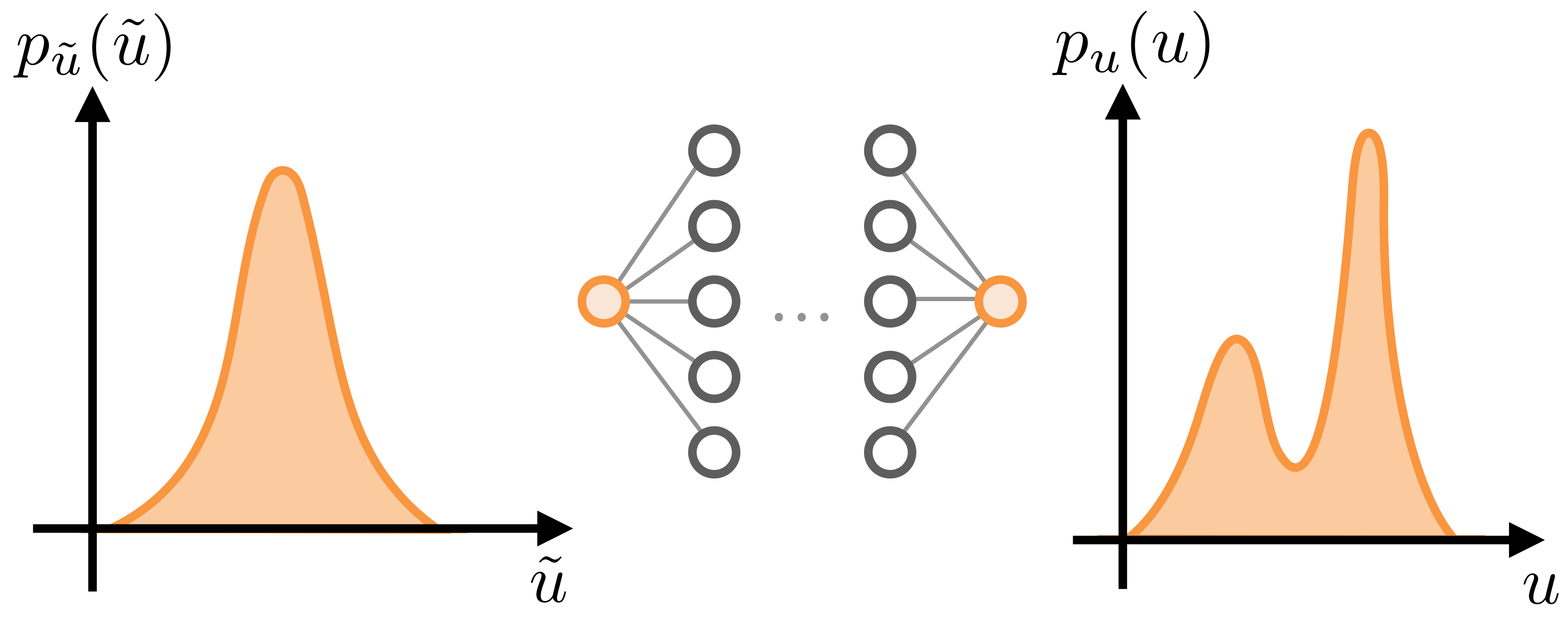

$\tilde{u} \sim p_{\tilde{u}}(\tilde{u})$ $\xleftrightarrow[h]{}$ u

n-dim. latents inv. NN n-dim. latents

$\mathcal{M}$-flows

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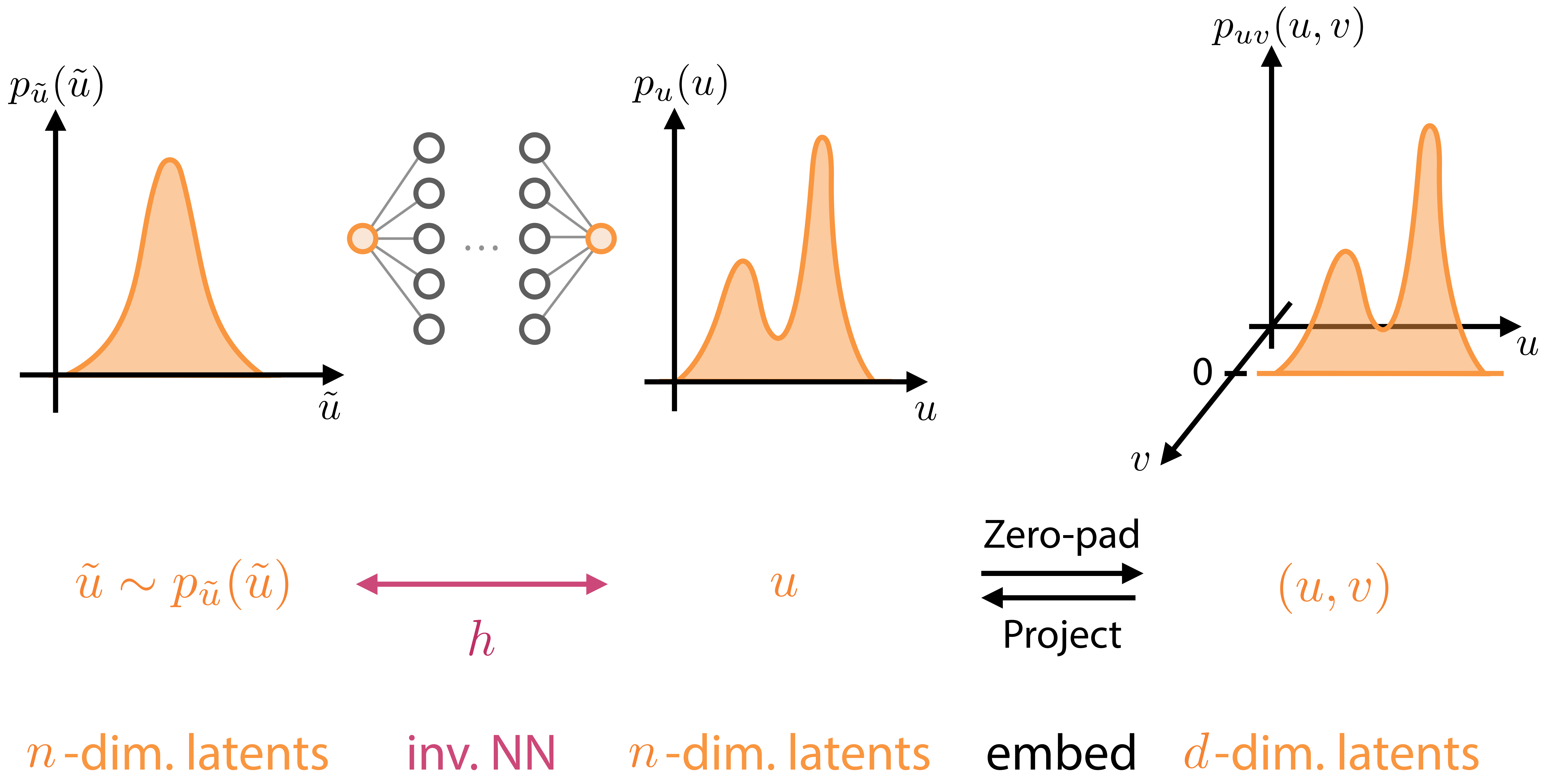

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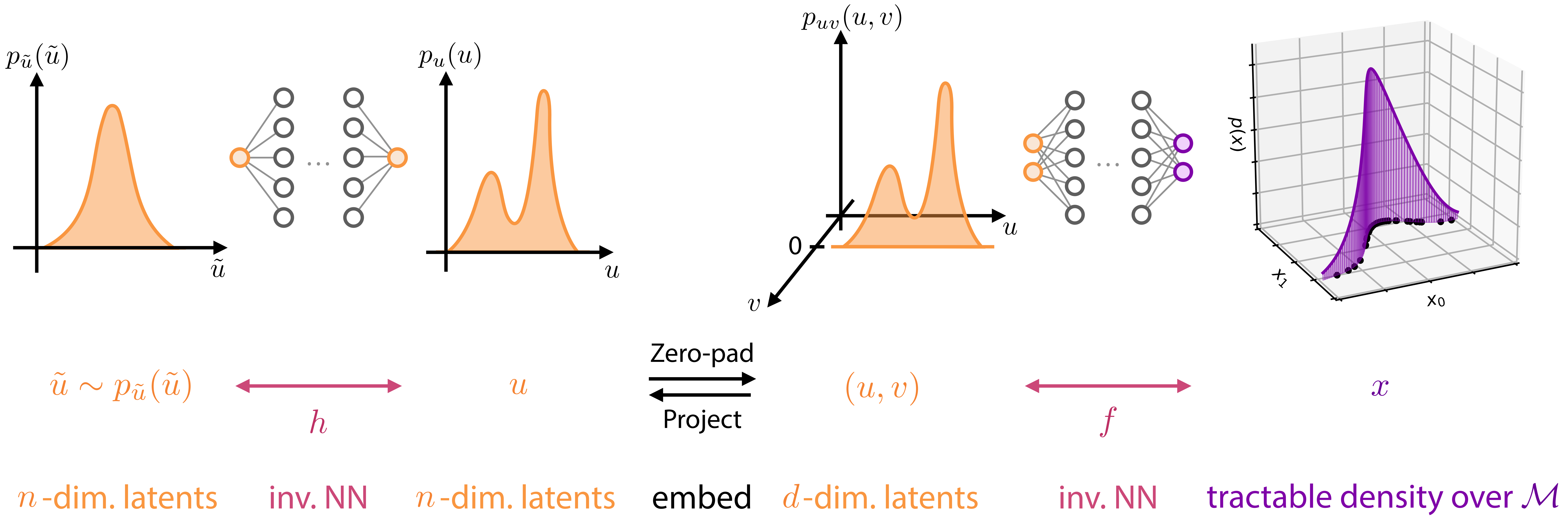
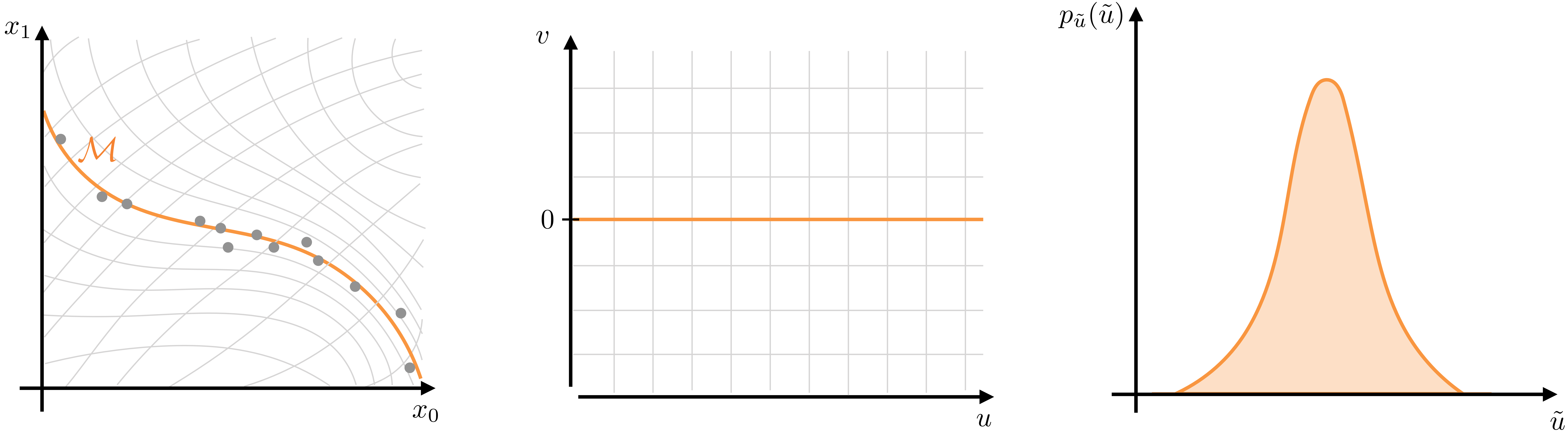


$$p_{\mathcal{M}}(x) = p_{\tilde u}(\tilde u)\,|\det J_h(\tilde u)|^{-1} \cdot \left|\det\left[\begin{pmatrix}\mathbb{1} & 0\end{pmatrix} J_f(u)^T J_f(u) \begin{pmatrix}\mathbb{1}\\ 0\end{pmatrix}\right]\right|^{-\frac{1}{2}}$$

Evaluating data on or off the manifold



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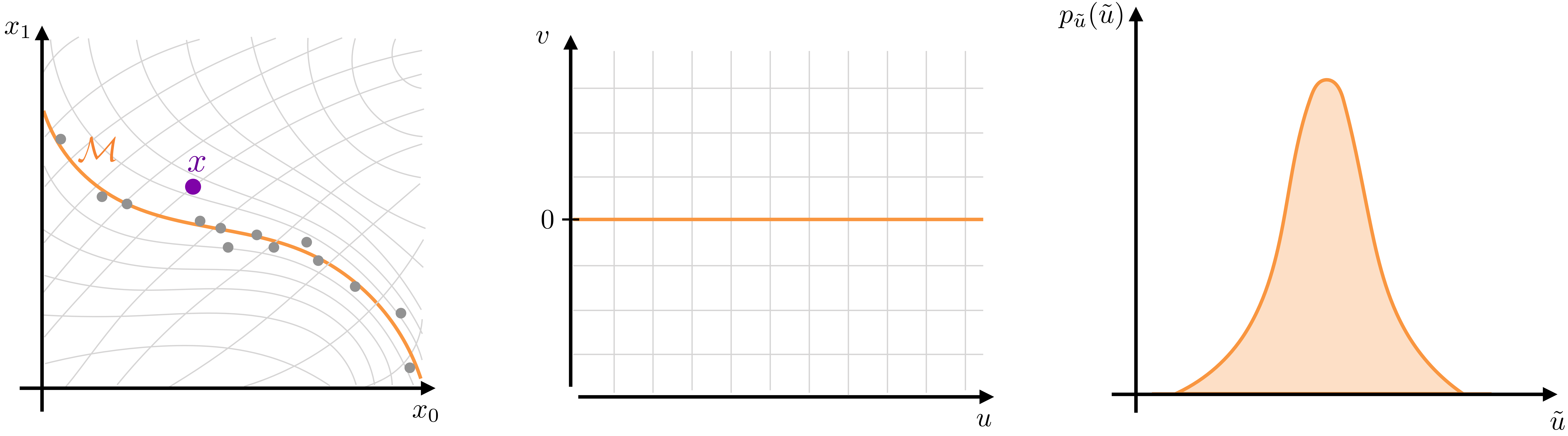

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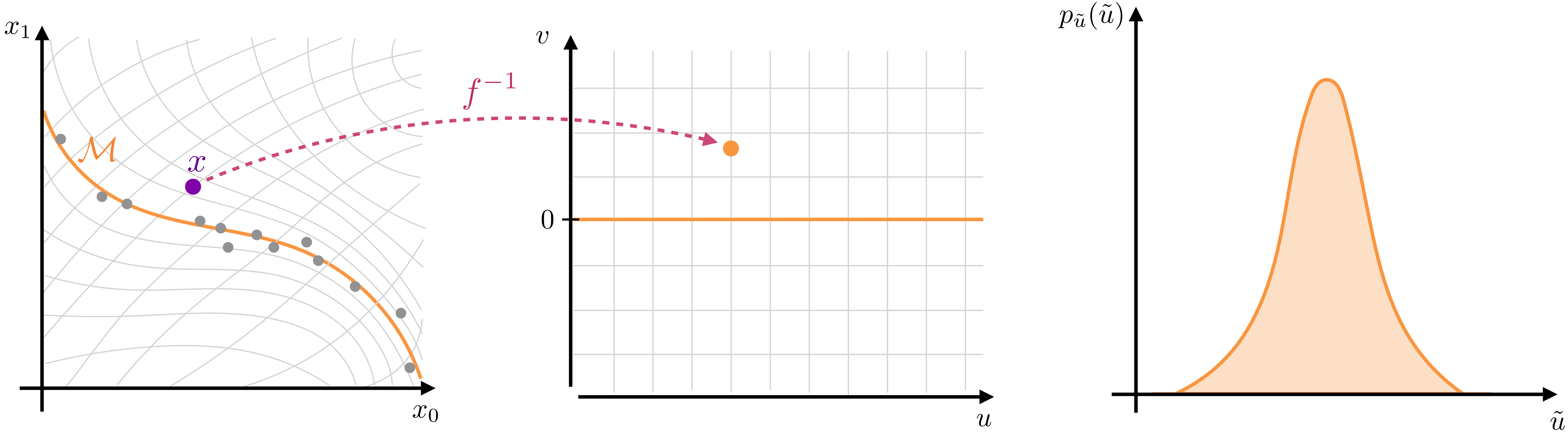

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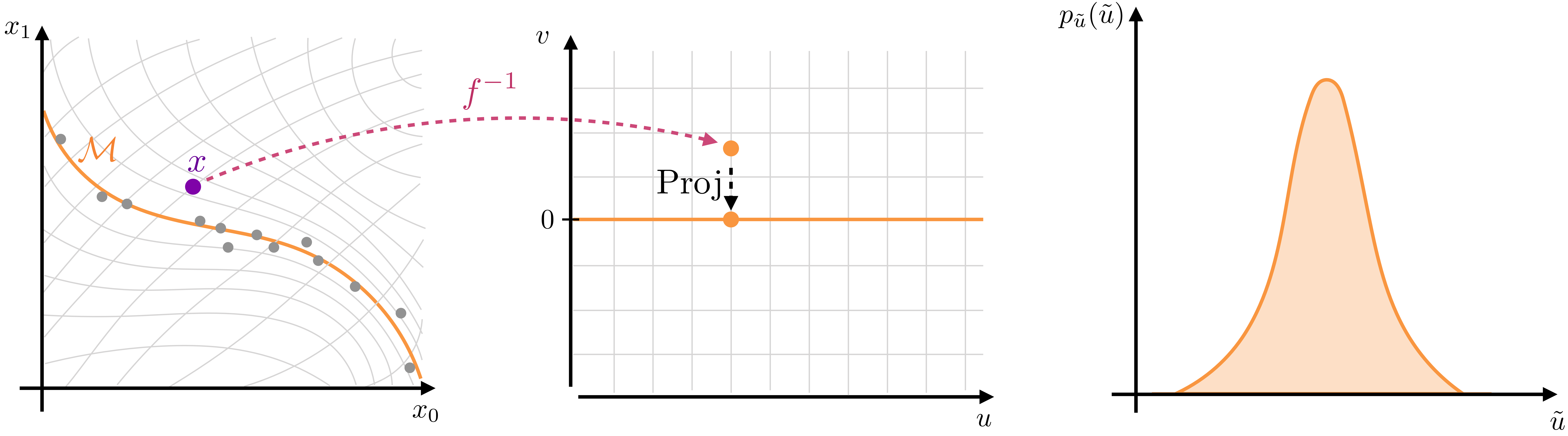

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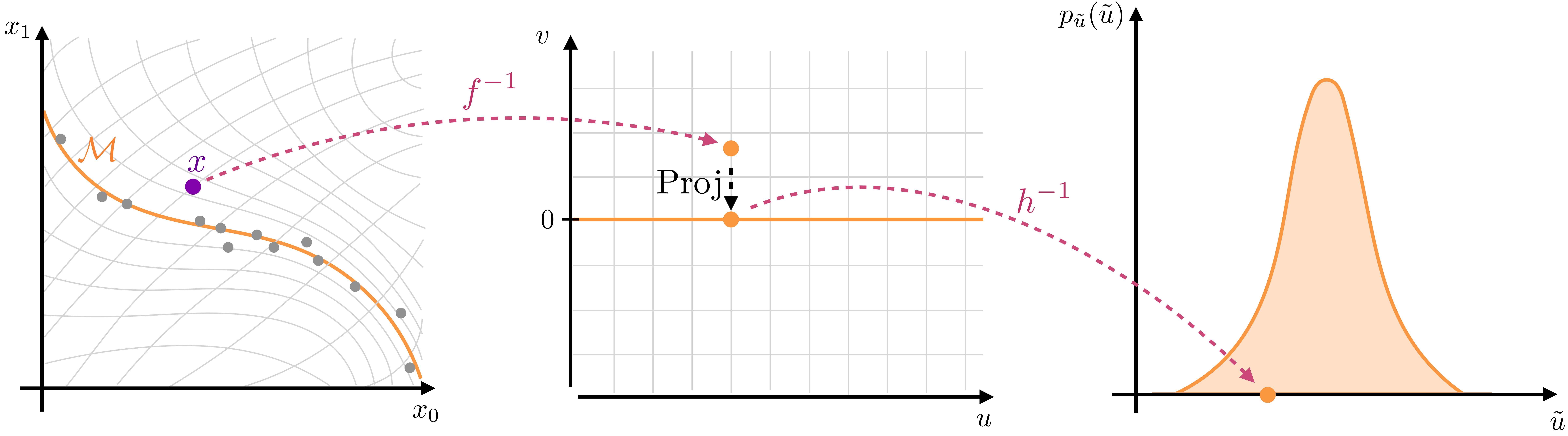

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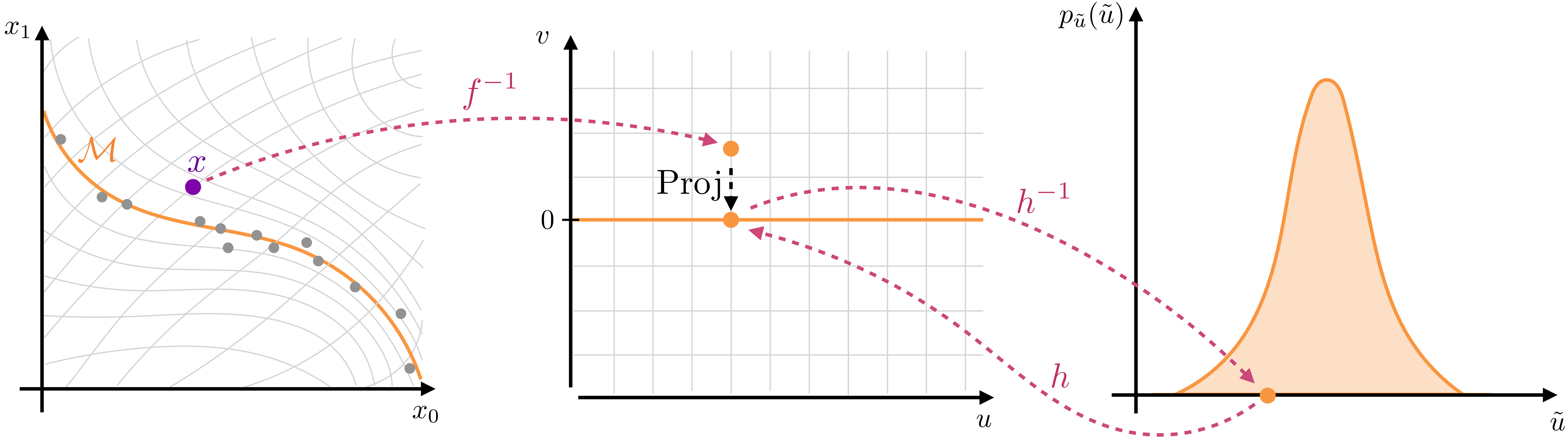

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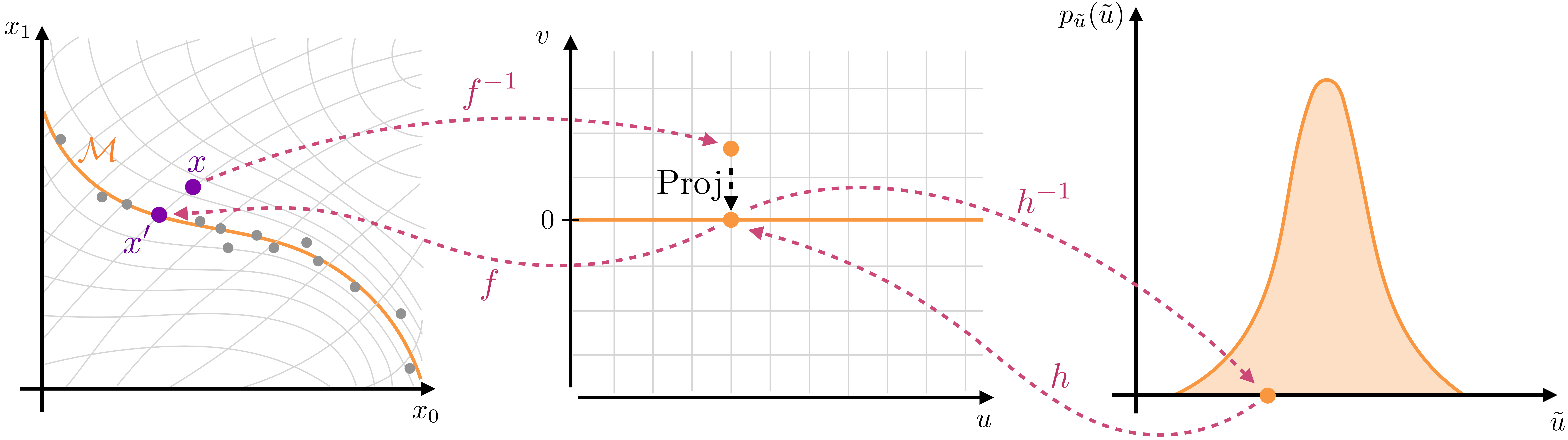

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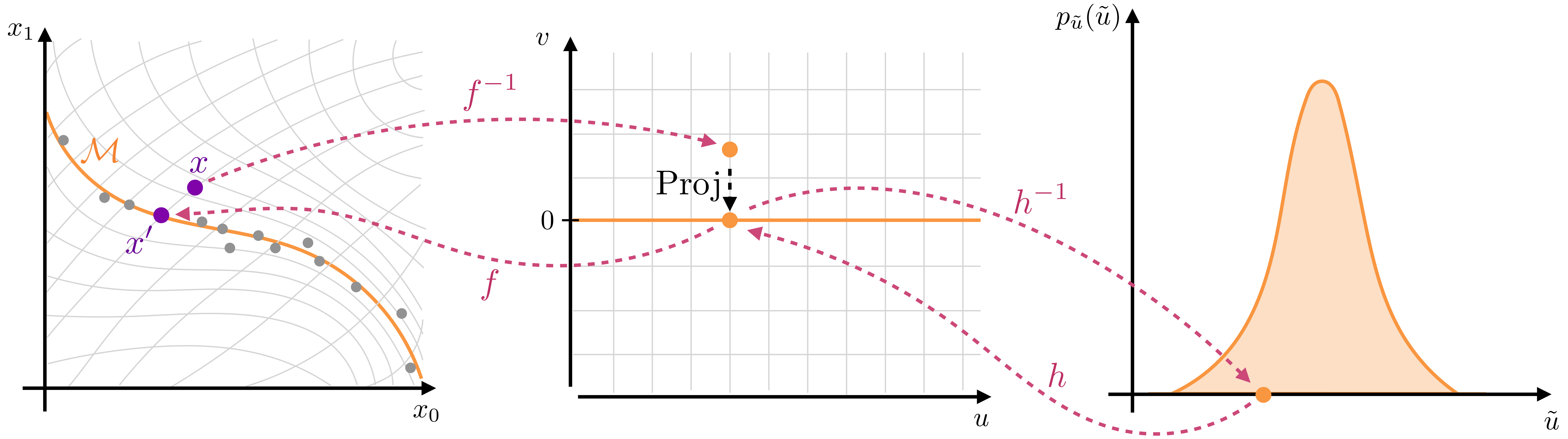


Input x	⇝ Representation $\tilde{u}$	(dimensionality reduction)
	⇝ Projection to manifold x'	(denoising)
	⇝ Reconstruction error $\|x - x'\|$	(training, OOD detection)
	⇝ Likelihood after projection $p_{\mathcal{M}}(x')$	(training, inference)

Related work

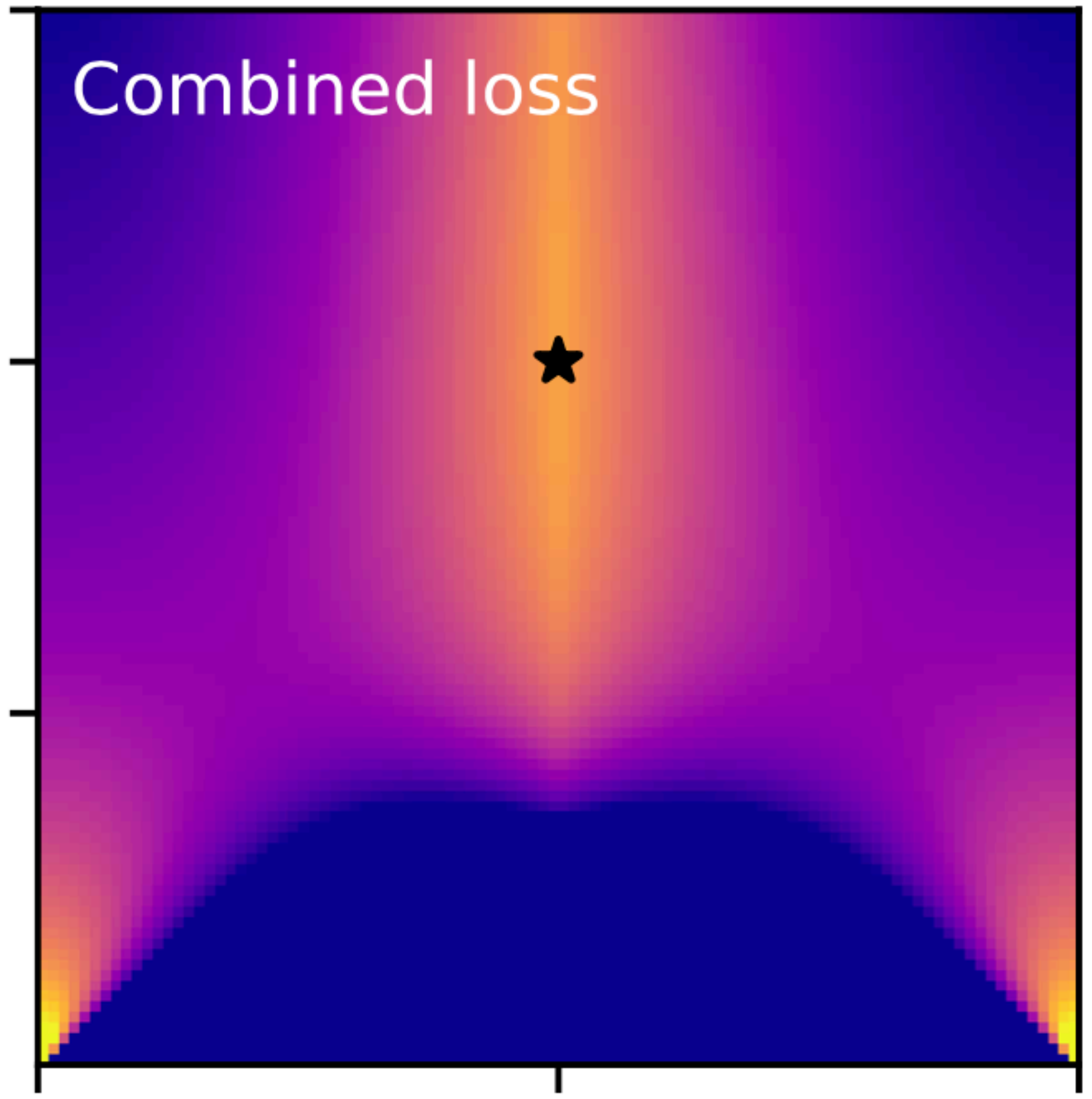
- Pseudo-Invertible Encoder (PIE):
  add "narrow" base density $p(v)$ for off-the-manifold latents,
  likelihood over ambient space (inconsistent with sampling)
  [J. J. Beitler, I. Sosnovik, A. Smeulders 2018]

- Probabilistic Auto-Encoder:
  classic autoencoder instead of flow f,
  likelihood intractable
  [V. Böhm, U. Seljak 2006.05479]

- Relaxed Injective Probability Flows:
  classic autoencoder + bounds on Jacobian,
  stochastic lower bound on likelihood
  [A. Kumar, B. Poole, K. Murphy 2002.08927]

Generative models vs. the data manifold

Model	Manifold	Chart	Generative	Tractable density	Restr. to manifold
Ambient flow (AF)	no	no	✓	✓	no
Flow on prescr. manifold	prescribed	prescribed	✓	✓	✓
GAN	learned	no	✓	no	✓
VAE	learned	no	✓	only ELBO	(no)
$\mathcal{M}$-flow	learned	learned	✓	✓ (potentially slow)	✓



Training $\mathcal{M}$-flows

Maximum likelihood is not enough

Likelihood defined after projection to $\mathcal{M}$,
which is defined through NN weights ϕ_f

Family of likelihoods $p_{\phi_f}(x|\phi_h)$
rather than one likelihood $p(x|\phi_f, \phi_h)$

$\Rightarrow$ Learning ϕ_f by maximum

likelihood is unstable

Maximum likelihood is not enough

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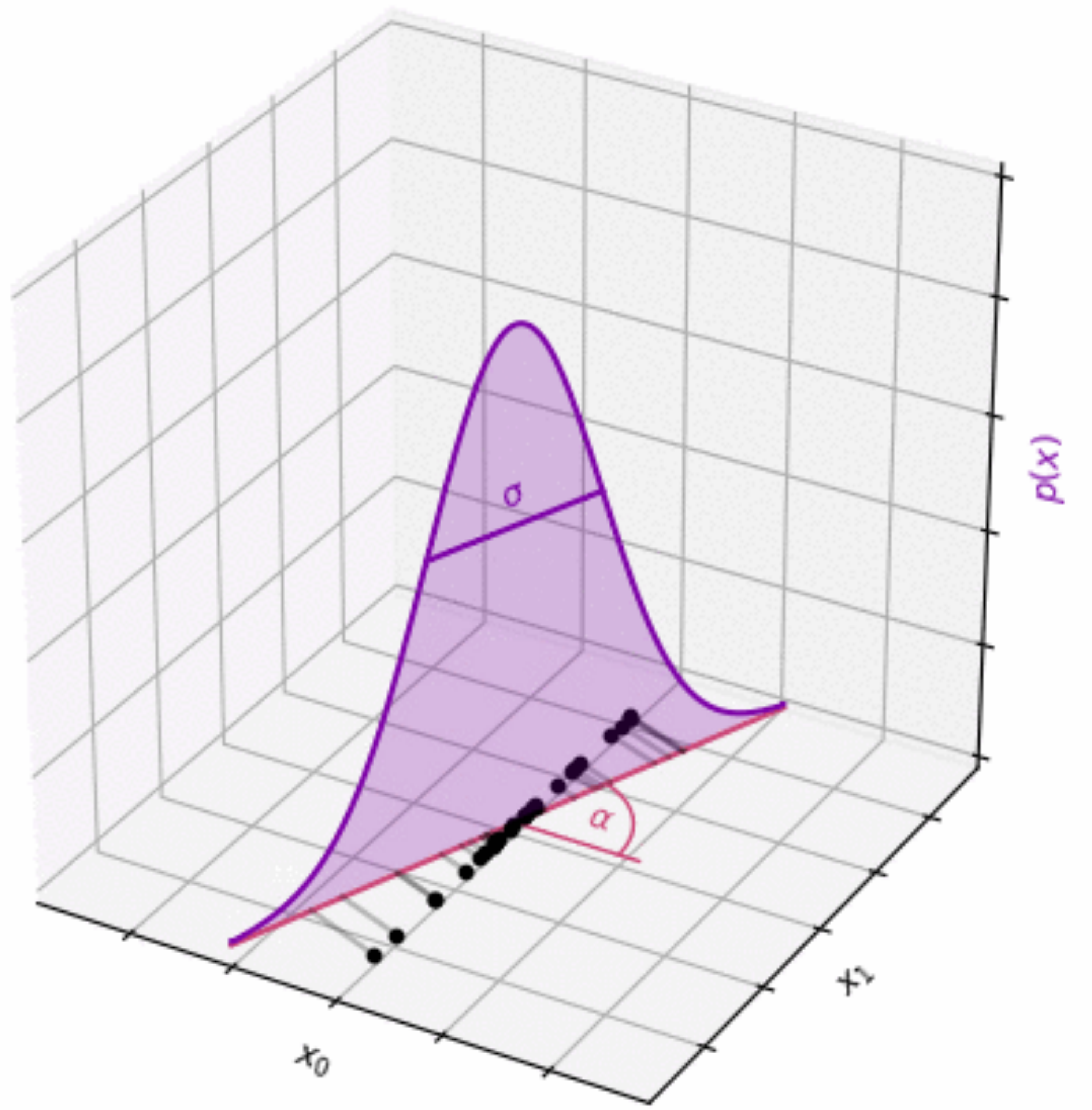

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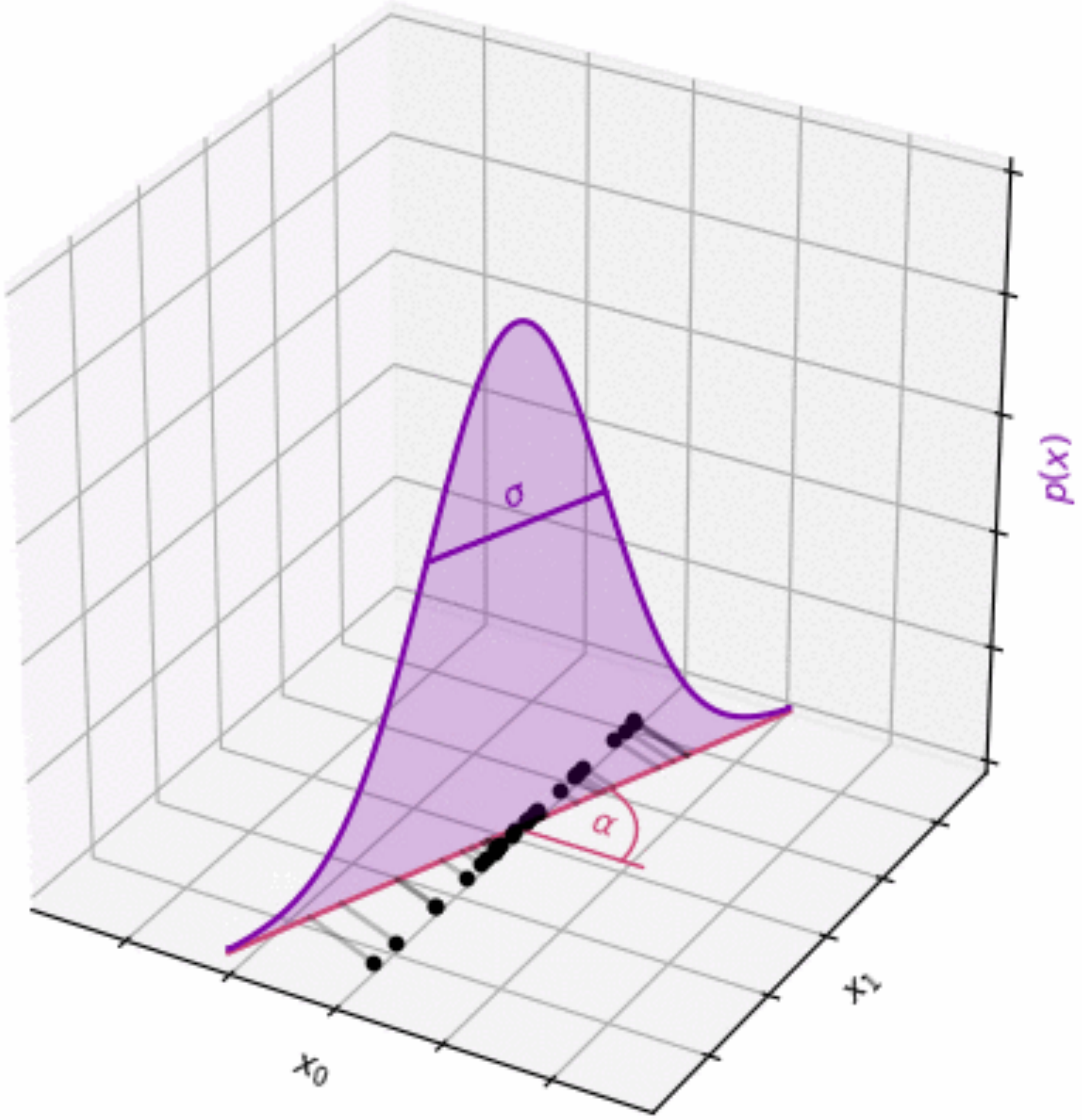
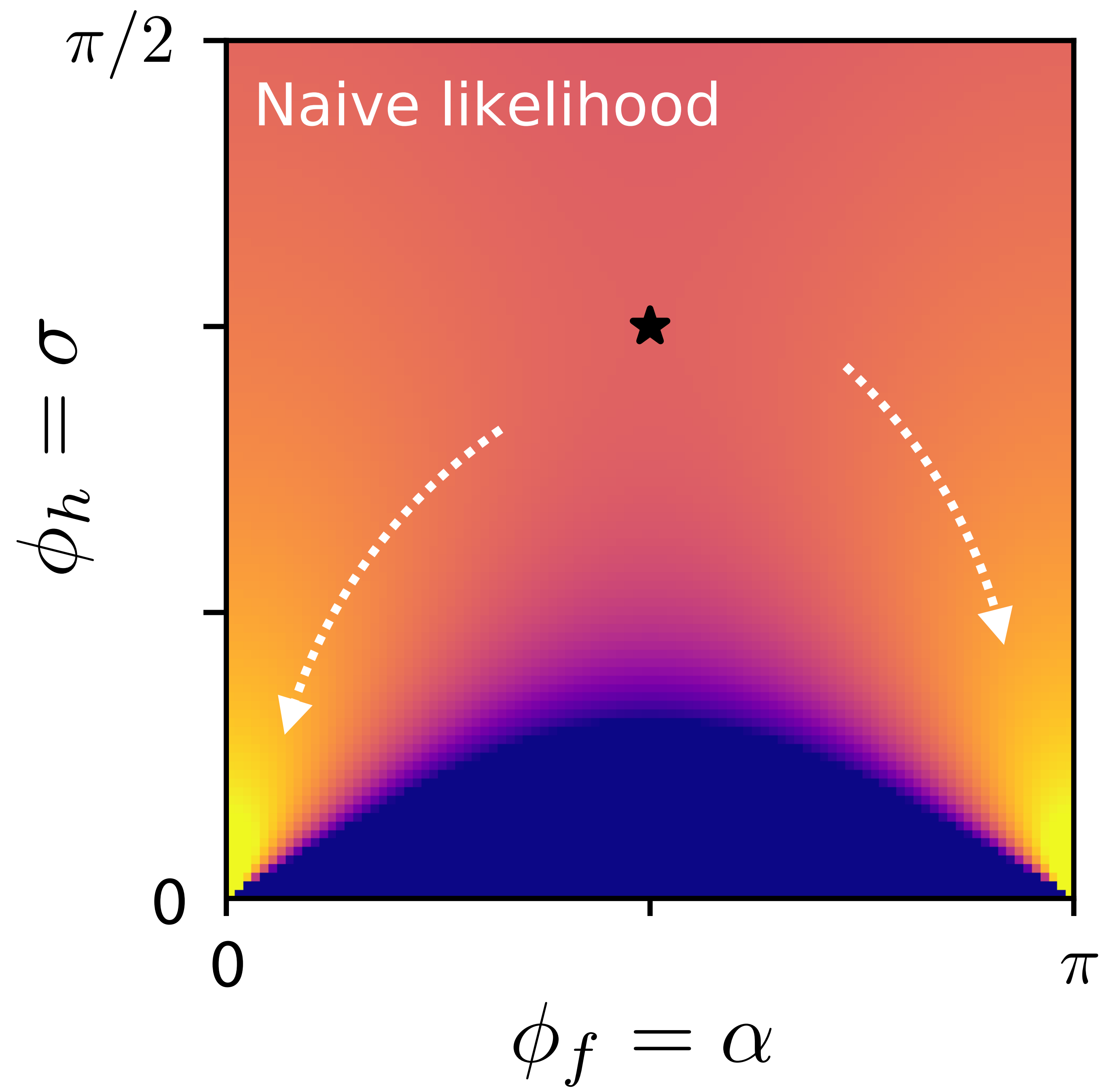
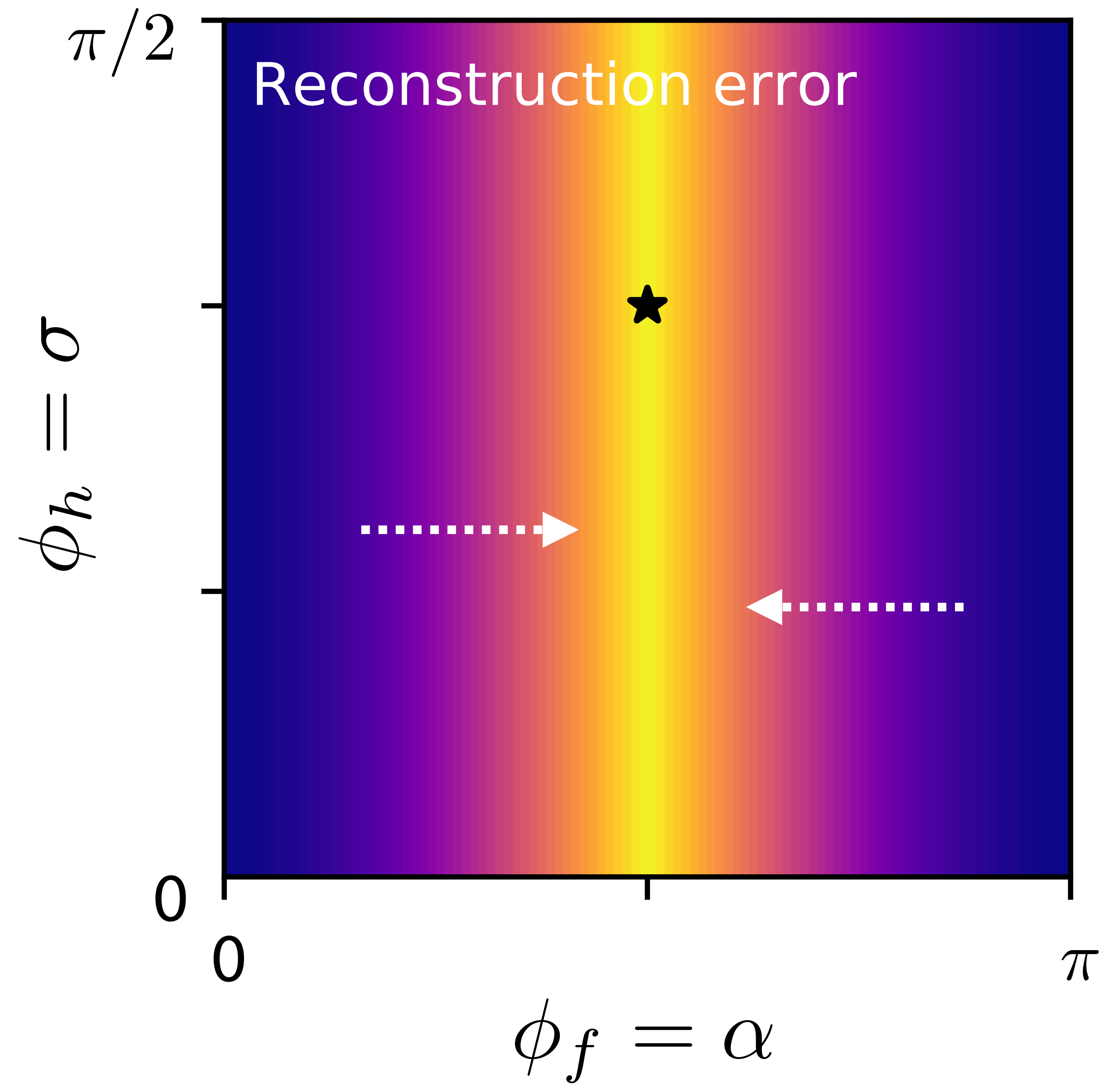




M/D training

Solution: separate training in two phases!

- Manifold phase:
  update ϕ_f (and thus $\mathcal{M}$) by minimizing $\|x - x'\|$



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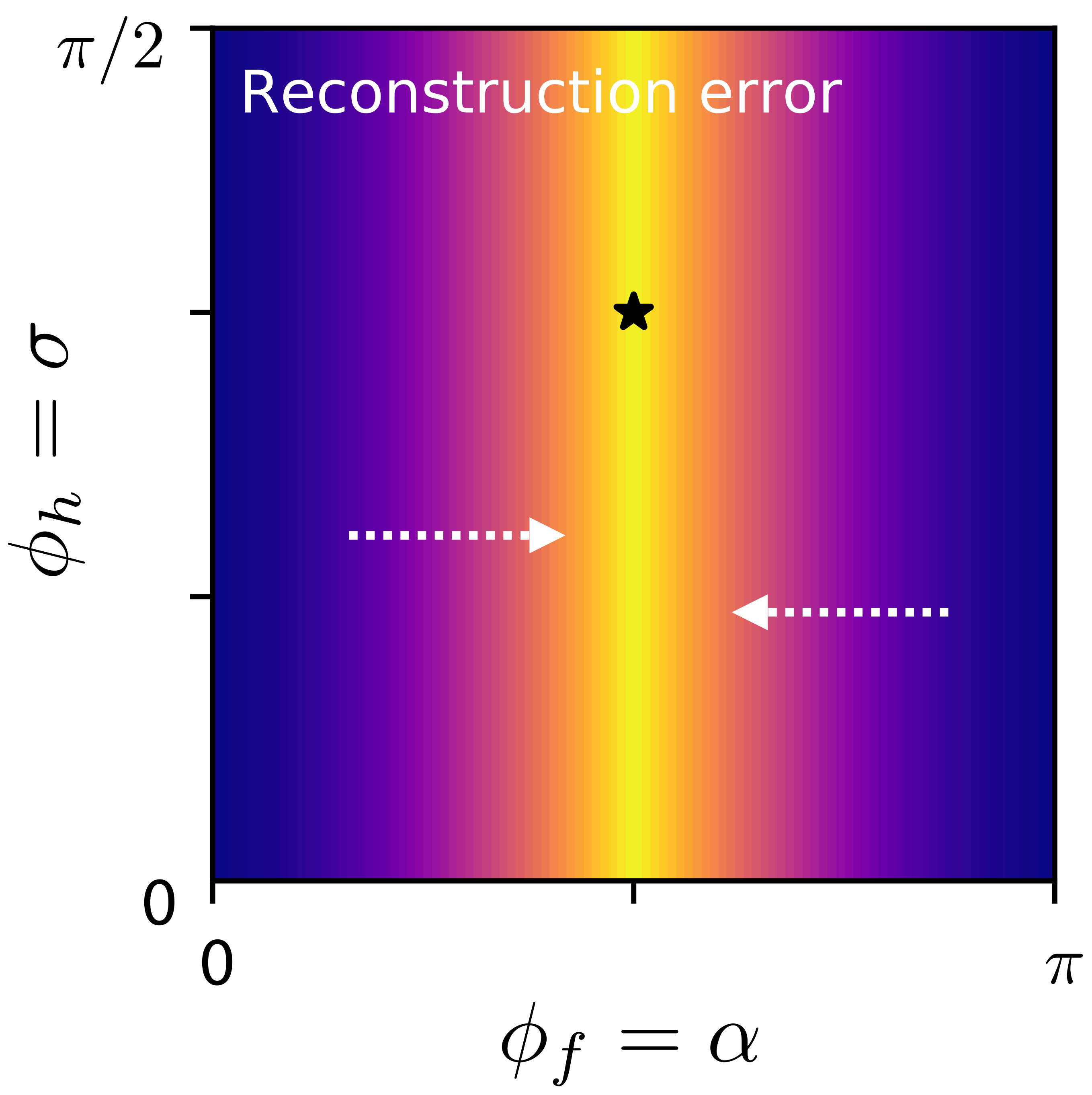
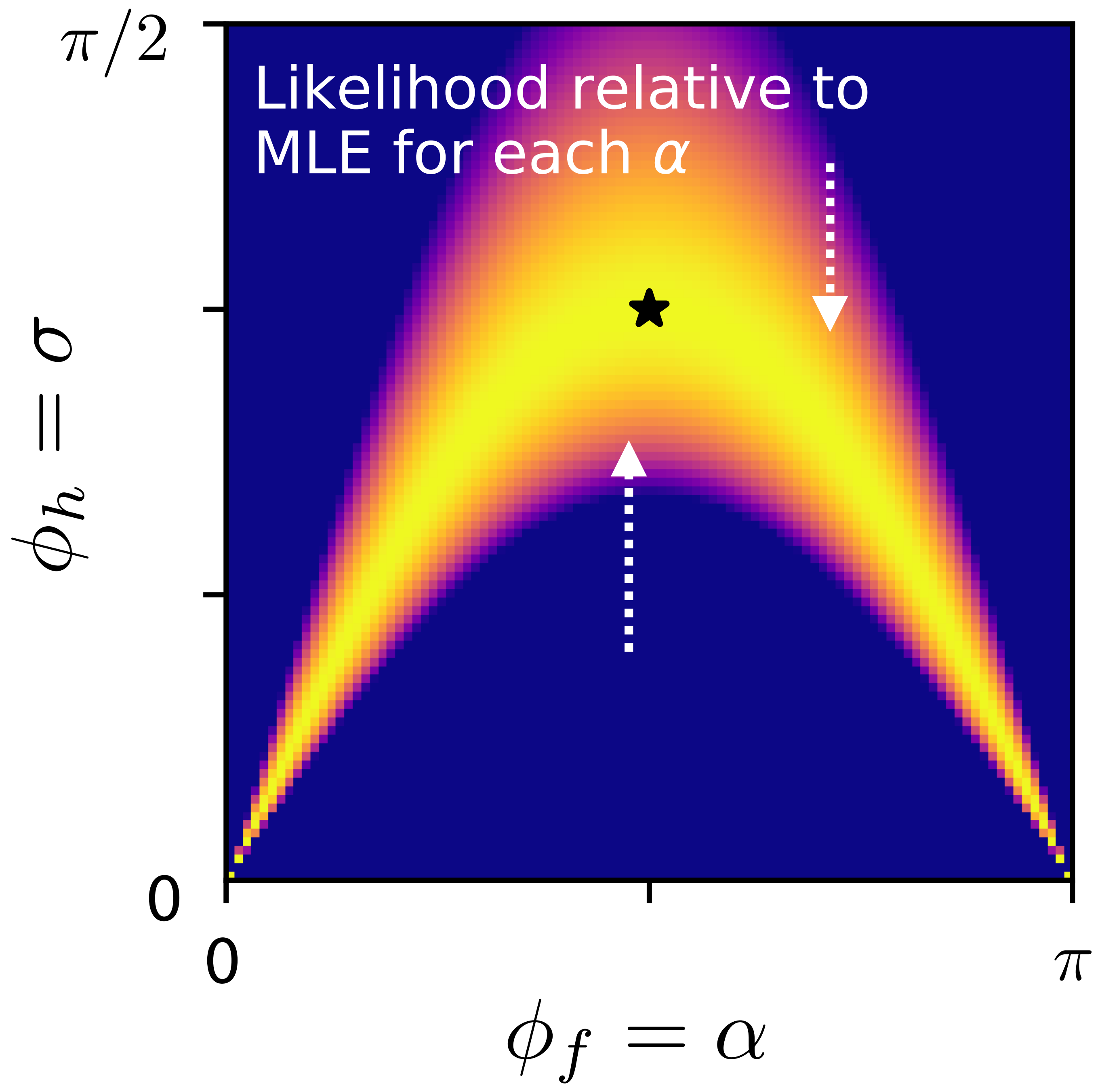


- Density phase:
  update ϕ_h (and thus $p_{\mathcal{M}}(x)$) by maximum likelihood (keeping $\mathcal{M}$ fixed)



A second problem… and an accidental solution

The likelihood becomes expensive to evaluate for high-dimensional x:

$$\log p_{\mathcal{M}}(x) = \log p_{\tilde{u}}(h^{-1}(u)) - \log\det J_h(h^{-1}(u)) - \frac{1}{2}\log \det \left[(\mathbb{1}\ 0)\, J_f^T(u)\, J_f(u) \begin{pmatrix} \mathbb{1} \\ 0 \end{pmatrix} \right]$$

Cannot separate determinant of product of non-square matrices

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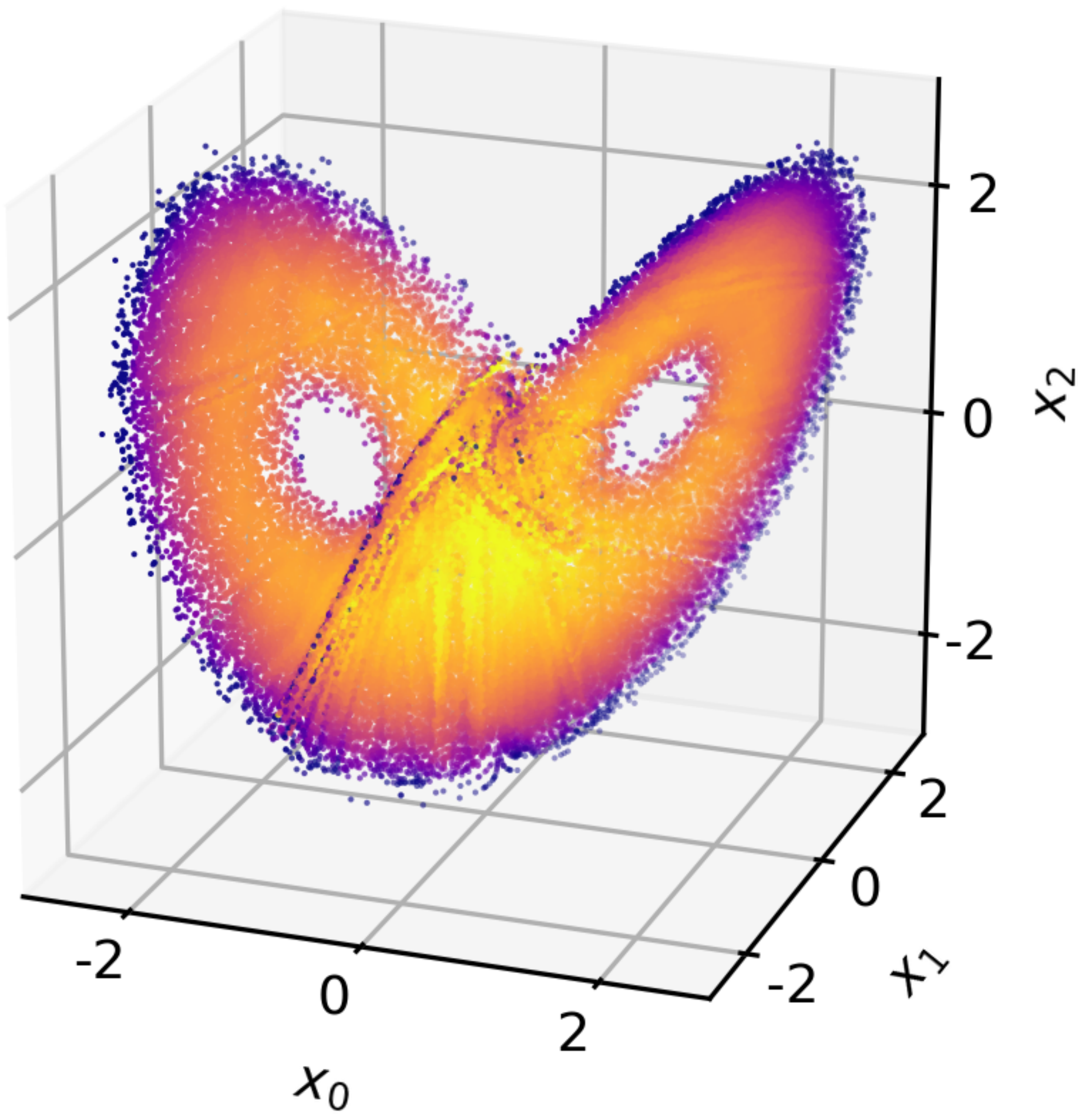
Cannot separate determinant of product of non-square matrices

M/D training sidesteps this problem: density phase only requires gradient

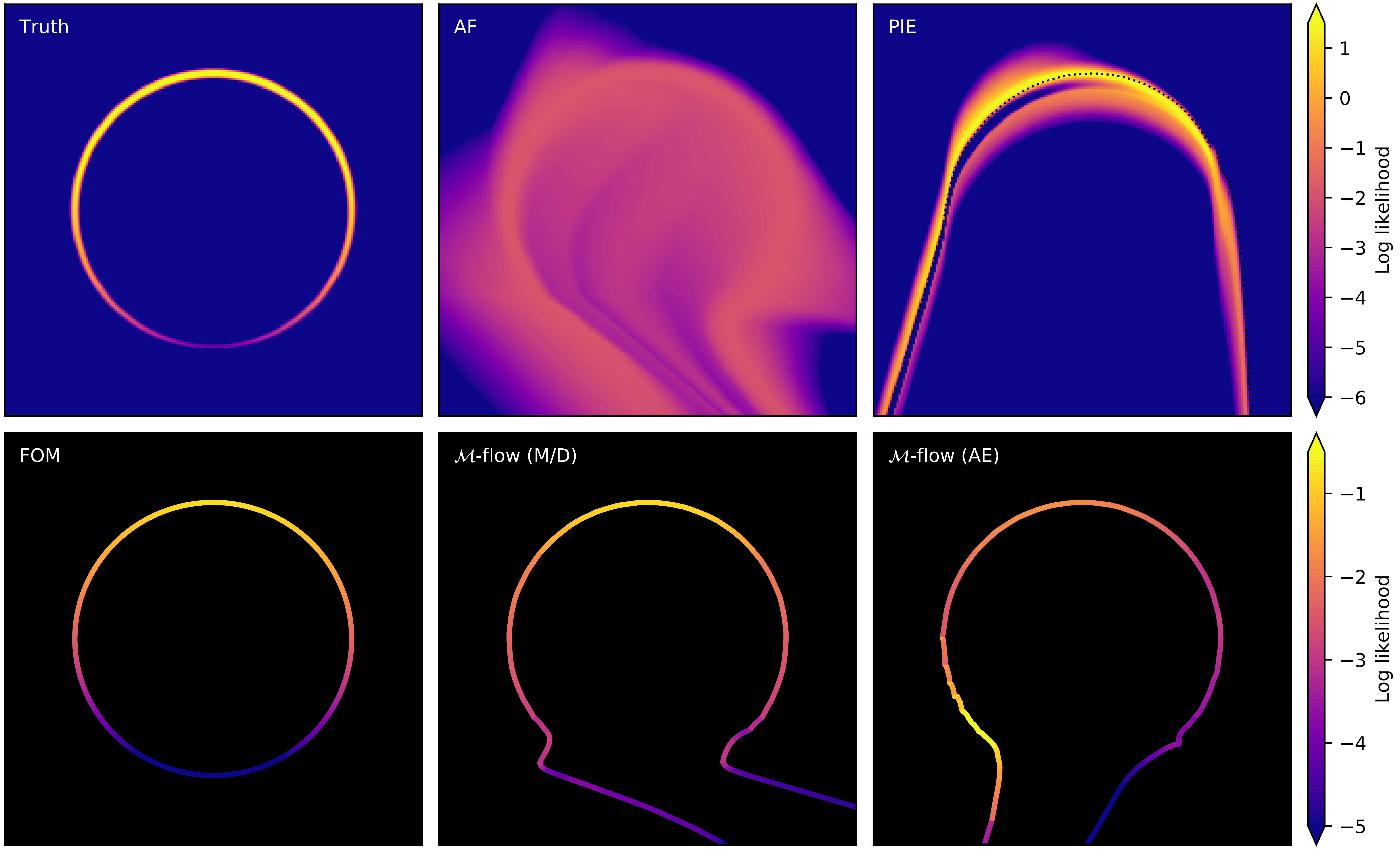
$$\nabla_{\phi_h}\left(\log p_{\mathcal{M}}(x)\right) = \nabla_{\phi_h}\left(\log p_{\tilde{u}}(h^{-1}(u))\right) - \nabla_{\phi_h}\left(\log\det J_h(h^{-1}(u))\right) - \underbrace{\nabla_{\phi_h}\frac{1}{2}\log\det\left[\begin{pmatrix}\mathbb{1} & 0\end{pmatrix} J_f^T(u)\, J_f(u)\begin{pmatrix}\mathbb{1}\\ 0\end{pmatrix}\right]}_{=0},$$

which can be computed efficiently!

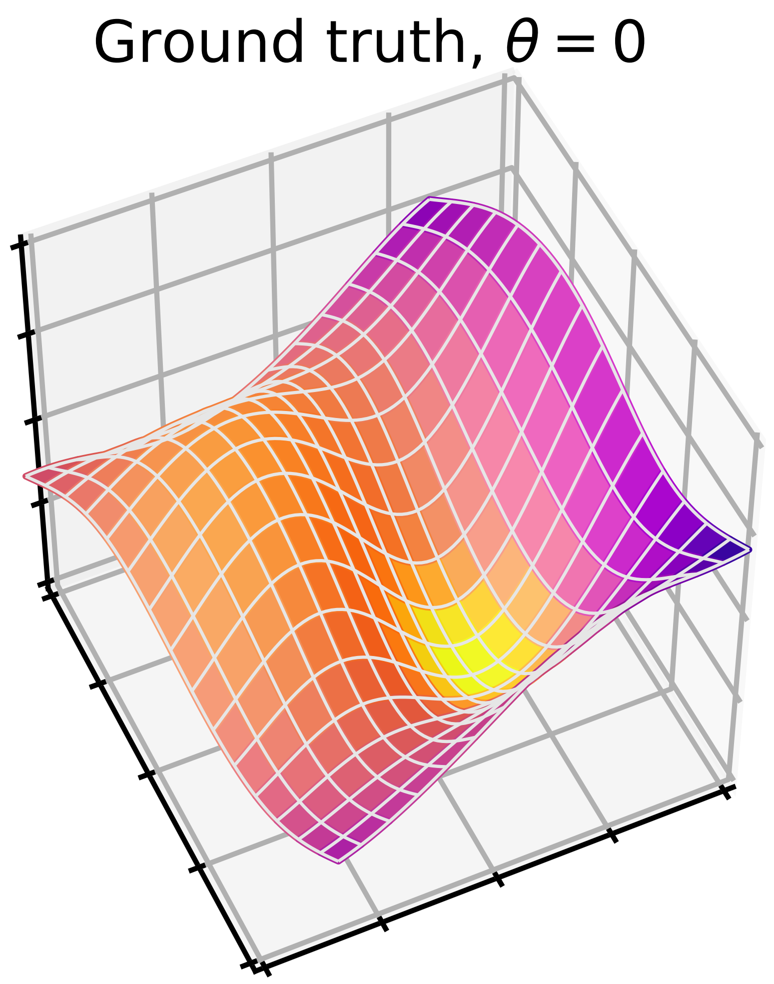


Experiments

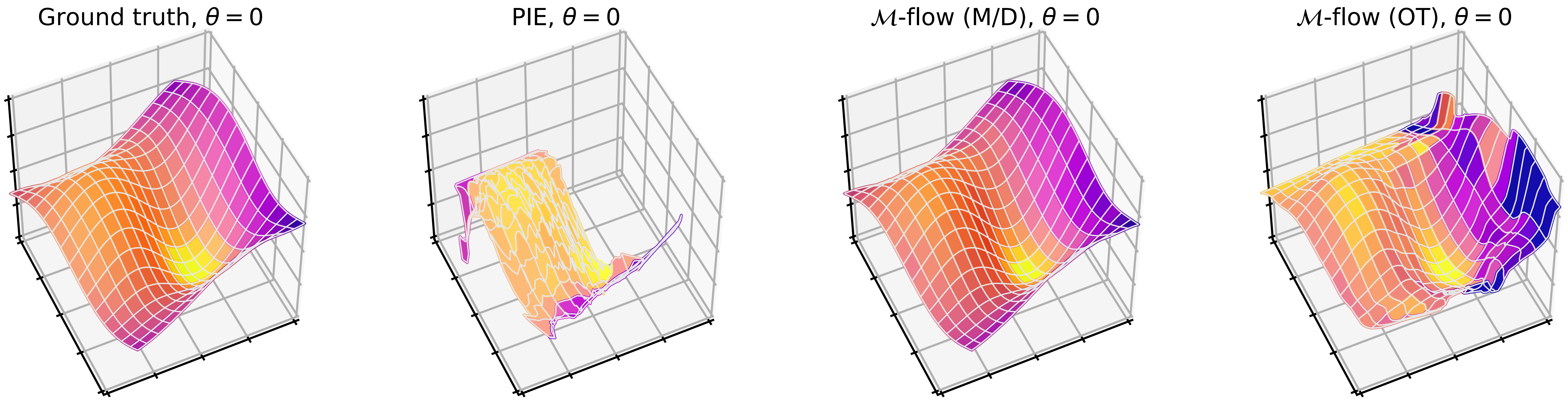
Gaussian on a circle



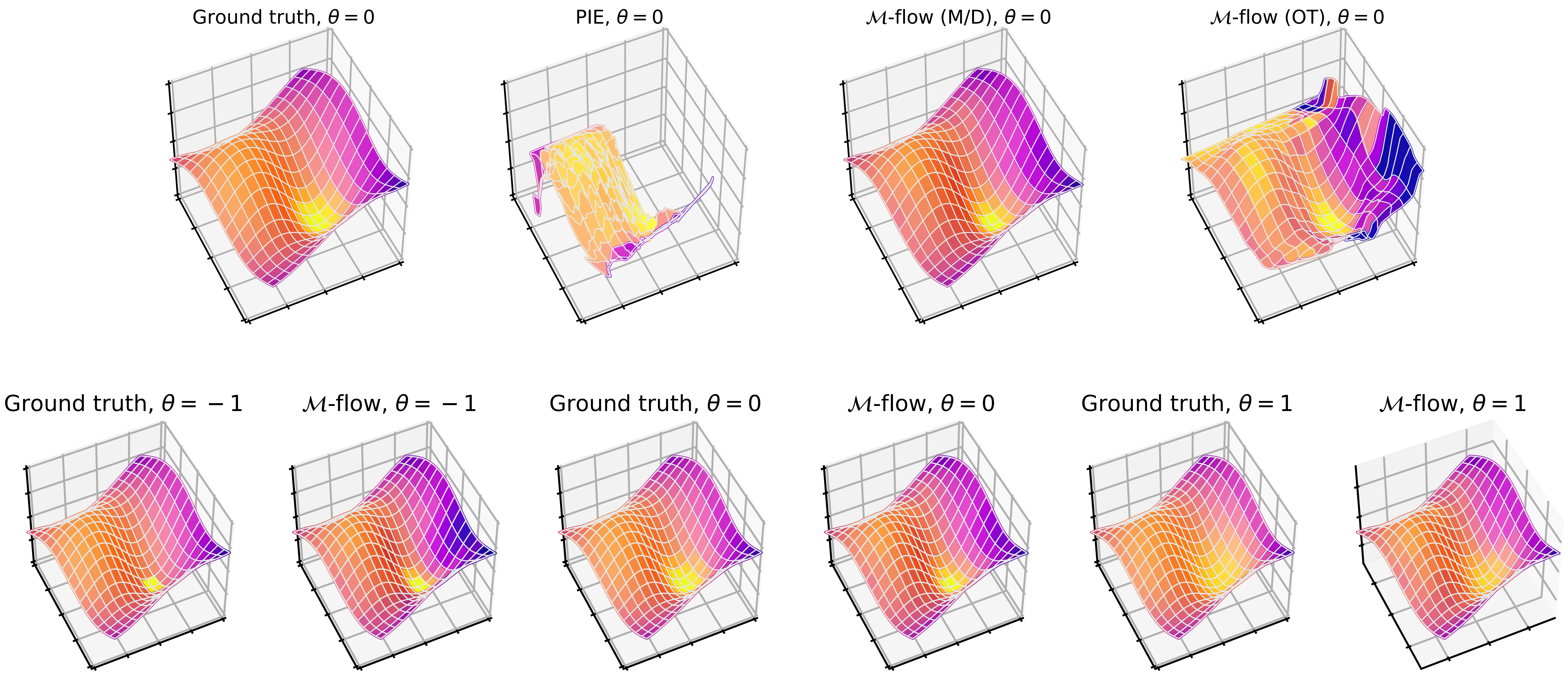
Mixture model on a polynomial surface



Mixture model on a polynomial surface

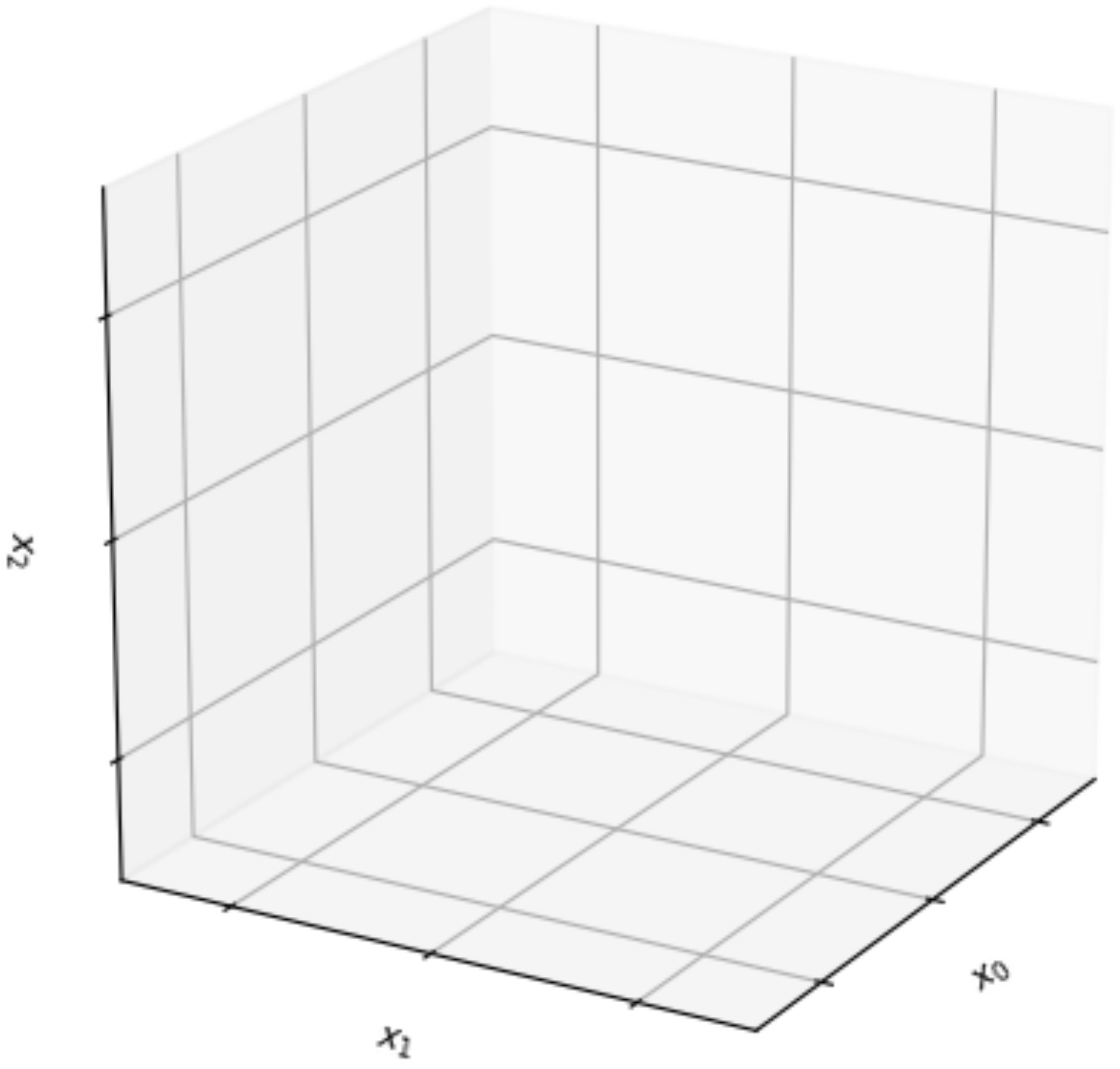


Mixture model on a polynomial surface



Lorenz attractor

[E. Lorenz 1963]



$$\frac{\mathrm{d}x_0}{\mathrm{d}t} = \sigma(x_1 - x_0)\,, \quad \frac{\mathrm{d}x_1}{\mathrm{d}t} = x_0(\rho - x_2) - x_1\,, \quad \frac{\mathrm{d}x_2}{\mathrm{d}t} = x_0 x_1 - \beta x_2\,.$$

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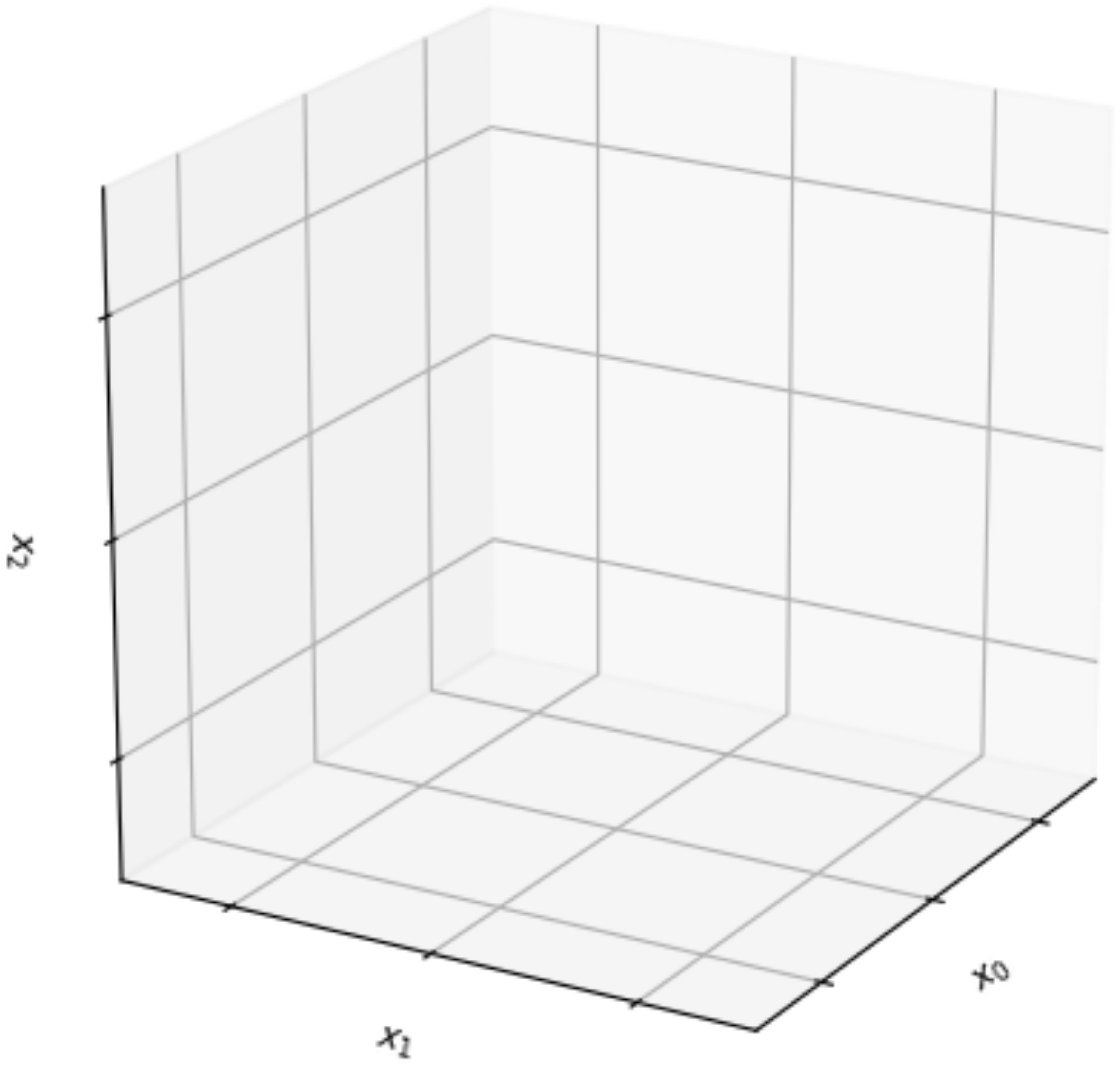

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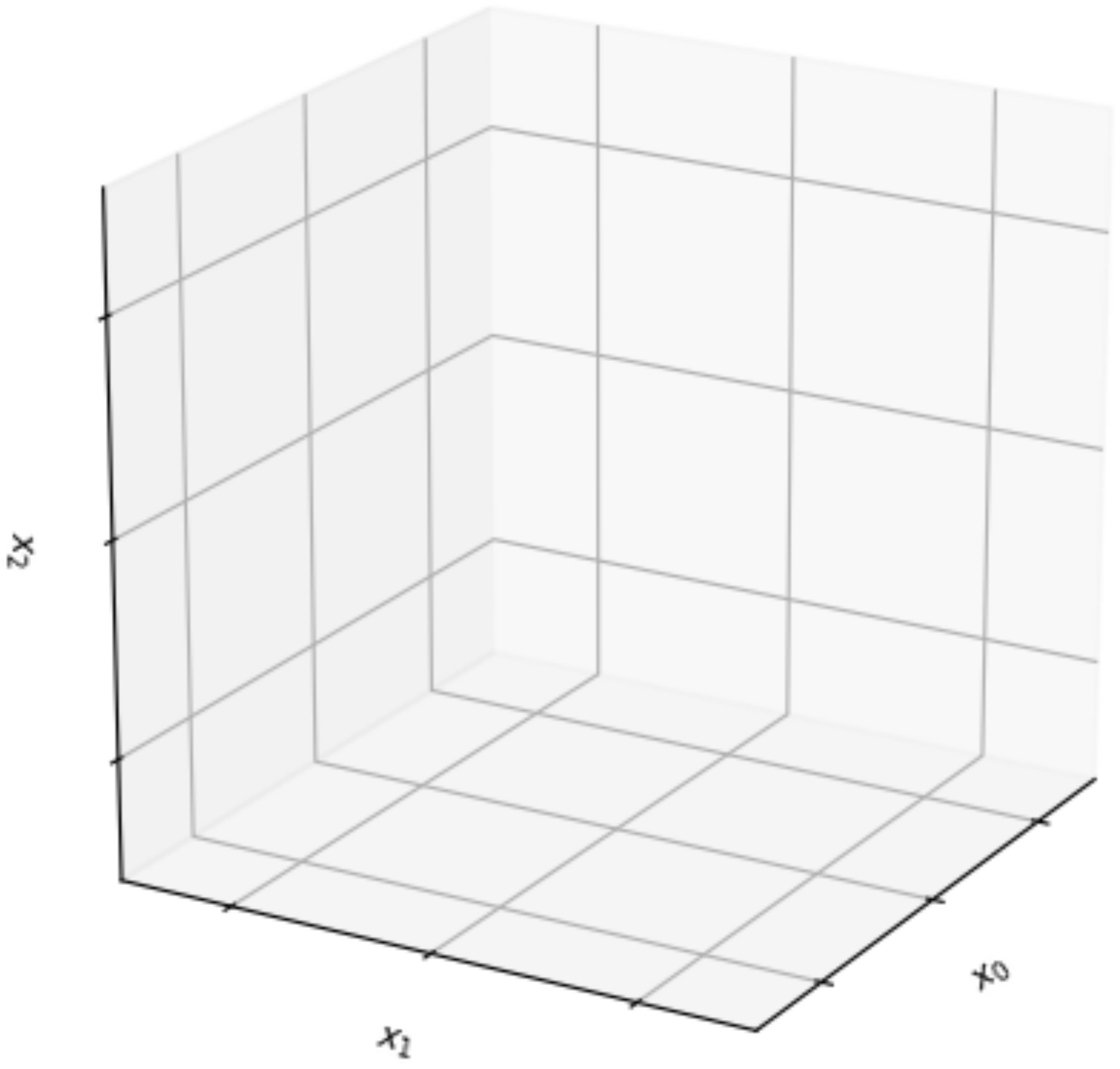

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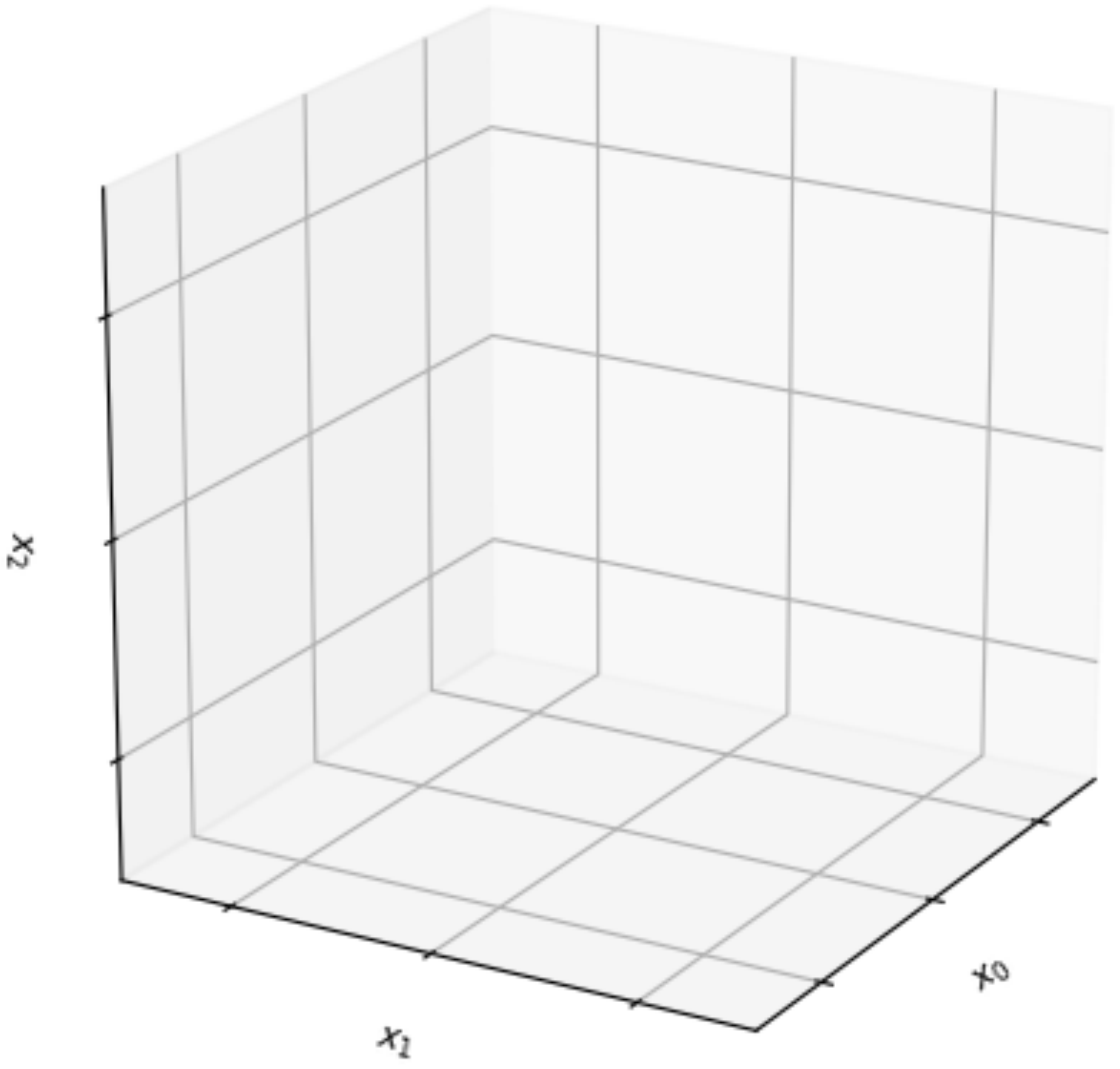

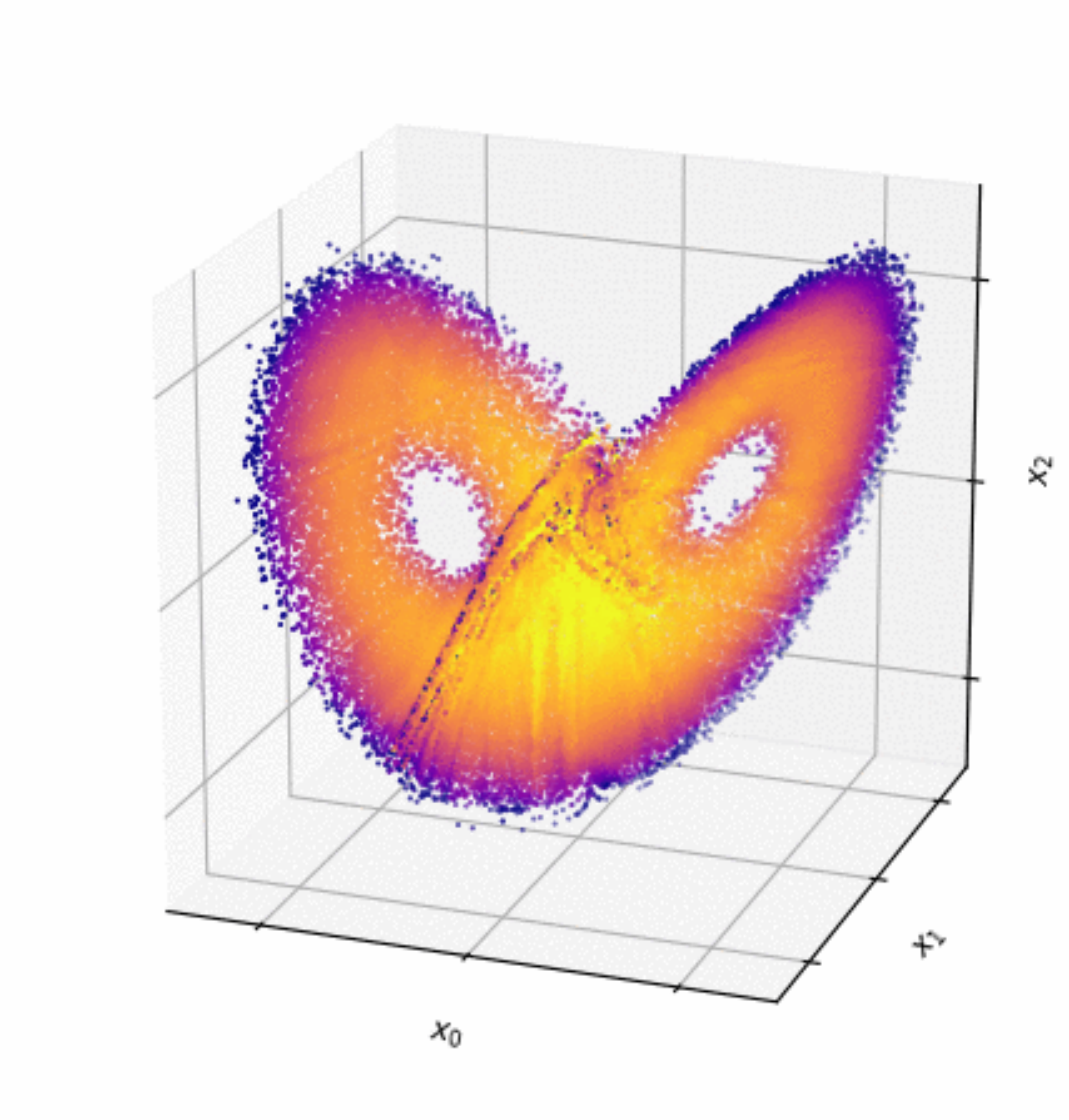

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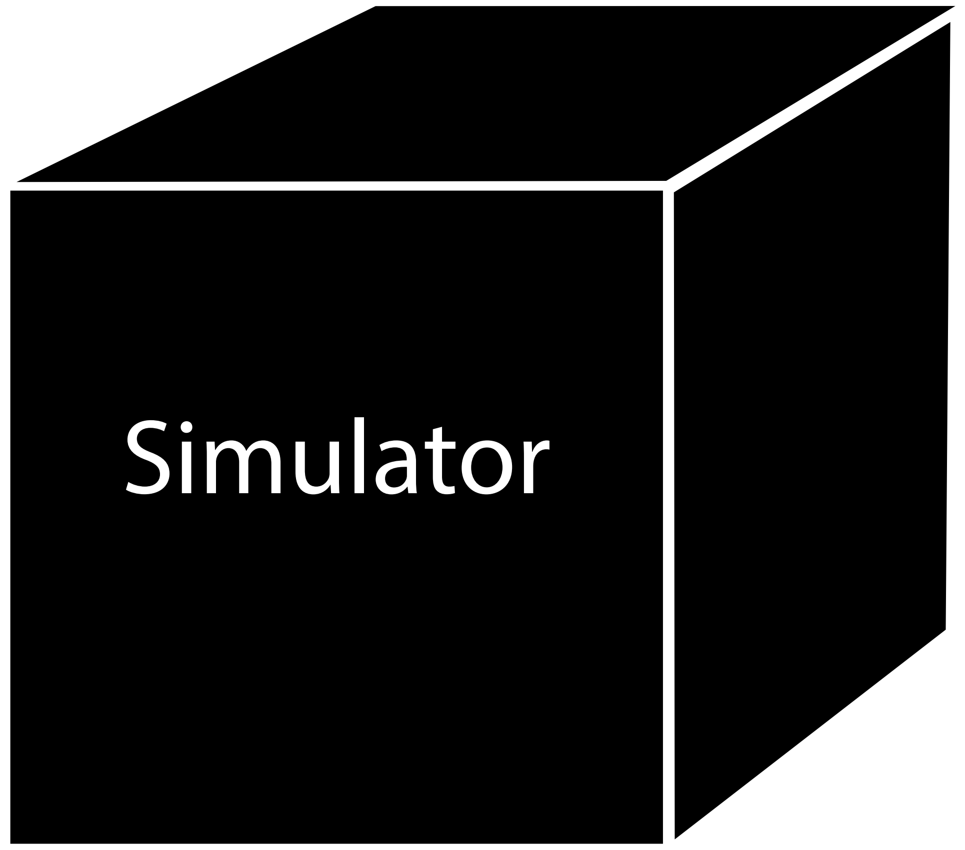
Particle physics as a likelihood-free inference problem

$\mathcal{O}(10)$ parameters θ

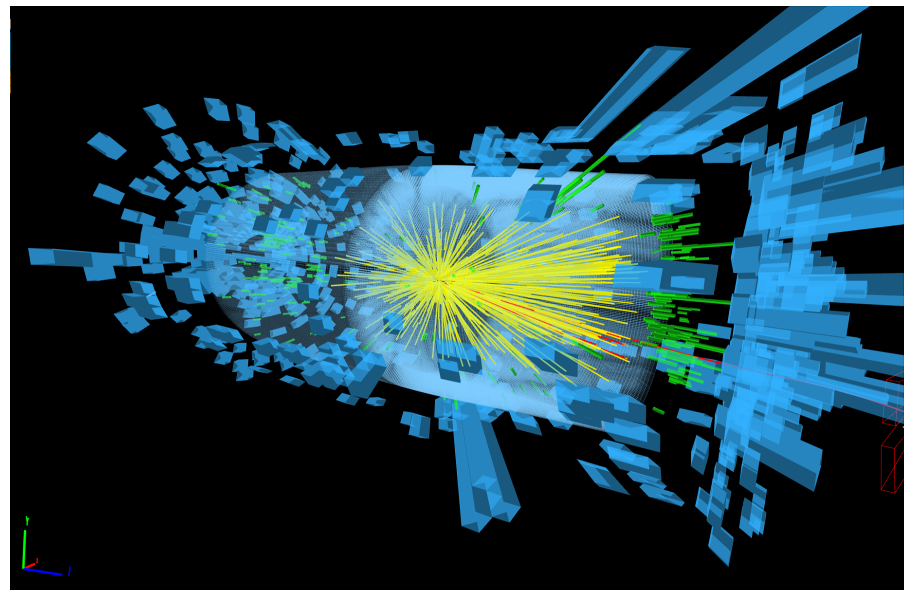
$$\begin{aligned} S = \int \mathrm{d}^4x \Bigg[& \mathcal{L}_{\mathrm{SM}} + \frac{f_{\phi,2}}{\Lambda^2}\,\frac{1}{2}\,\partial_\mu(\phi^\dagger\phi)\,\partial^\mu(\phi^\dagger\phi) + \frac{f_{\phi,3}}{\Lambda^2}\,\frac{1}{3}(\phi^\dagger\phi)^3 \\ & + \frac{f_{GG}}{\Lambda^2}\,(\phi^\dagger\phi)\,G^a_{\mu\nu}\,G^{\mu\nu\,a} - \frac{f_{BB}}{\Lambda^2}\,\frac{g'^2}{4}\,(\phi^\dagger\phi)\,B_{\mu\nu}\,B^{\mu\nu} - \frac{f_{WW}}{\Lambda^2}\,\frac{g^2}{4}\,(\phi^\dagger\phi)\,W^a_{\mu\nu}\,W^{\mu\nu\,a} \\ & + \frac{f_B}{\Lambda^2}\,\frac{\mathrm{i}g'}{2}\,(D^\mu\phi)^\dagger\,D^\nu\phi\,B_{\mu\nu} + \frac{f_W}{\Lambda^2}\,\frac{\mathrm{i}g}{2}\,(D^\mu\phi)^\dagger\,\sigma^a\,D^\nu\phi\,W^a_{\mu\nu} \\ & + \frac{f_\ell}{\Lambda^2}\,(\phi^\dagger\phi)\,\overline{L}_L\phi\,\ell_R + \frac{f_u}{\Lambda^2}\,(\phi^\dagger\phi)\,\overline{Q}_L\tilde{\phi}\,u_R + \frac{f_d}{\Lambda^2}\,(\phi^\dagger\phi)\,\overline{Q}_L\phi\,d_R \\ & + \frac{f_{G\widetilde{G}}}{\Lambda^2}\,(\phi^\dagger\phi)\,G^a_{\mu\nu}\,\widetilde{G}^{\mu\nu\,a} - \frac{f_{B\widetilde{B}}}{\Lambda^2}\,\frac{g'^2}{4}(\phi^\dagger\phi)\,B_{\mu\nu}\,\widetilde{B}^{\mu\nu} - \frac{f_{W\widetilde{W}}}{\Lambda^2}\,\frac{g^2}{4}(\phi^\dagger\phi)\,W^a_{\mu\nu}\,\widetilde{W}^{\mu\nu\,a} \Bigg] \end{aligned}$$

$\longrightarrow$



$\longrightarrow$

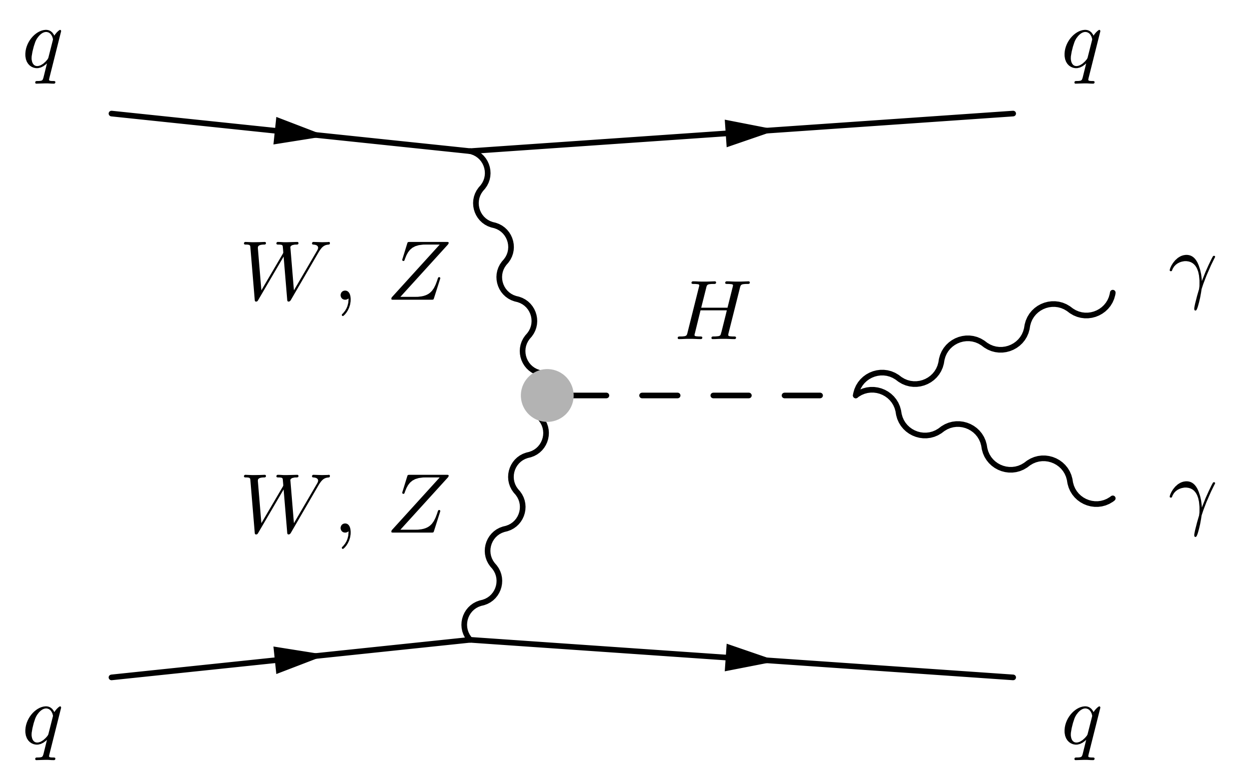
$\mathcal{O}(10\ldots1000)$ observables x



Prediction: Simulator can sample $x \sim p(x|\theta)$

Inference: Simulator likelihood $p(x|\theta)$ is intractable, but we can train ambient flows or $\mathcal{M}$-flows as surrogate

Particle physics: structure

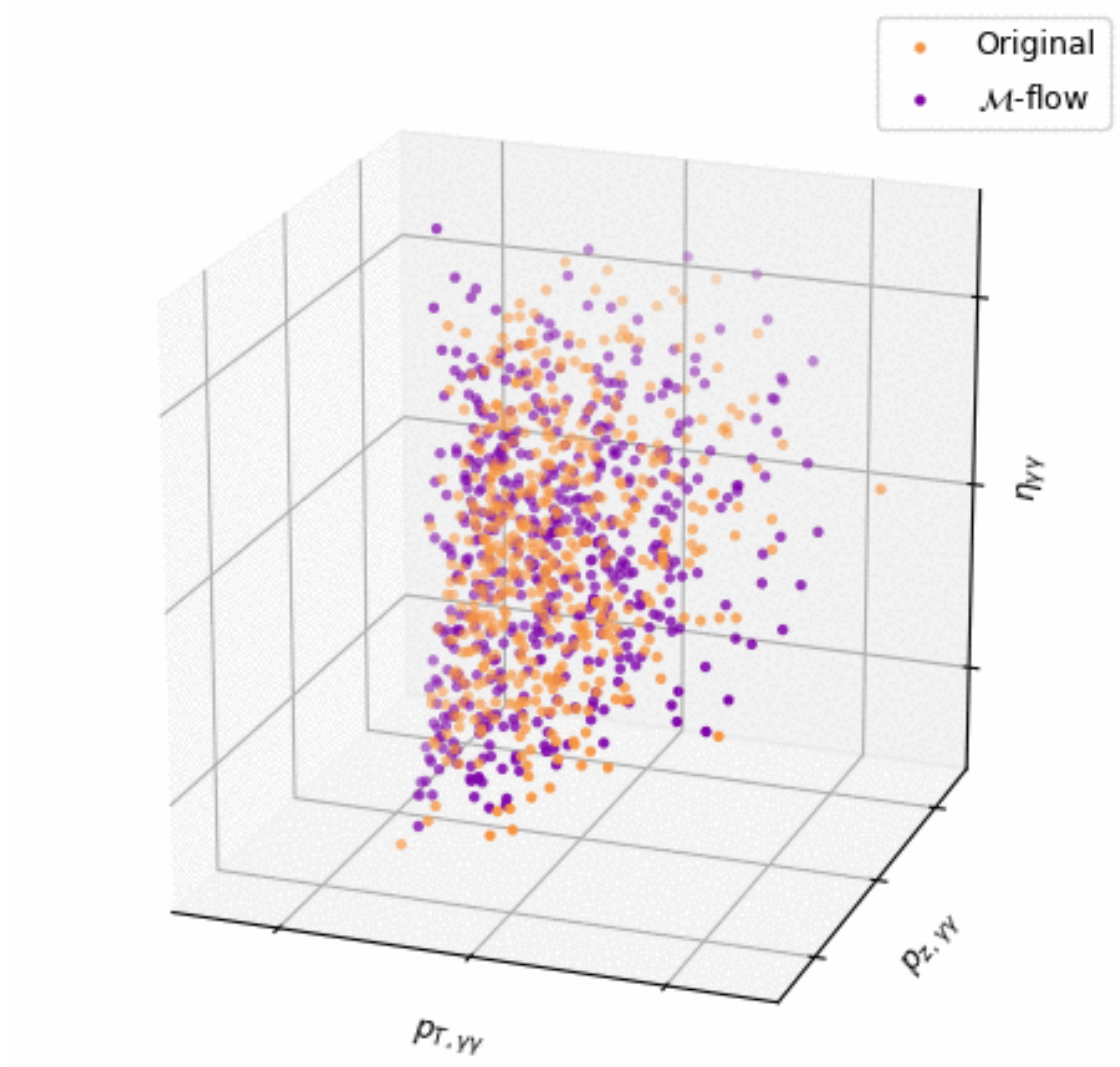


particle masses
("on-shell condition")

redundant
observables

energy-momentum
conservation

14-dimensional manifold
embedded in 40-dimensional
data space



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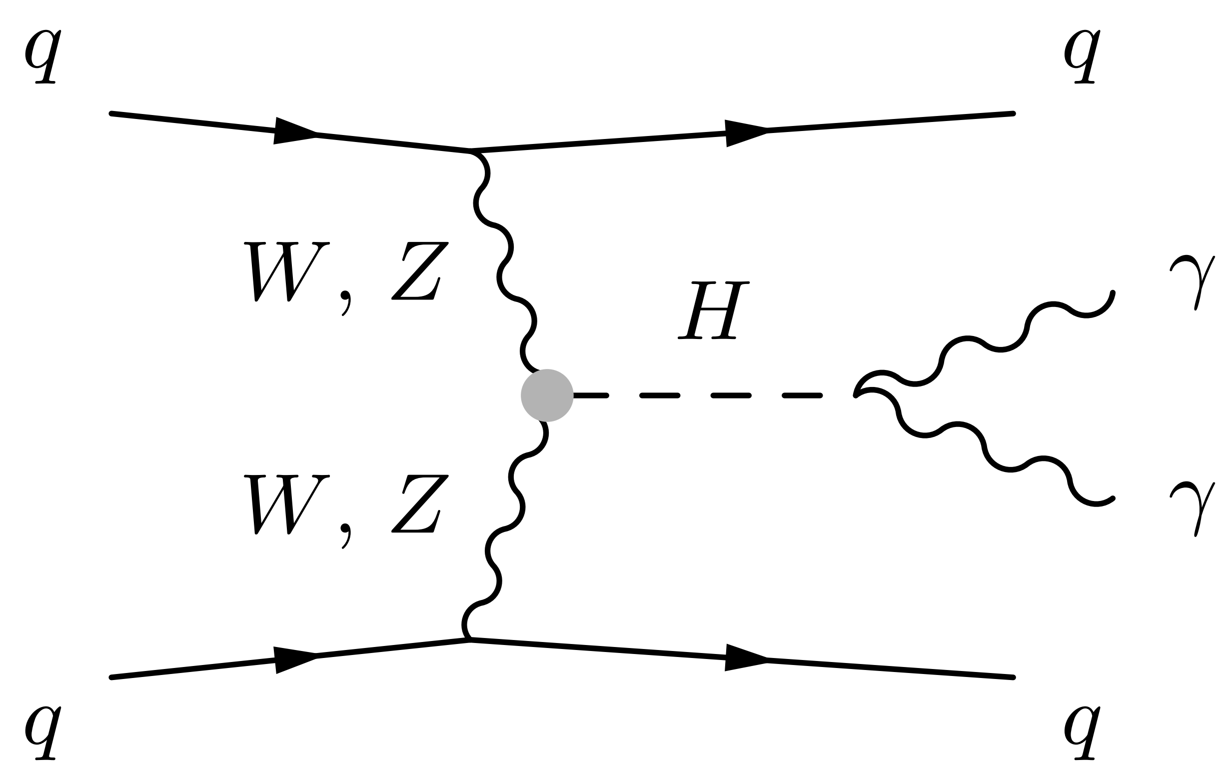

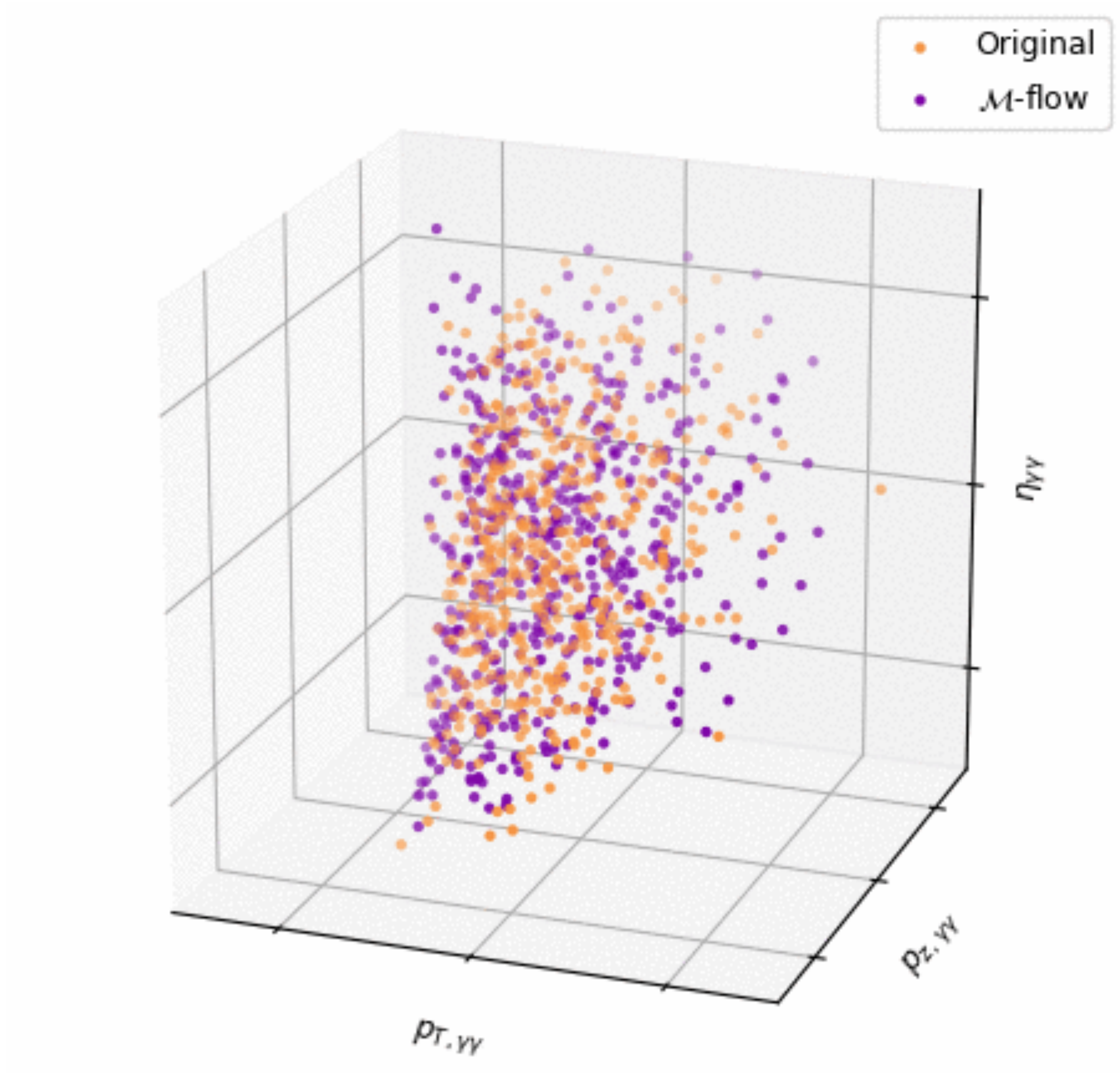

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Particle physics: results

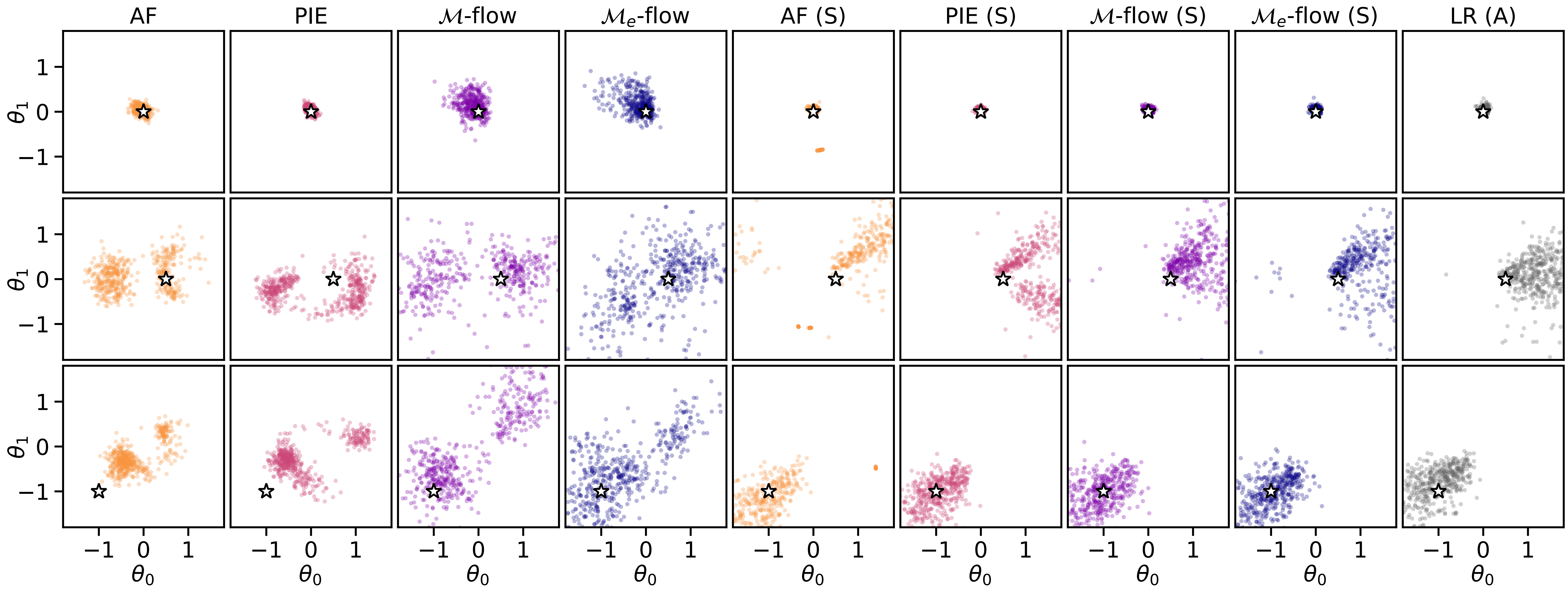
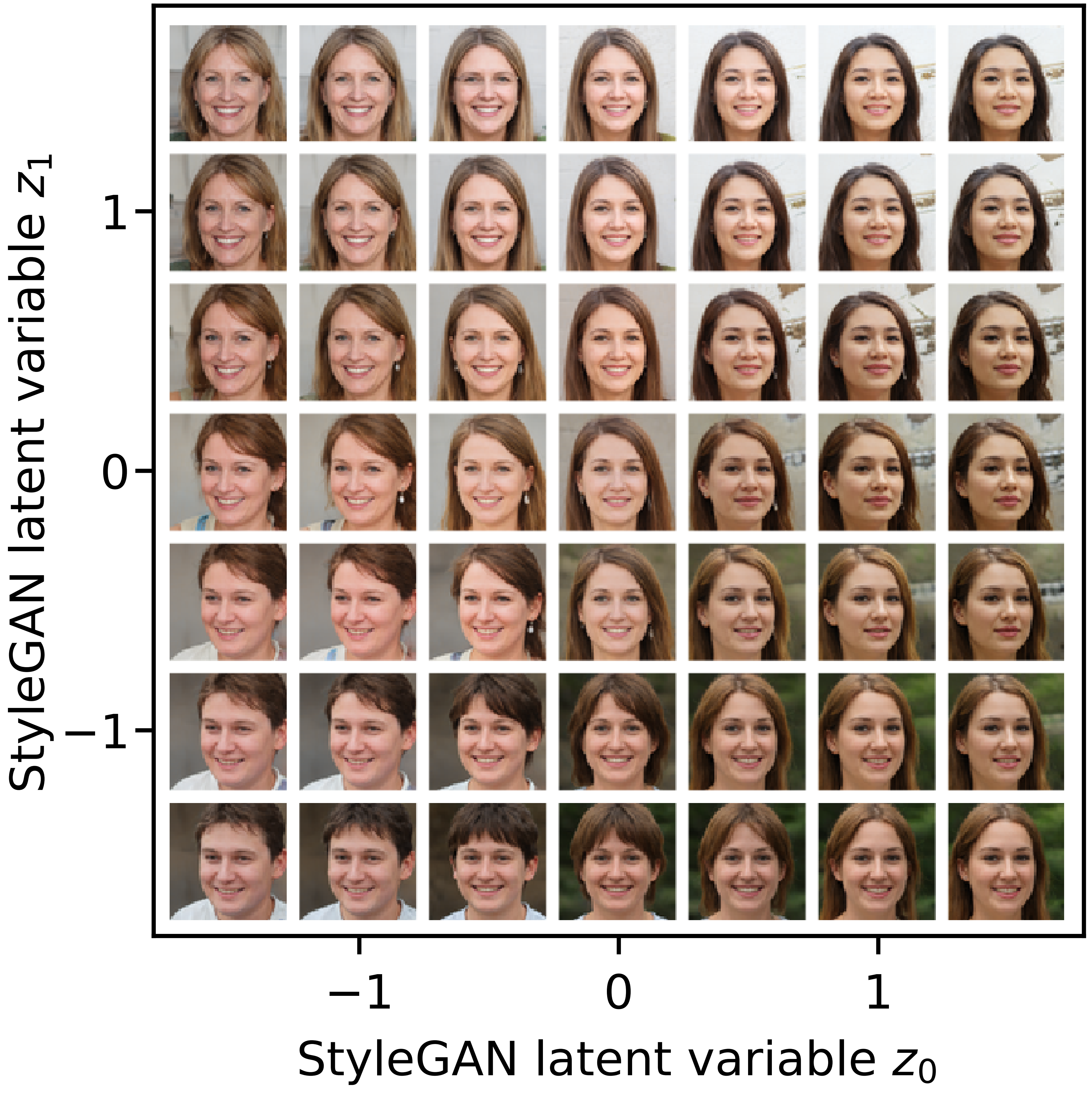


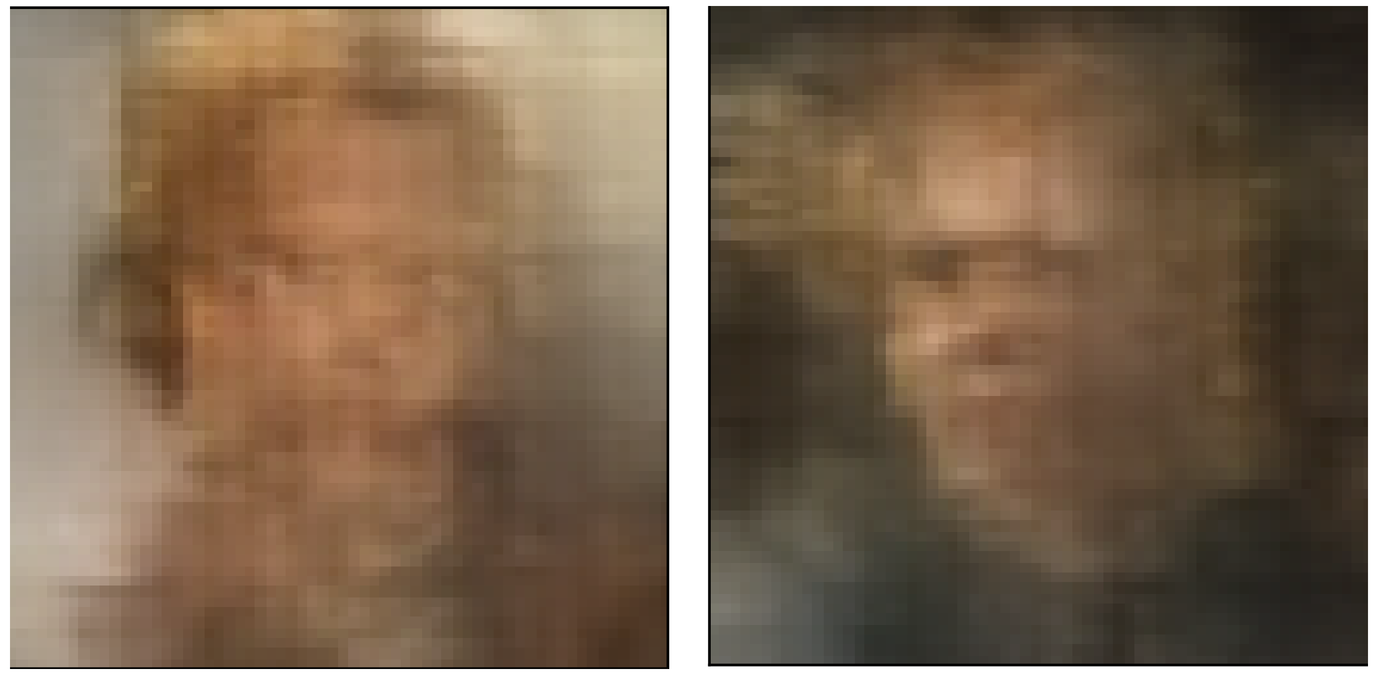
Image manifolds

Q: How to make image datasets where we **know** that data lives on an n -dimensional manifold?

A: take a pretrained GAN model, sample n of its latent variables, and keep all others fixed

$n = 2$





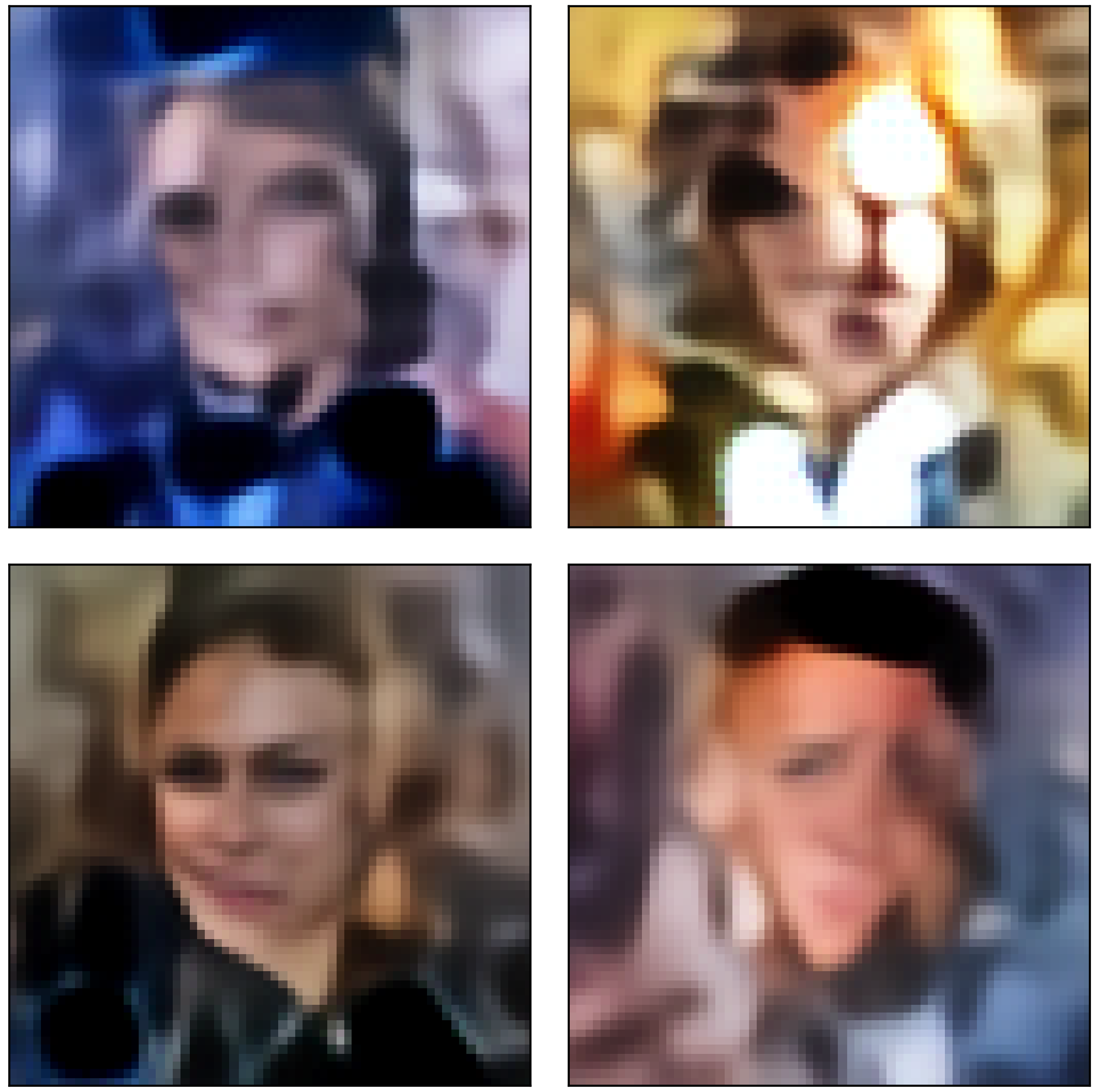
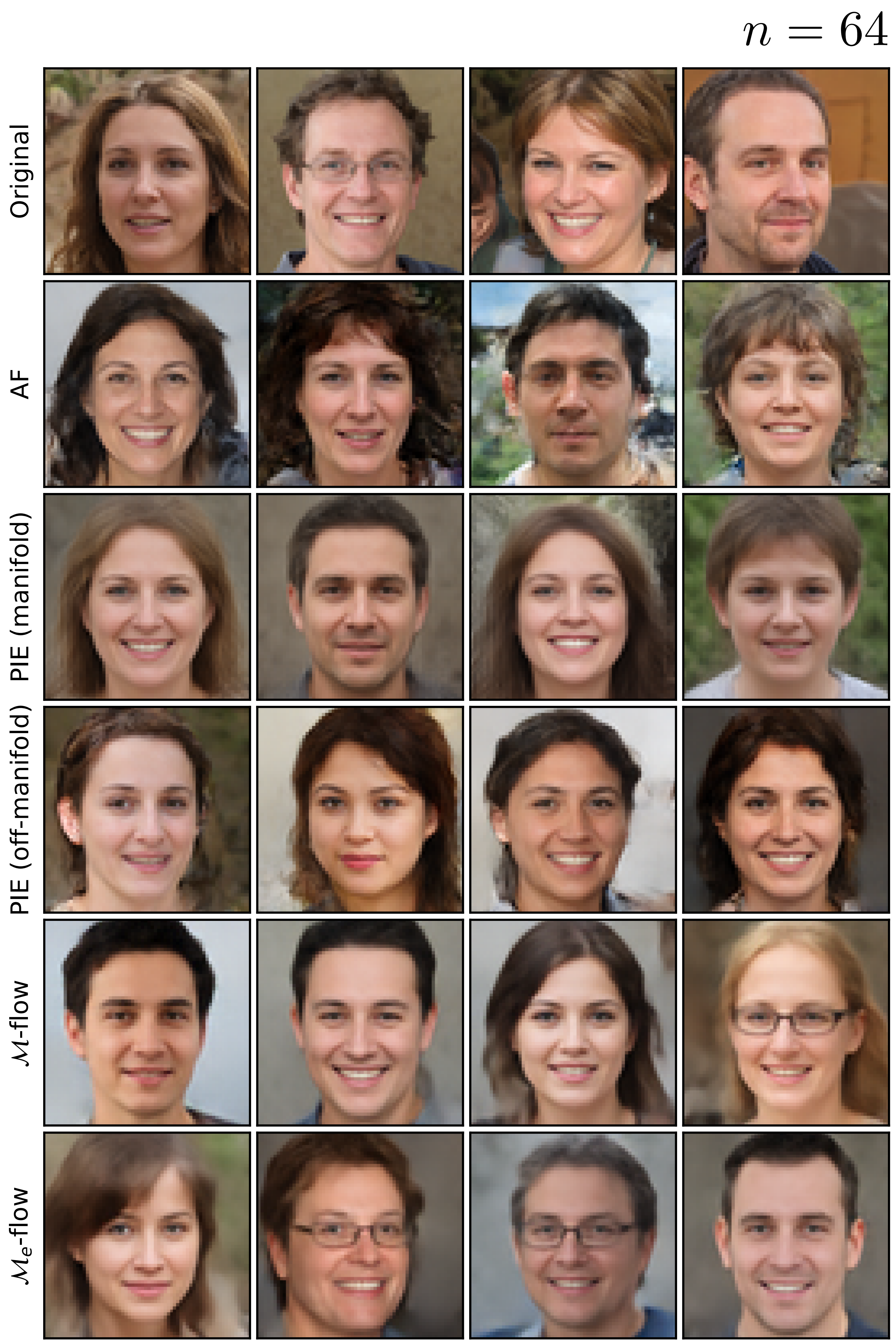


Image manifold results



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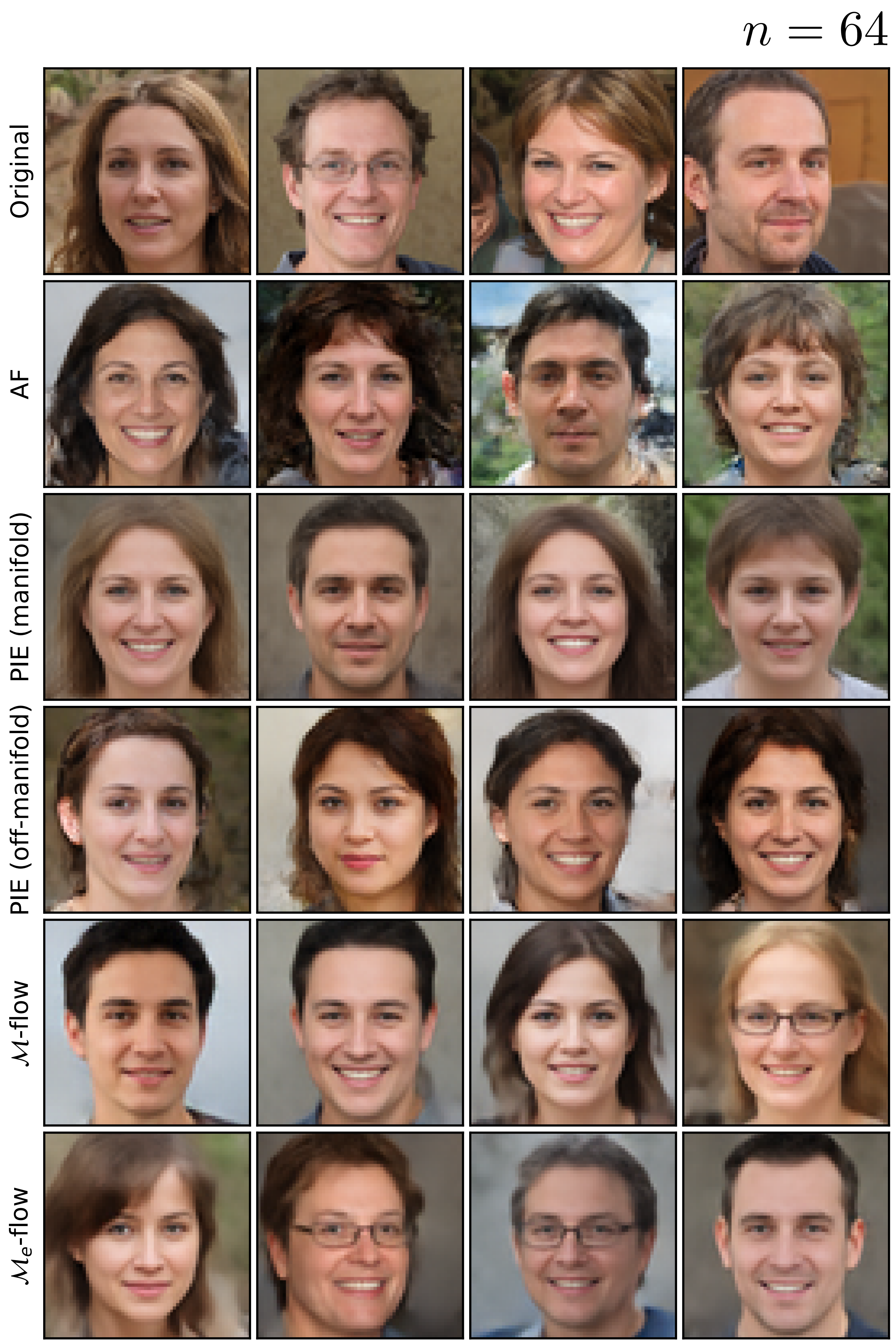


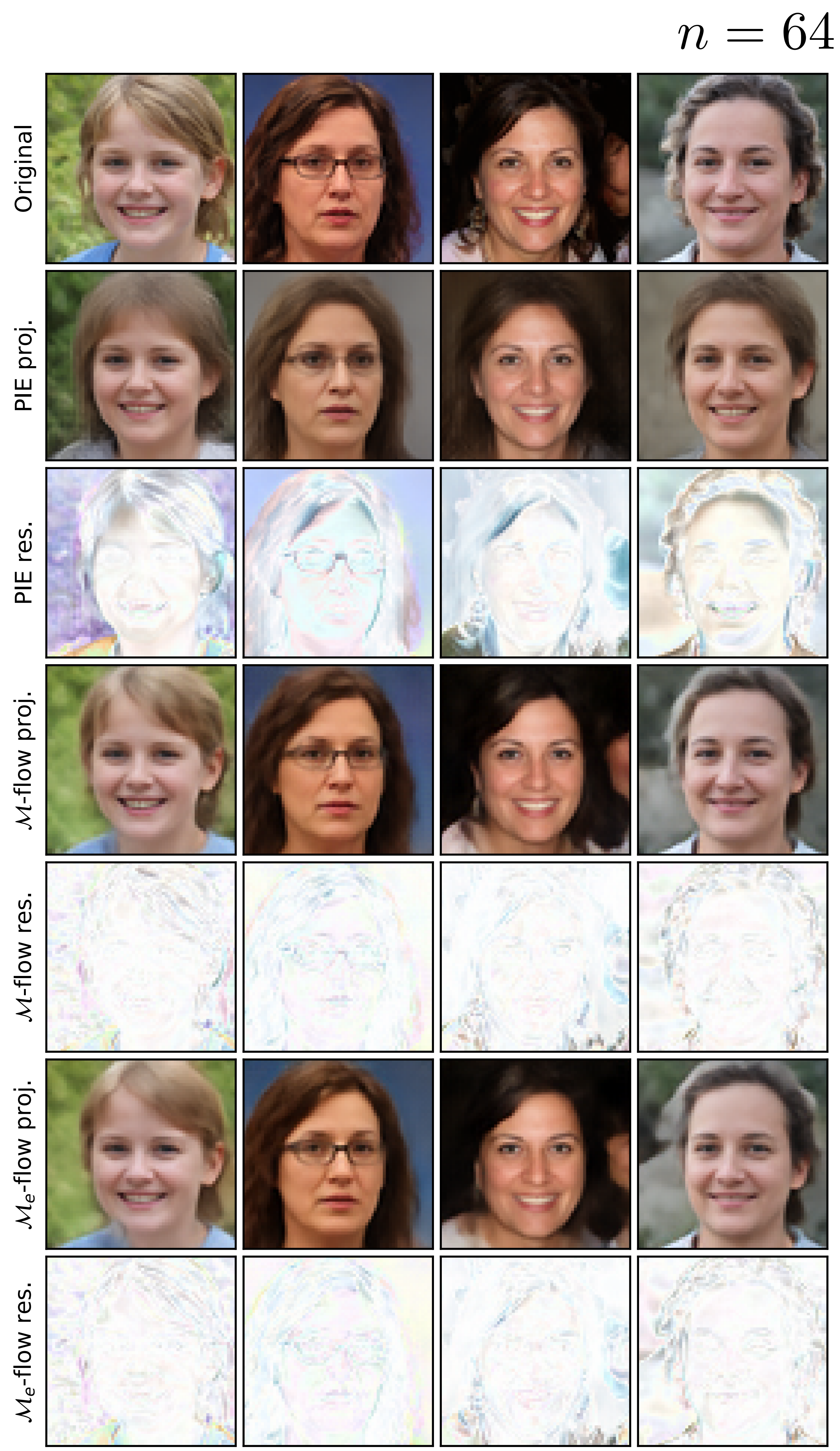
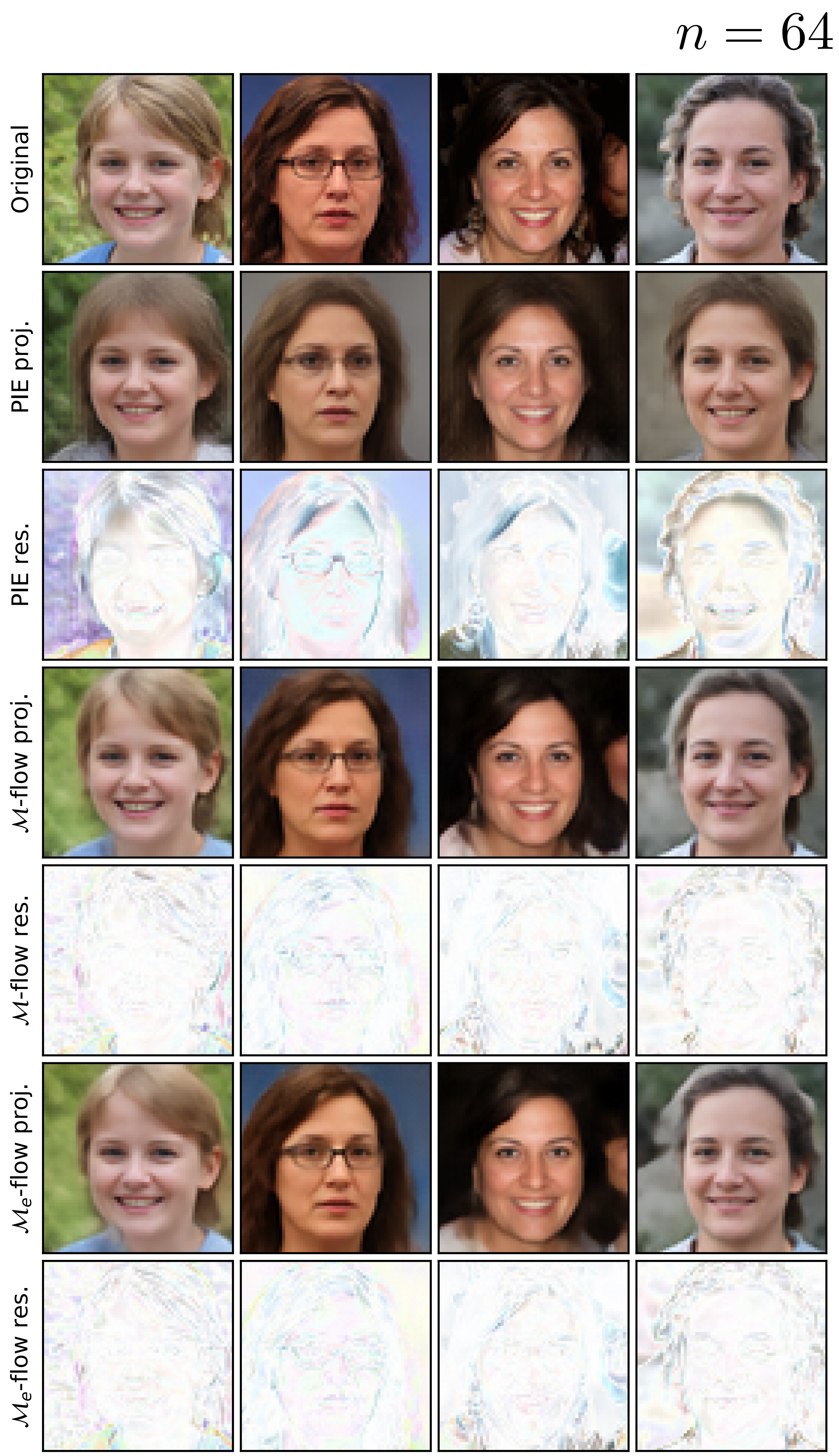
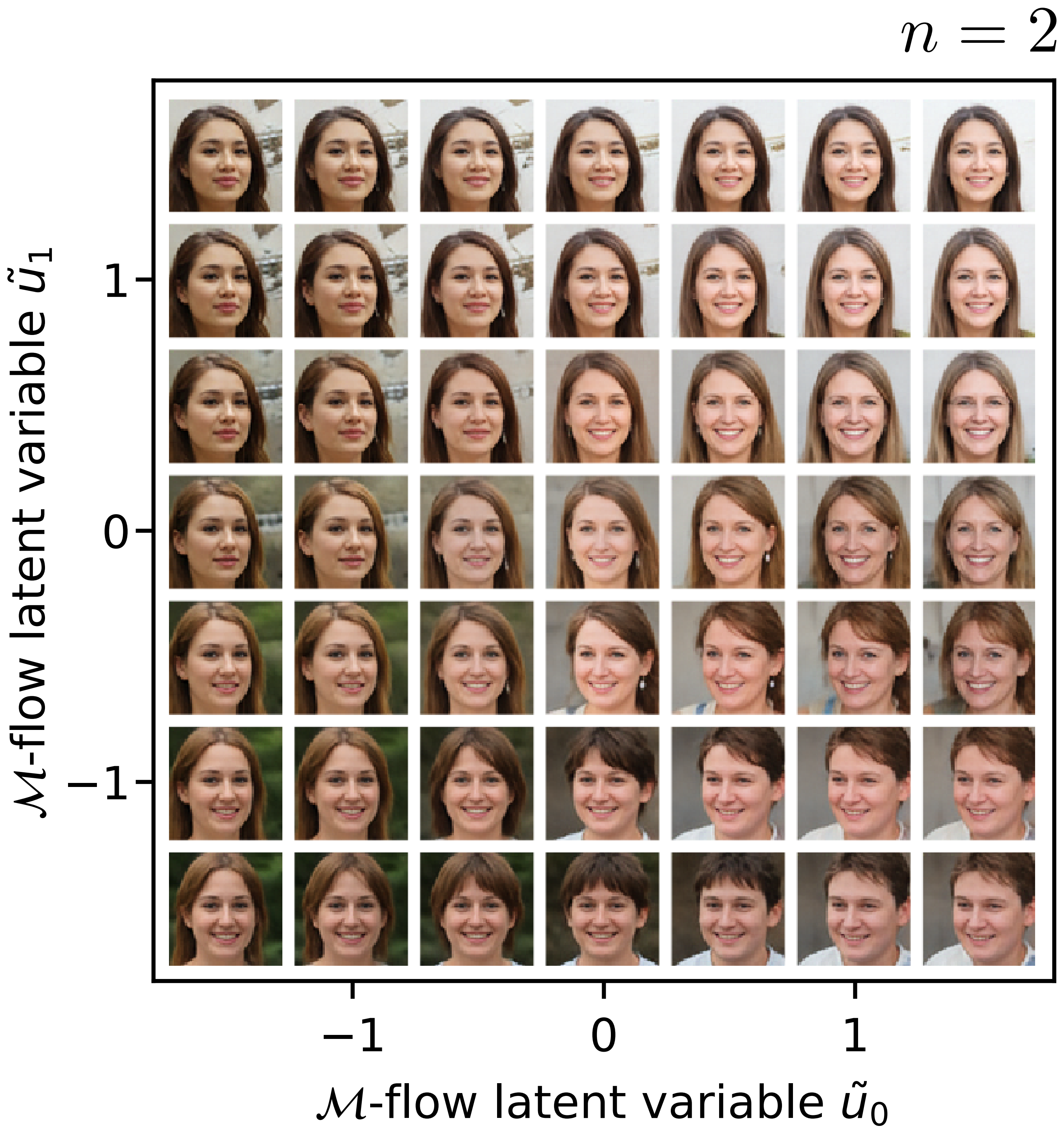


Image manifold results





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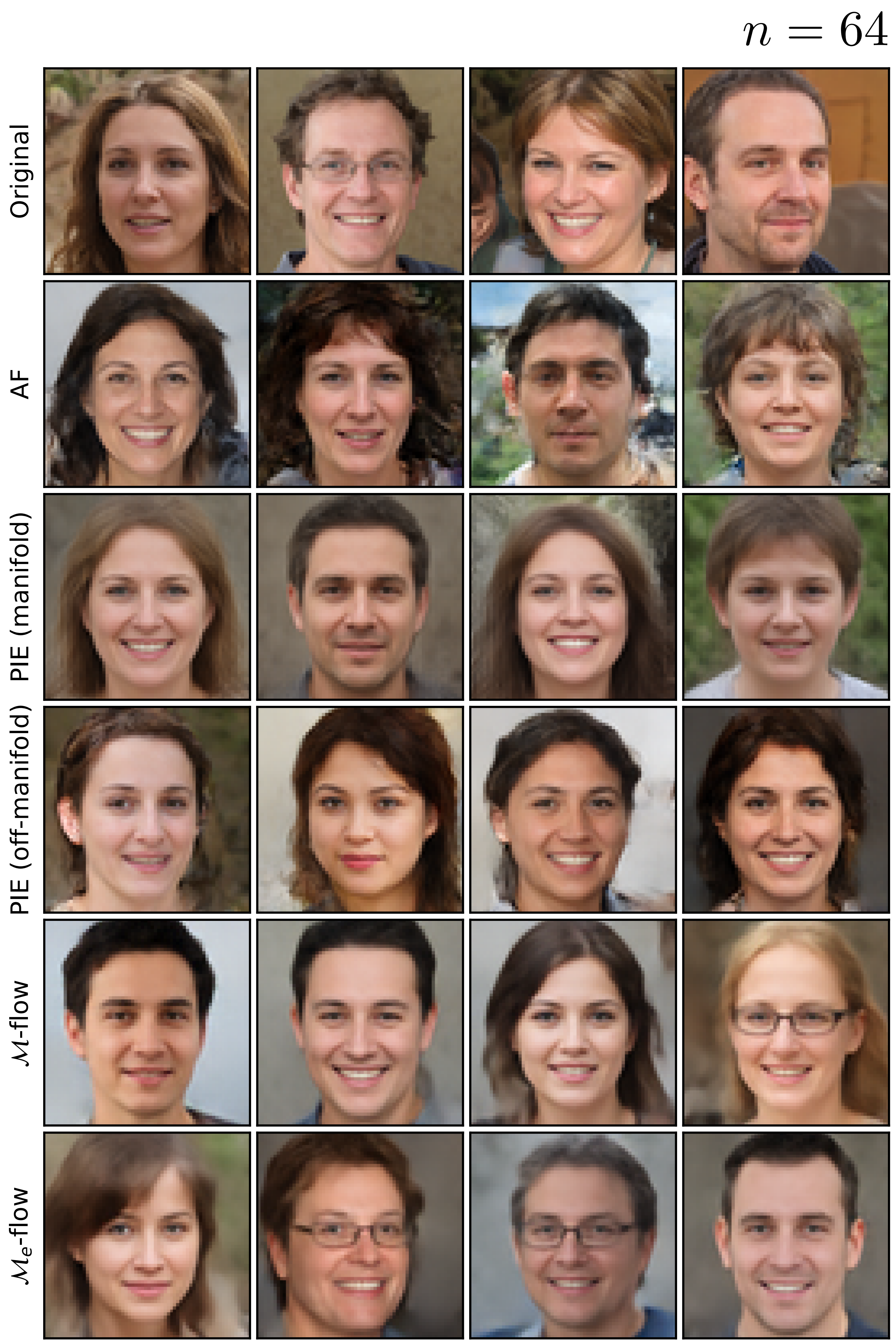

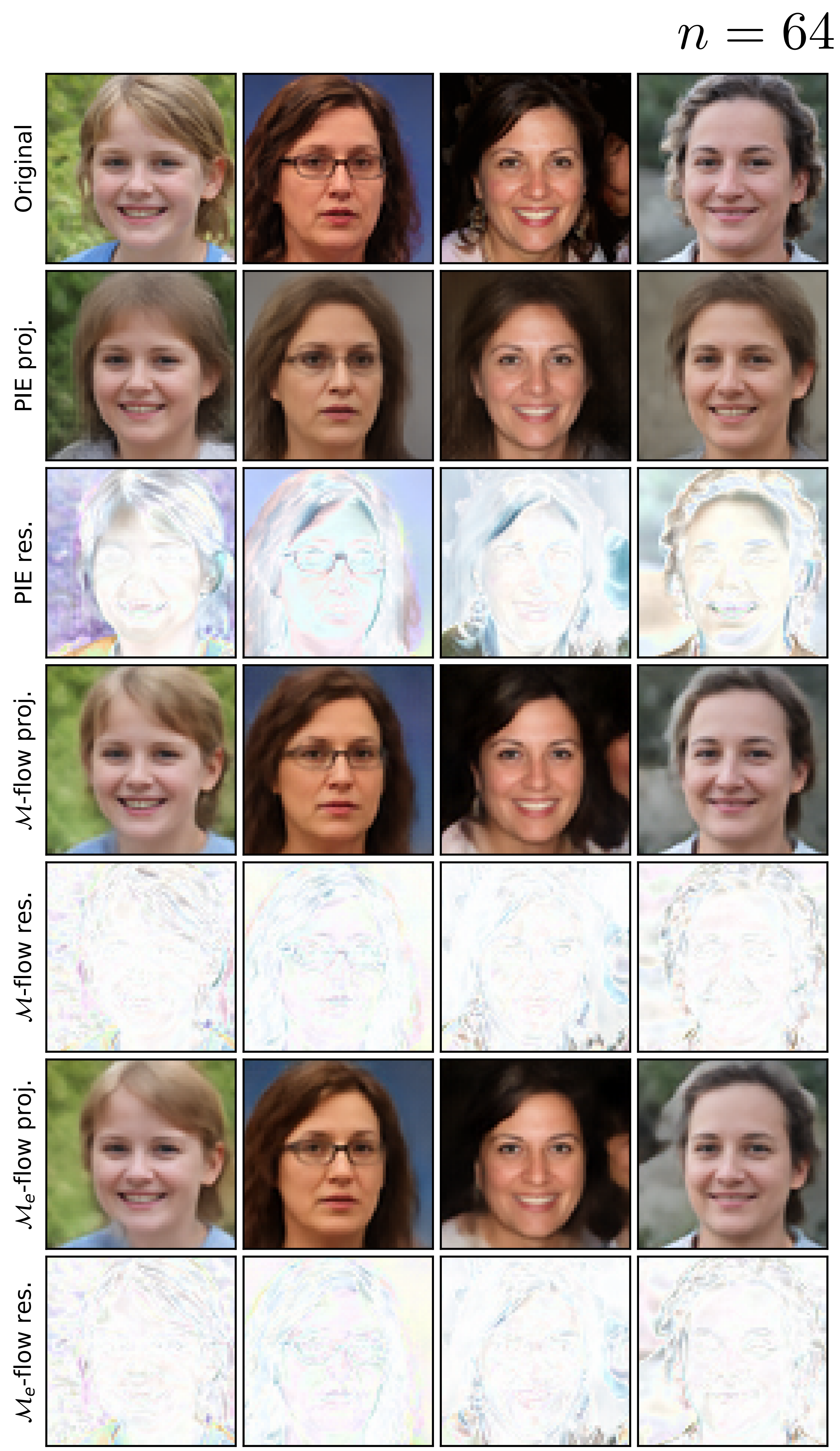

Real-world images: CelebA

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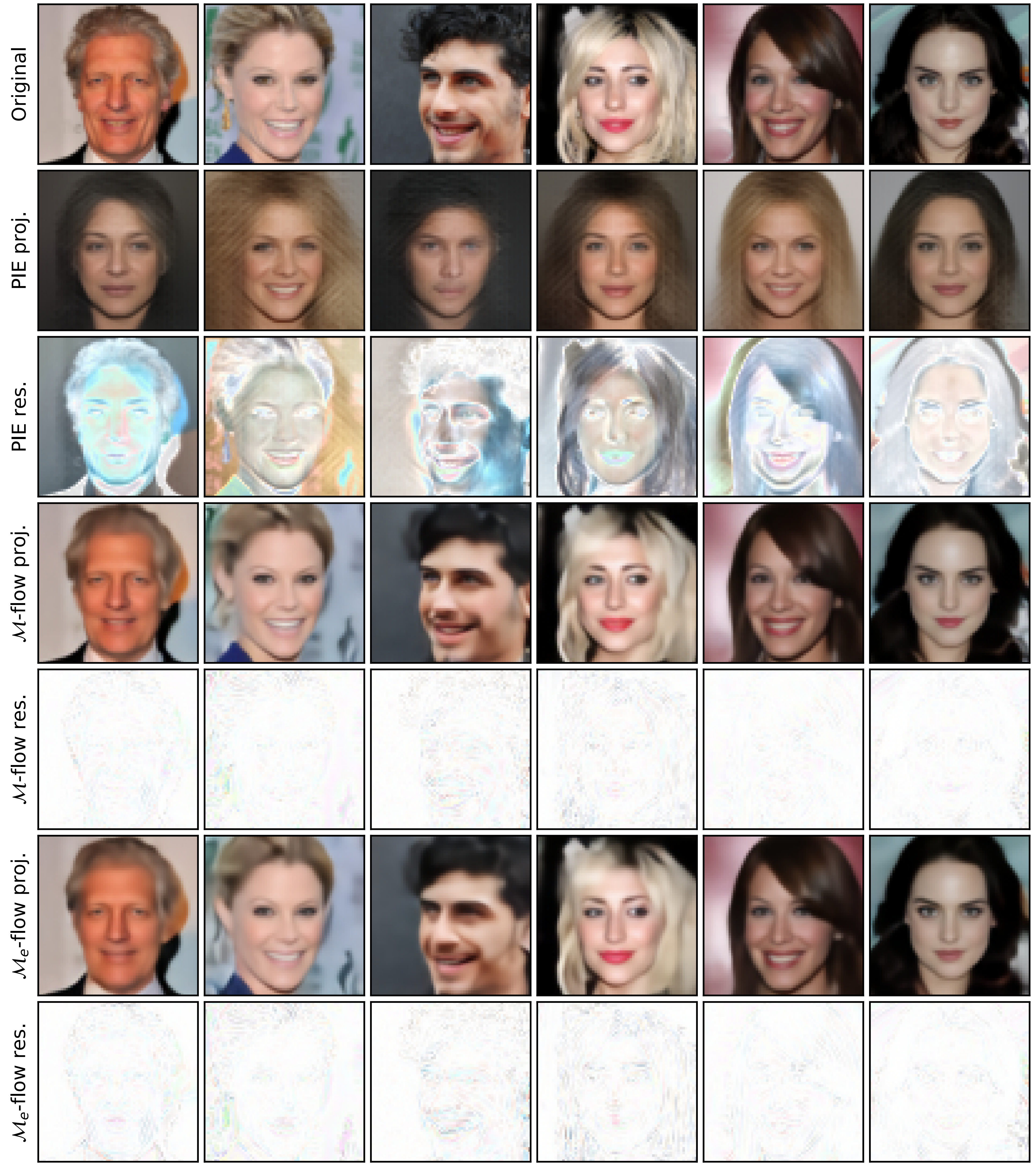


Metrics

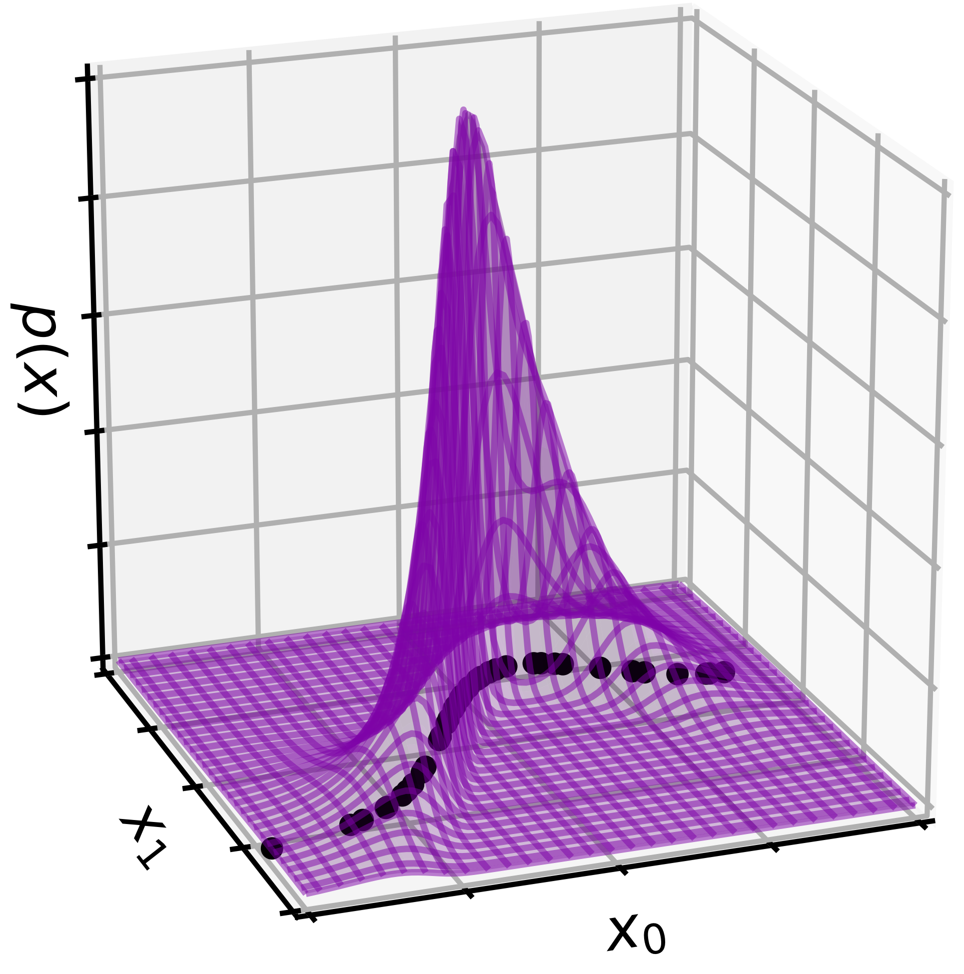
Model	Polynomial surface			Particle physics			Images			
	Distance	RE	MMD	Closure	RE	$\log p(\theta^*)$	$n = 2$ FID	$n = 64$ FID	$n = 64$ $\log p(\theta^*)$	CelebA FID
AF	0.005	–	0.071	**0.0019**	–	-3.94	58.3	24.0	0.17	**33.6**
PIE	0.035	1.278	0.131	0.0023	2.054	-4.68	139.5	32.2	-6.40	75.7
$\mathcal{M}$-flow	**0.002**	**0.003**	0.020	0.0045	**0.012**	-1.71	43.9	**20.8**	**2.67**	37.4
$\mathcal{M}_e$-flow	**0.002**	**0.002**	**0.007**	0.0046	0.029	$-\mathbf{1.44}$	**43.5**	23.7	1.81	35.8

Open questions

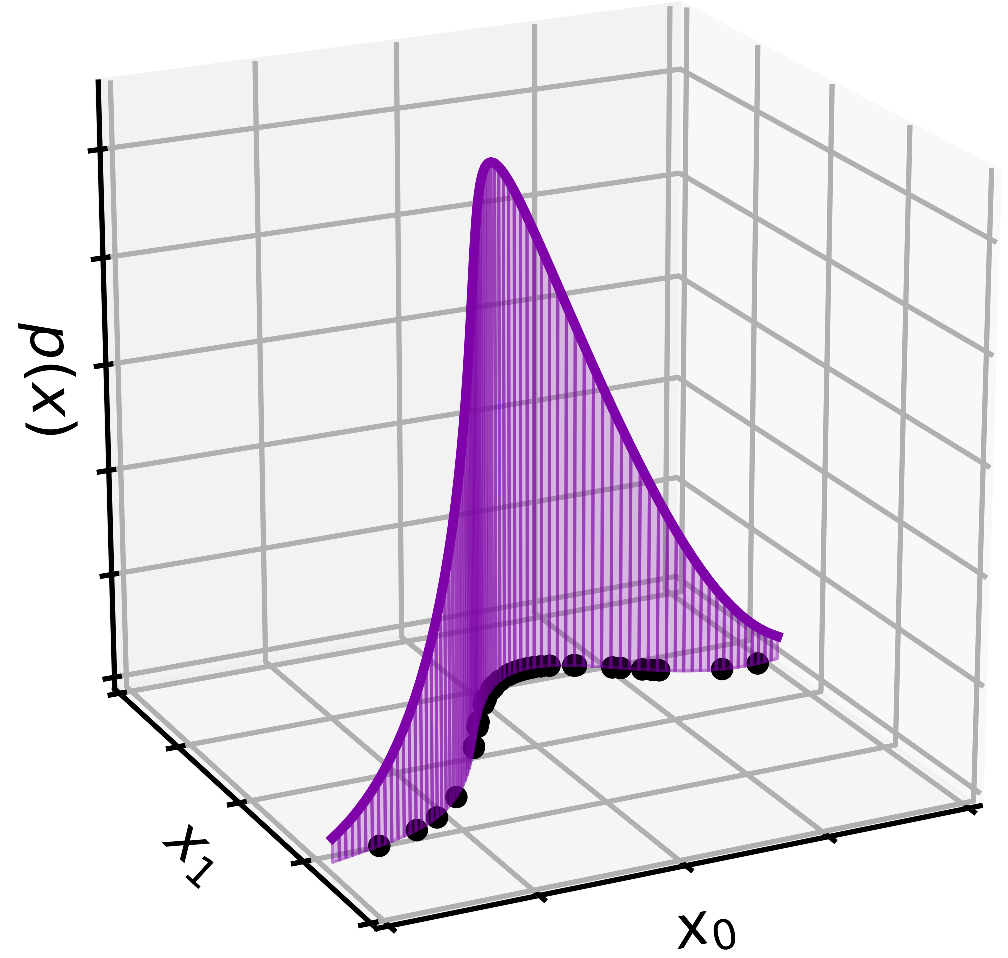
How do you learn n ?

What are good architectures for image data?

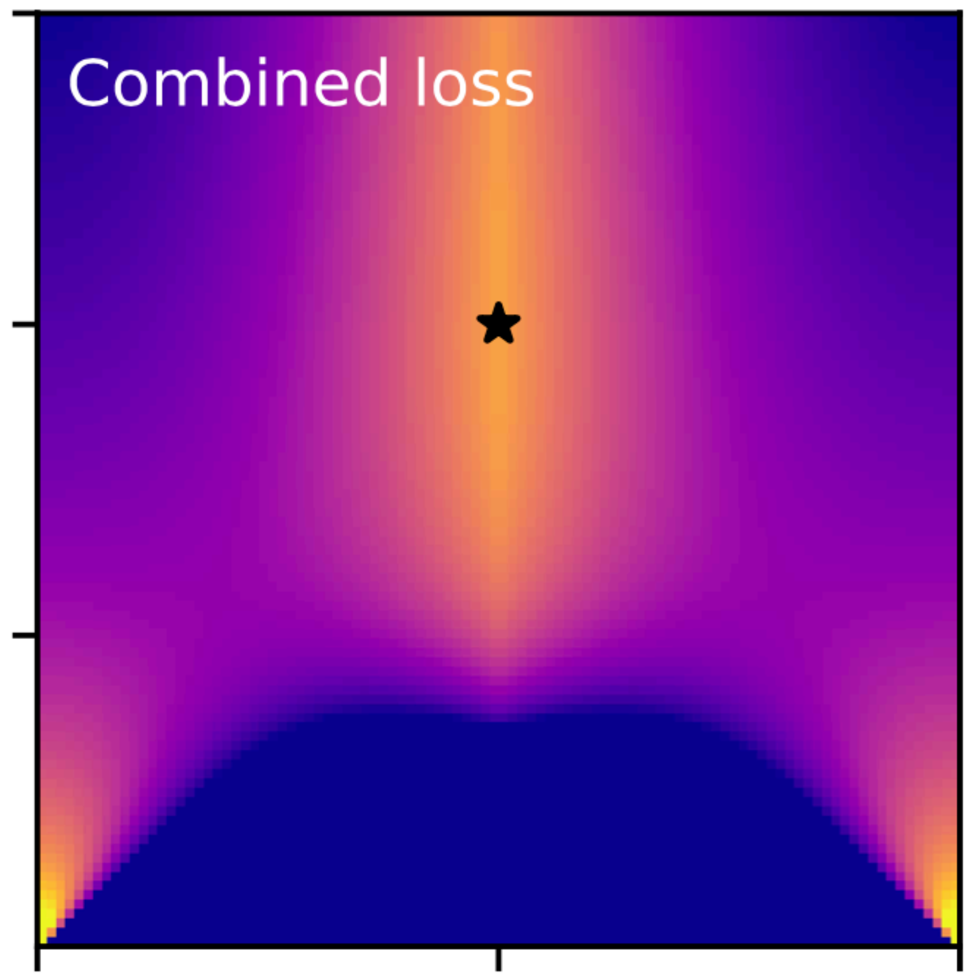
Are there transformations f for which the likelihood can be computed faster?



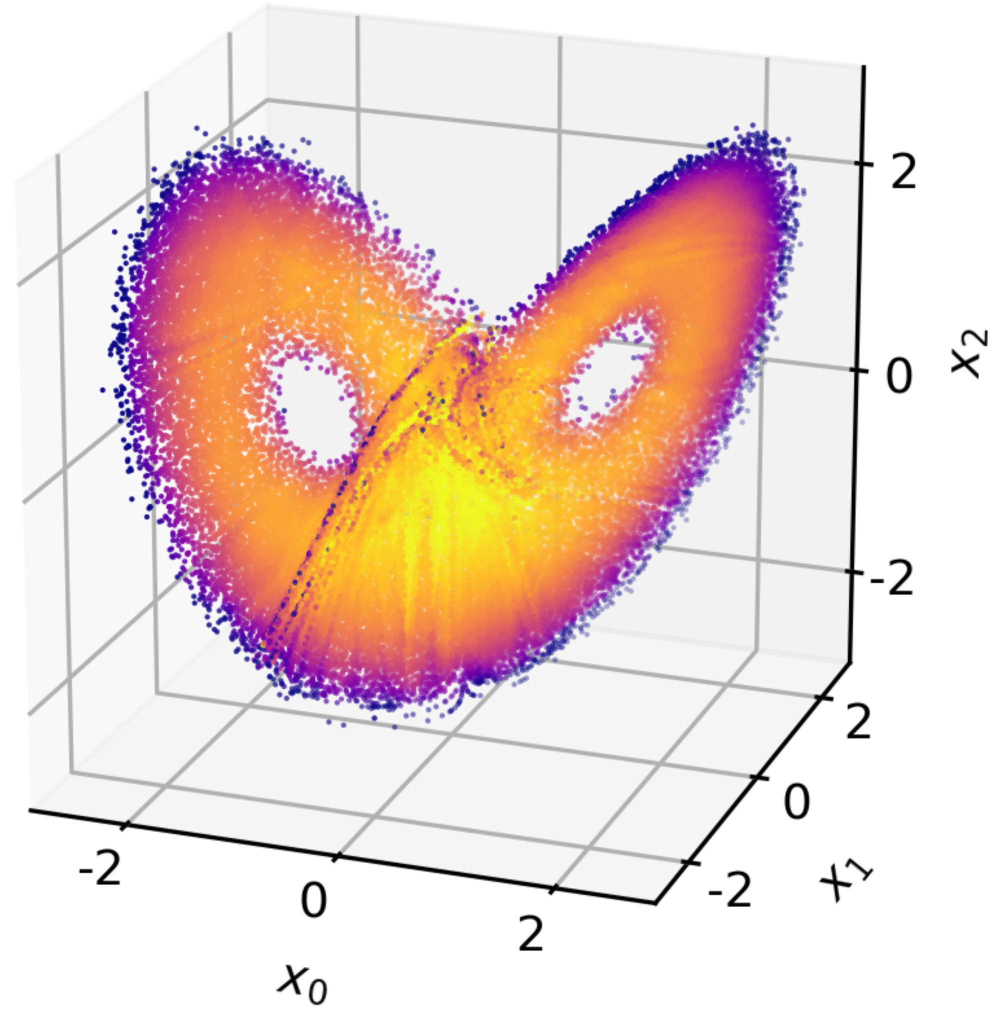
Standard ambient flows cannot represent lower-dim. data manifolds



$\mathcal{M}$-flows learn data manifold and a tractable density on it



Maximum likelihood is not enough, but $\mathcal{M}$-flows can be trained with M/D algorithm



First experiments: $\mathcal{M}$-flows learn data manifolds well, good performance on inference tasks

[JB, Kyle Cranmer 2003.13913]