Towards Improving Generative Model
from Dynamical System Perspective

Tianrong Chen

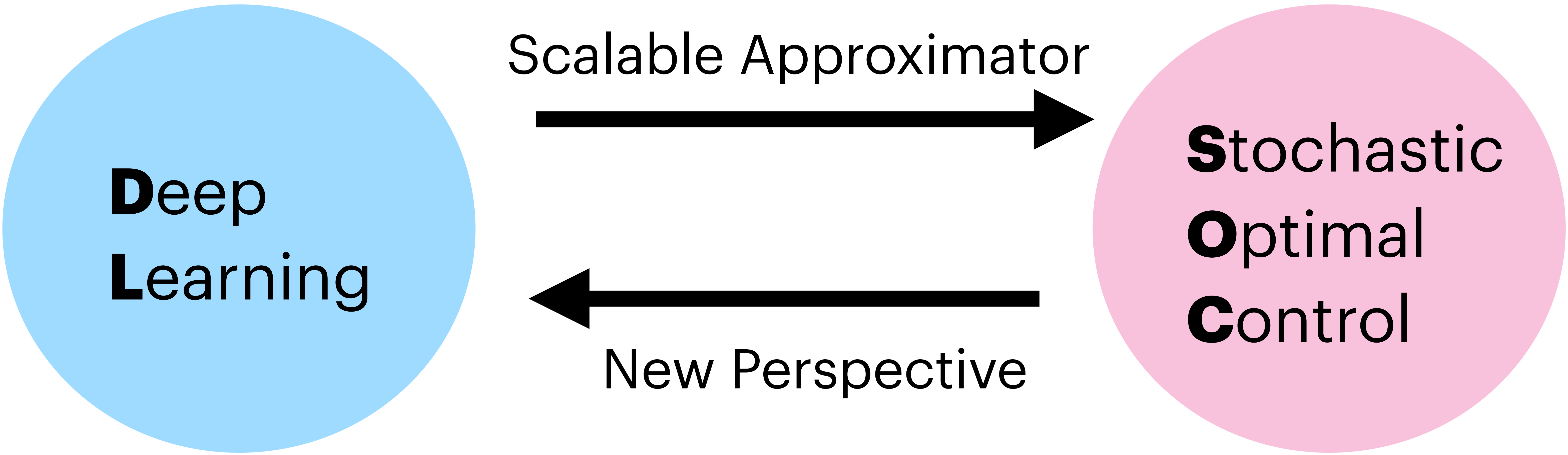
01/24/2024

About me

I am a senior PhD at ACDS Lab from Gatech supervised Professor Evangelos Theodorou.

I was extremely fortune to intern at Apple MLR, working with many talented researchers including (Apple) Jiatao Gu, Laurent Dinh, Joshua Susskind, Shuangfei Zhai, (Google Deepmind) Valentin De Bortoli, Microsoft (Chenru Duan) and (Georgia Tech) Molei Tao.

Research Topics:



Selected Work

- **Solving Stochastic Differential Game (DL—> SOC)**

  Large-Scale Multi-Agent Deep FBSDEs

  [**Tianrong Chen**, Ziyi Wang, Ioannis Exarchos, Evangelos Theodorou. ICML2021 spotlight]

  Deep Graphic FBSDEs for Social Opinion Dynamics Control

  [**Tianrong Chen**, Ziyi Wang, Evangelos Theodorou. CDC 2022]

- **SOC Inspired Optimizer(SOC—>DL)**

  DDPNOpt: Differential Dynamic Programming Neural Optimizer

  [Guan-horng Liu, **Tianrong Chen,** Evangelos Theodorou. ICLR2022 Oral]

  Second-Order Neural ODE Optimizer

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  …

- **Generative Modeling(SOC—>DL)**

  Likelihood Training of Schrödinger Bridge using Forward-Backward SDEs Theory

  [**Tianrong Chen*,**Guan-horng Liu***,** Evangelos Theodorou. ICLR 2022]

  Multi-marginal momentum Schrödinger Bridge

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  Generative Modeling with Phase Stochastic Bridges (Apple Intern)

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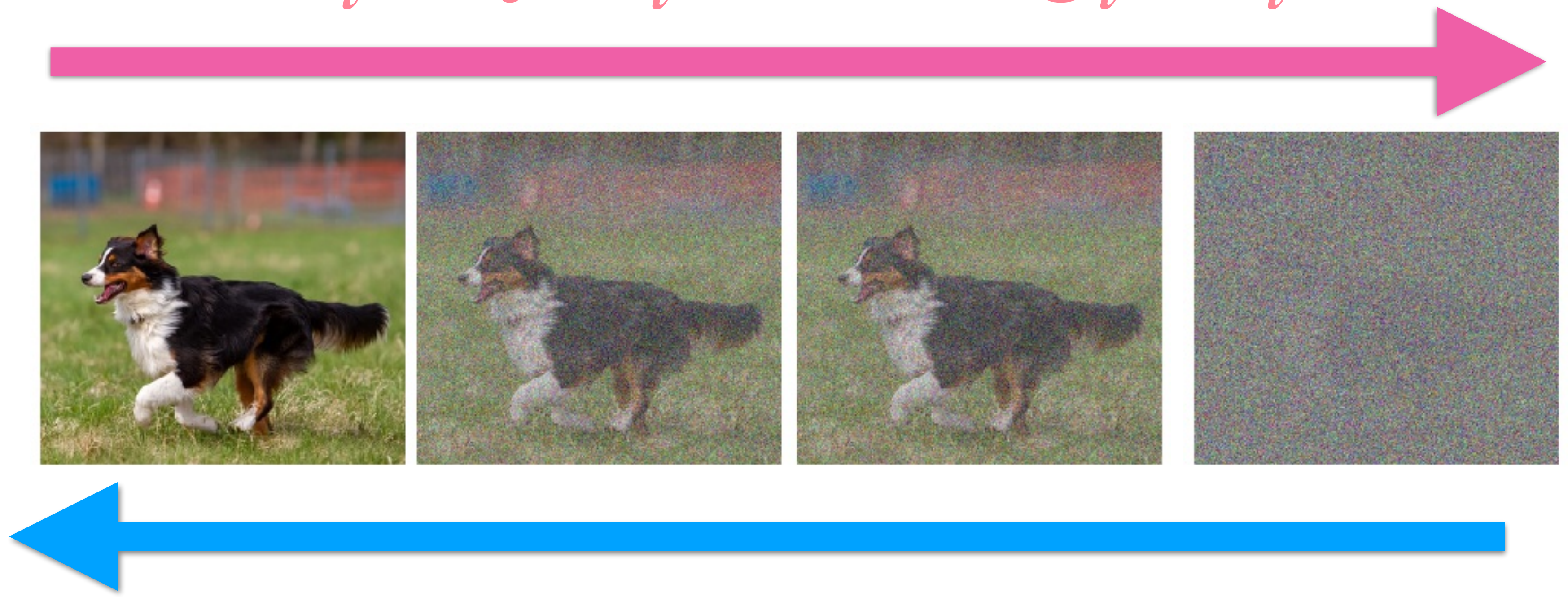
- **Gentle Introduction.**
- Generative Modeling with Phase Stochastic Bridges
- Momentum Schrödinger Bridge for AI4Science (Biology)
- Future Directions
- Q&A

Introduction

Dynamical Generative Model

$$dx_t = f(x_t, t)dt + g_t dw_t$$

$x_0 \sim p_0$  $x_1 \sim p_1$

$$dx_t = b(x_t, t)dt + g_t dw_t$$

Task:

1. **Generative Modeling:** Sample data from data distribution p_0
2. **Trajectory Inference:** sample data and intermediate trajectories in between.

How: Construct transportation map between prior p_1 and p_0 by Dynamical System: SDE (Diffusion Model [1]), ODE (Flow Matching[2]).

[1] Song, Yang, et al. "Score-based generative modeling through stochastic differential equations." *arXiv preprint arXiv:2011.13456* (2020).
[2] Lipman, Yaron, et al. "Flow matching for generative modeling." *arXiv preprint arXiv:2210.02747* (2022).

Dynamical Generative Model

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$x_0 \sim p_0$

$x_1 \sim p_1$

$$dx_t = b(x_t, t)dt + g_t dw_t$$

Diffusion Model:

Predefine diffusion process.

1. Choose $f(\cdot)$ and $g_t(\cdot)$

Learn the reverse process (Time reversal Theorem)

1. $b(\cdot) := f - g^2 \nabla_x \log p(\cdot)$

Dynamical Generative Model

$$dx_t = f(x_t, t)dt + g_t dw_t$$

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Flow Matching:

Predefine data pairing $(x_0, x_1) \sim p_0 \otimes p_1$

1. Construct linear interpolation vector field $f(\cdot, t \,|\, x_0, x_1) := x_1 - x_0,\ g_t \equiv 0$

Learn the reverse process

1. $b(\cdot) := -f(\cdot)$

Dynamical Generative Model

$$dx_t = f(x_t, t)dt + g_t dw_t$$

$x_0 \sim p_0$

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~~1. Construct linear interpolation vector field~~ $\cancel{f(\cdot, t \mid x_0, x_1) := x_1 - x_0, g_t \equiv 0}$

Learn the vector field

$b(\cdot) := -(x_1 - x_0)$ Alert!

Dynamical Generative Model

$$dx_t = f(x_t, t)dt + g_t dw_t$$

$x_0 \sim p_0$

$x_1 \sim p_1$

$$dx_t = b(x_t, t)dt + g_t dw_t$$

Connection?

Diffusion Model:

<u>**Predefine**</u> diffusion process.

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<u>**Learn**</u> the reverse process

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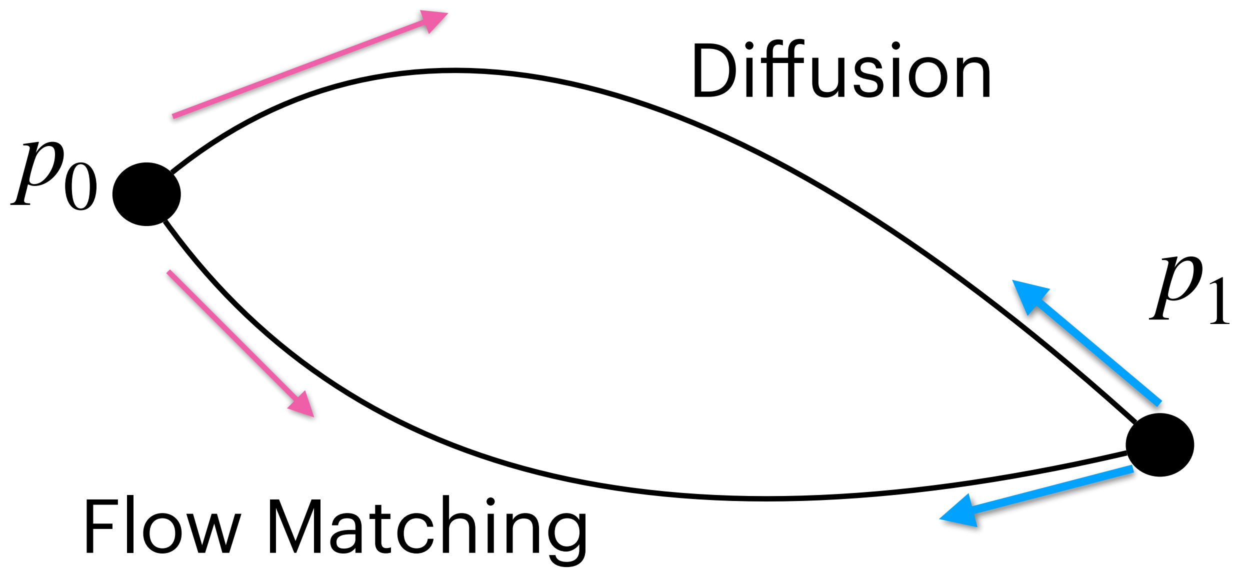
Learn the reverse process

1. $b(\cdot) := f - g^2 \nabla_x \log p(\cdot)$

Fokker Planck Equation

$$\frac{\partial p_t}{\partial t} = -\frac{\partial}{\partial x}[\boxed{f(x,t)}p(x,t)] + \frac{\partial^2}{\partial x^2}tr[\boxed{\frac{1}{2}}g^2 p(x,t)]$$



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Learn the reverse process

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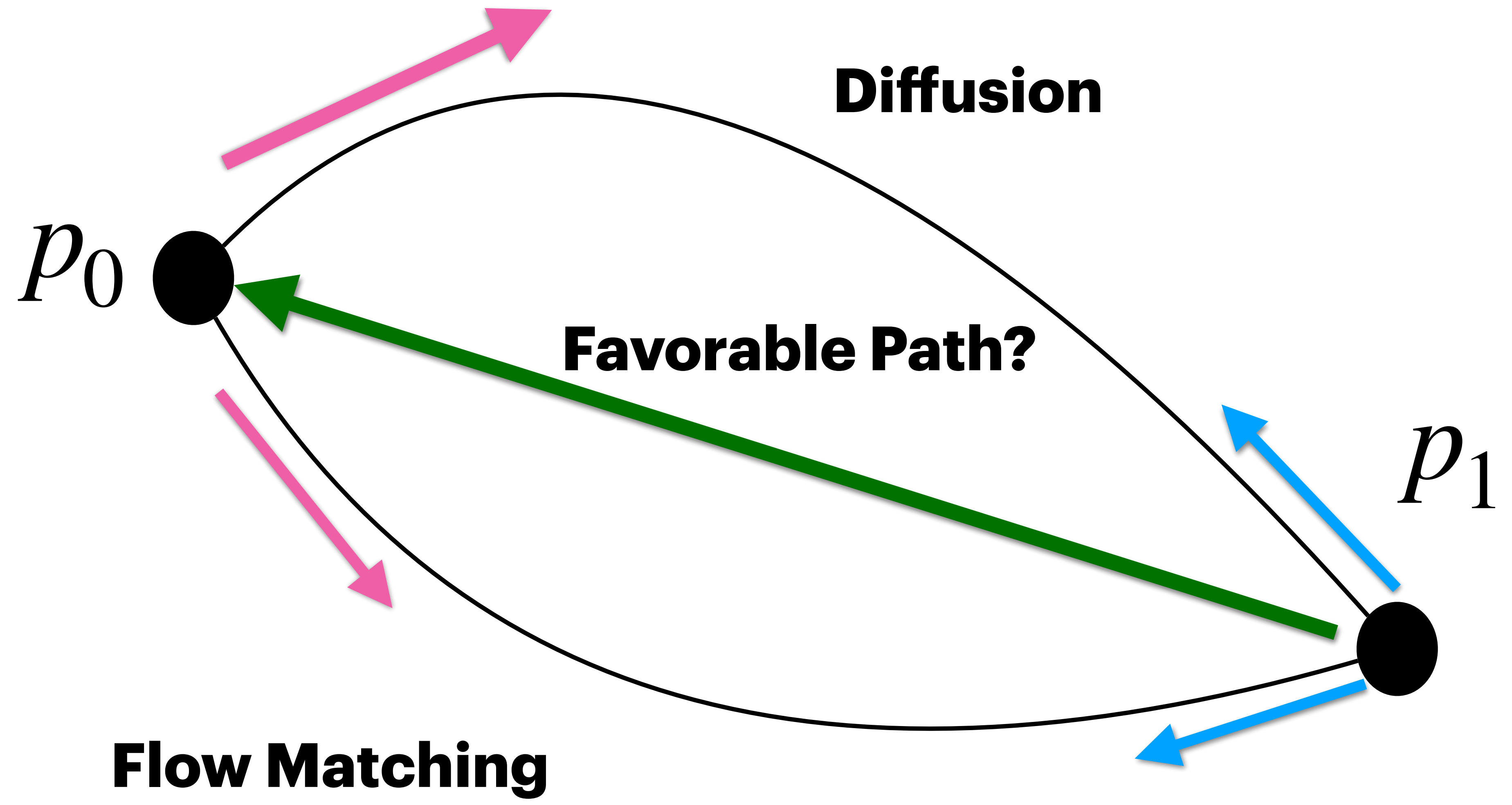
Yaron Lipman et al. "flow matching"

Design Space

1. **Take aways**
   - path measure: not unique.
   - Prior: has to be Gaussian.



Q: What is the ***favorable*** Path and Prior?

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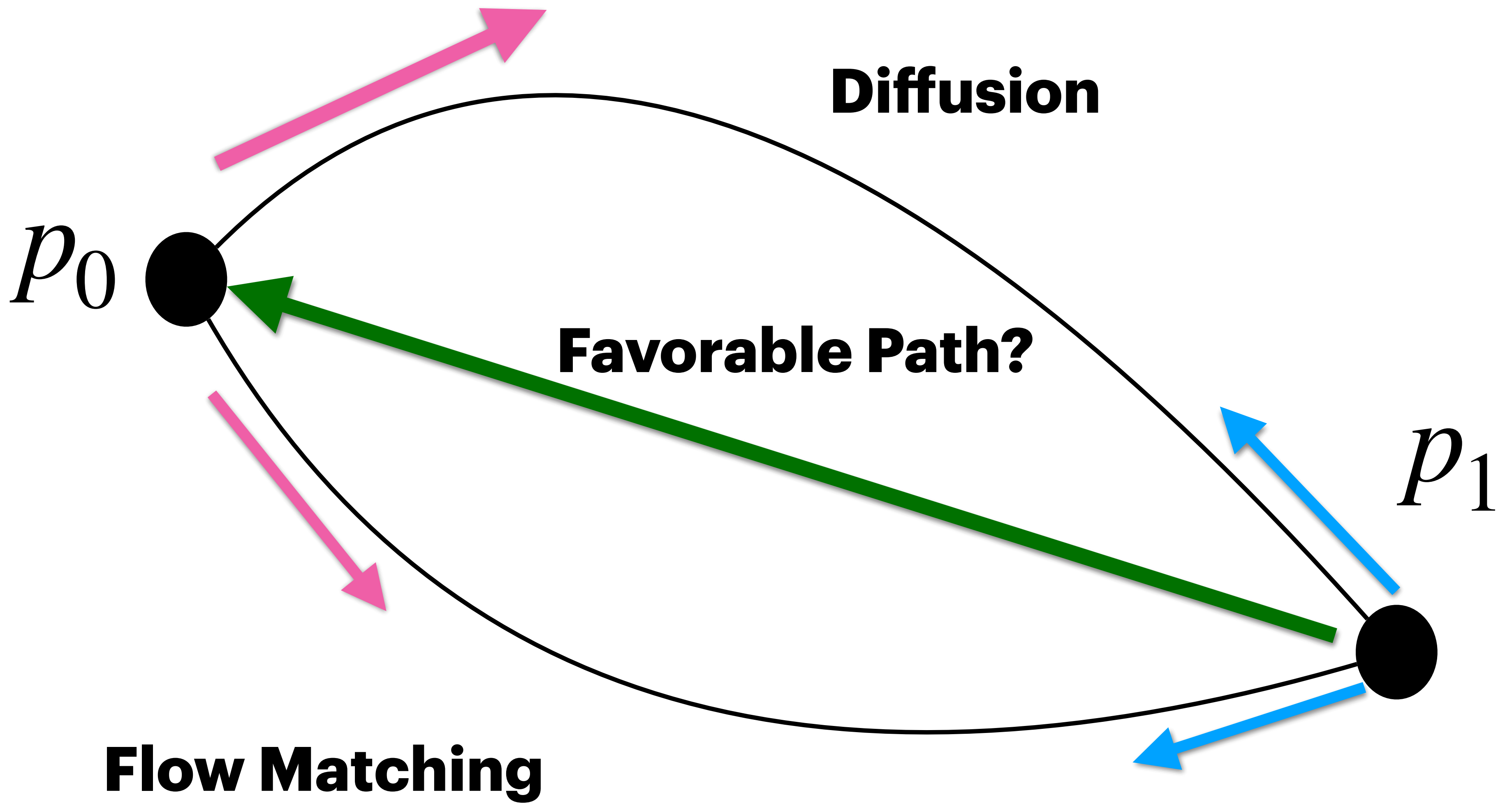

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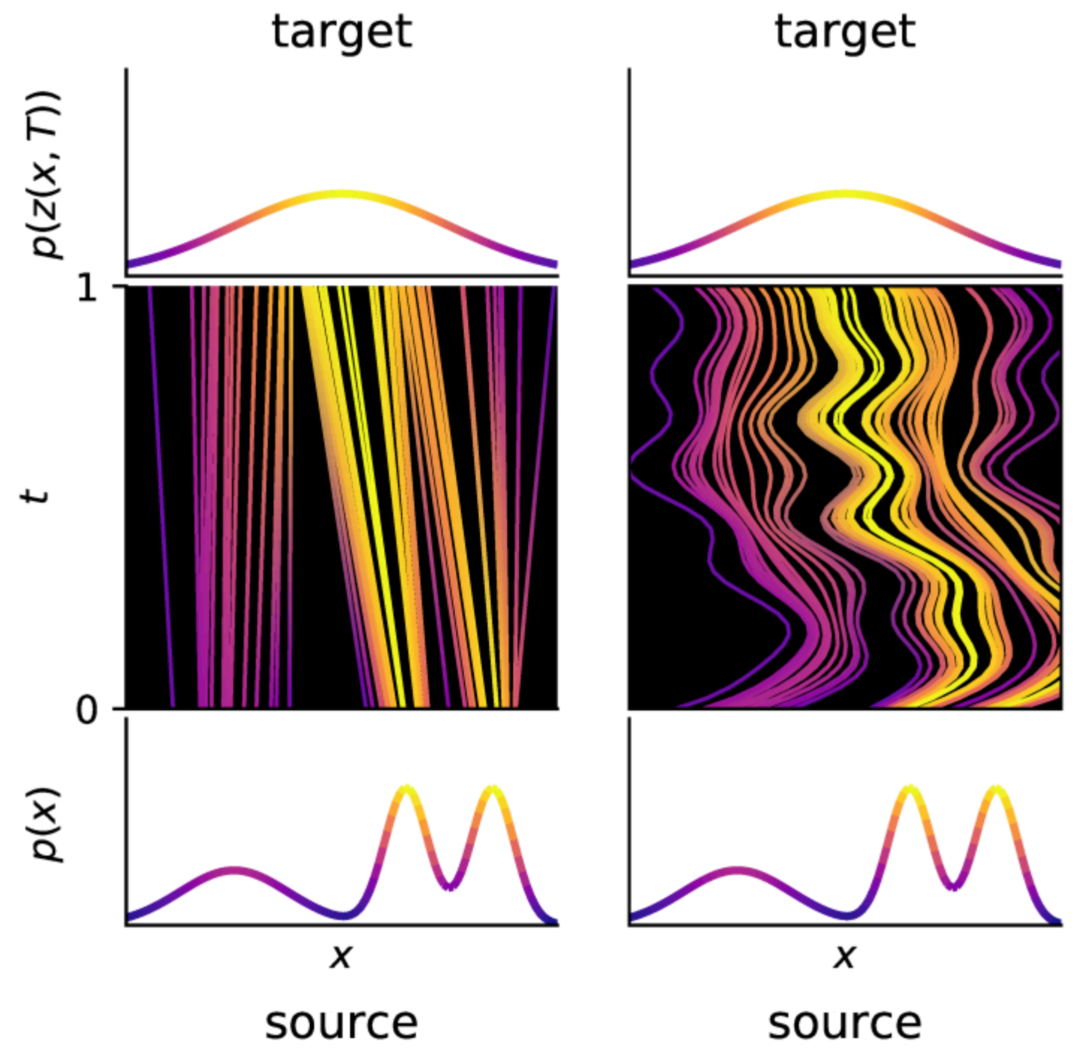
A: Task Specific:

1. **Generative Modeling:**
   1. smooth and straight **path** For fast sampling.



PC to Chris Finlay et al. 'How to Train Your Neural ODE: the World of Jacobian and Kinetic Regularization'

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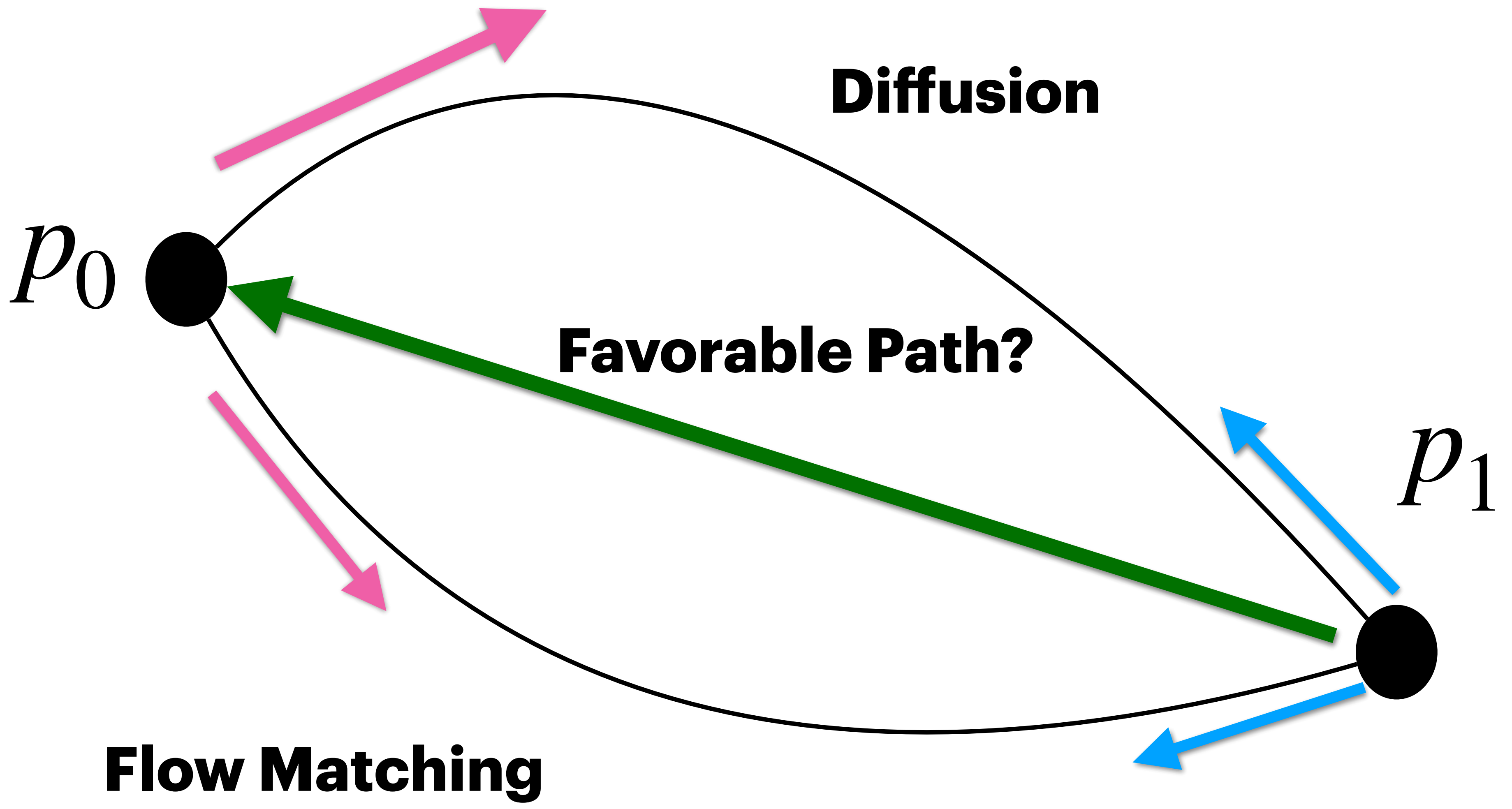

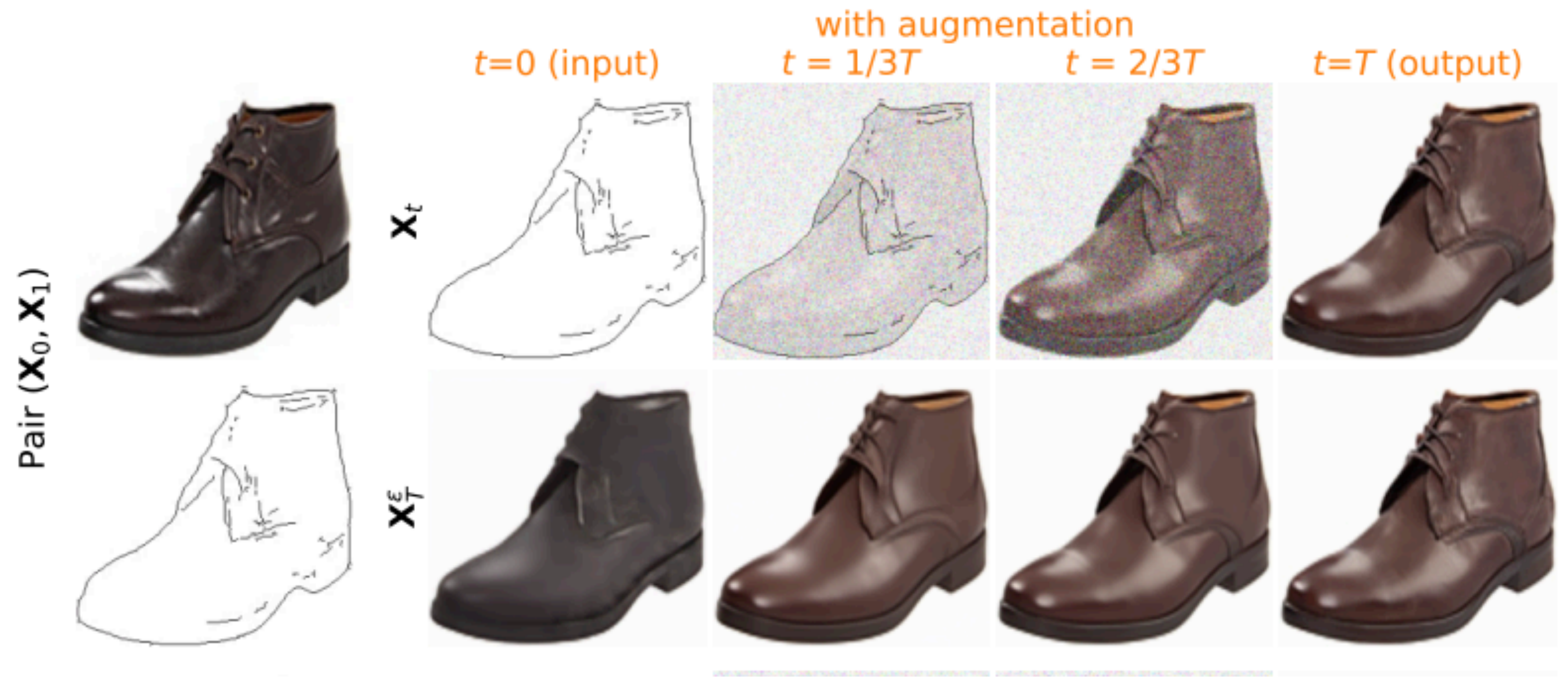

PC to Valentin et al. 'AUGMENTED BRIDGE MATCHING'

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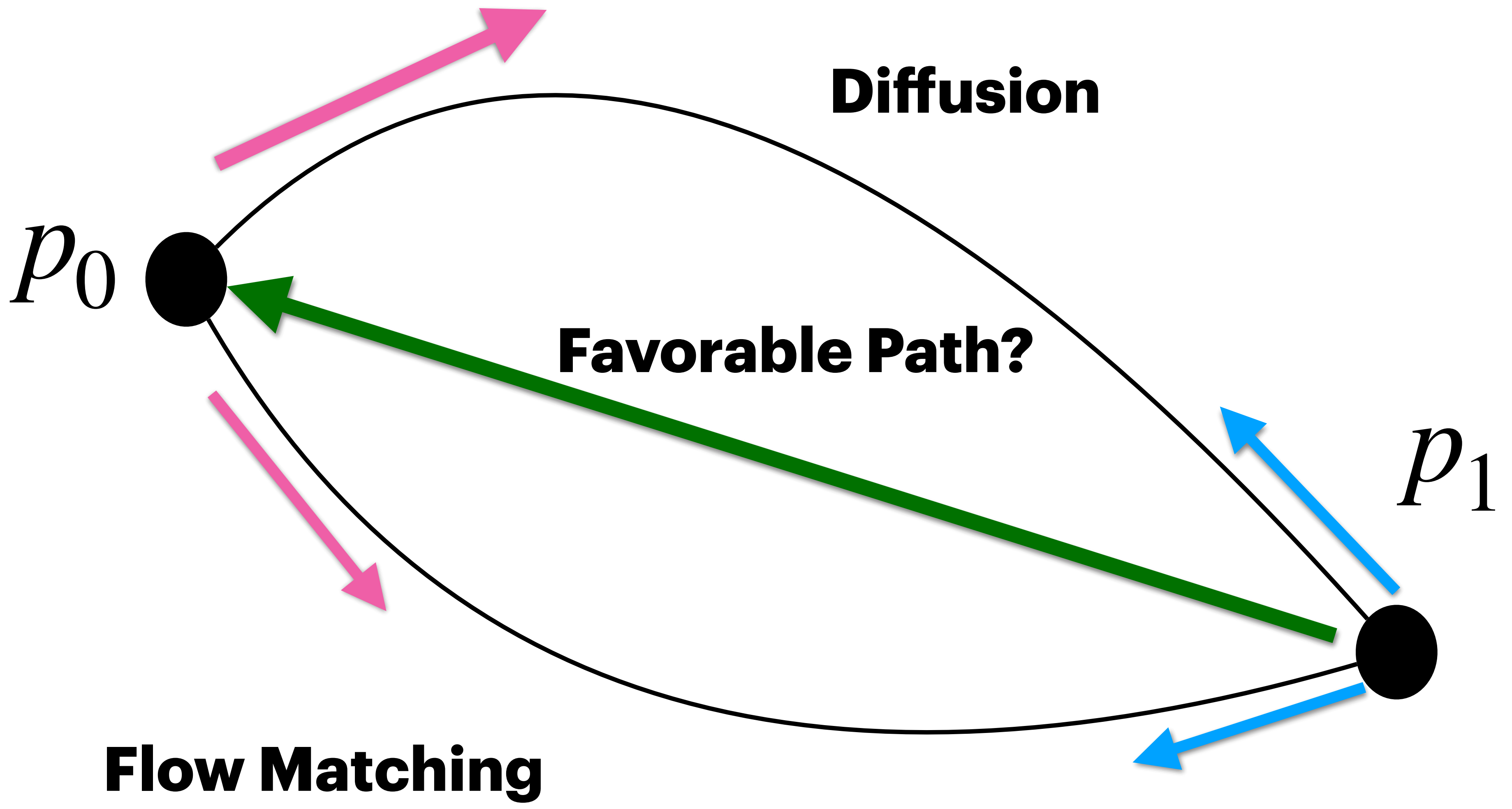

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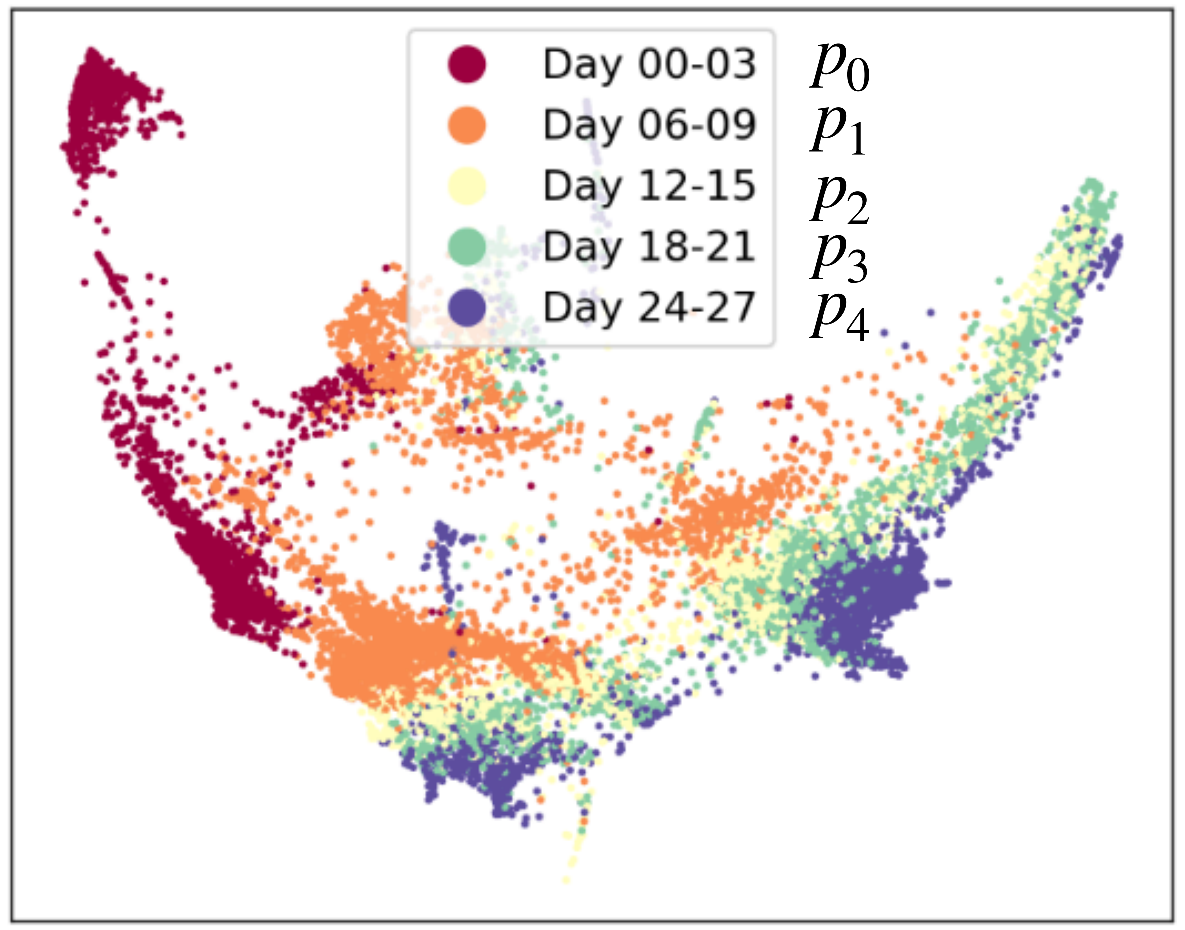
2. **Trajectory Inference:** 'Natural' Interpolation **path** between non-Gaussian distributions $p_0, p_1..., p_N$.



PC to Alex Tong et al. 'TrajectoryNet'

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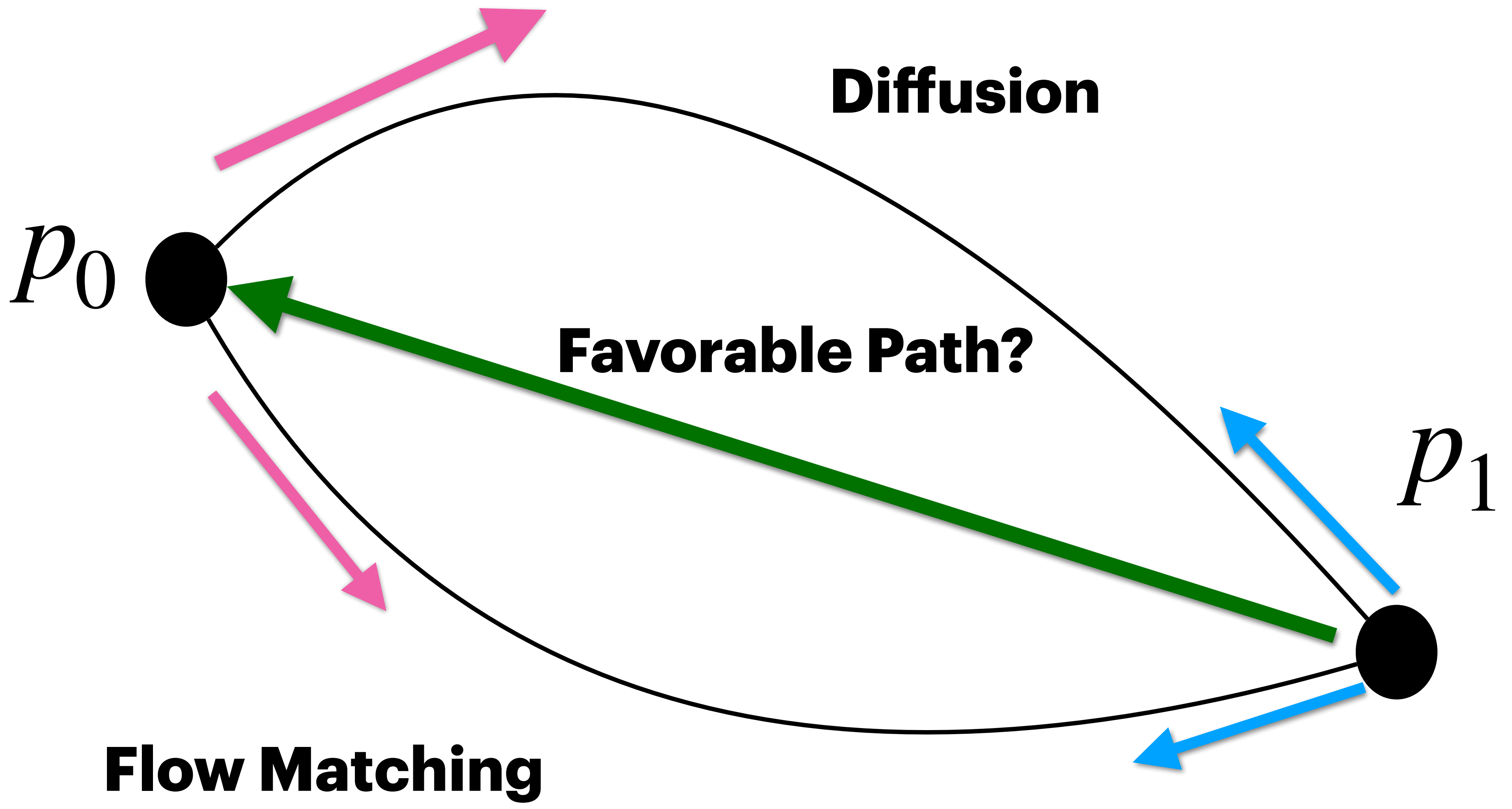
Optimality



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- Gentle Introduction.
- **Fast Sampling: Generative Modeling with Phase Stochastic Bridges**
- momentum Schrödinger Bridge for Biology
- Future Directions
- Q&A

Generative Modeling with Phase Stochastic Bridge

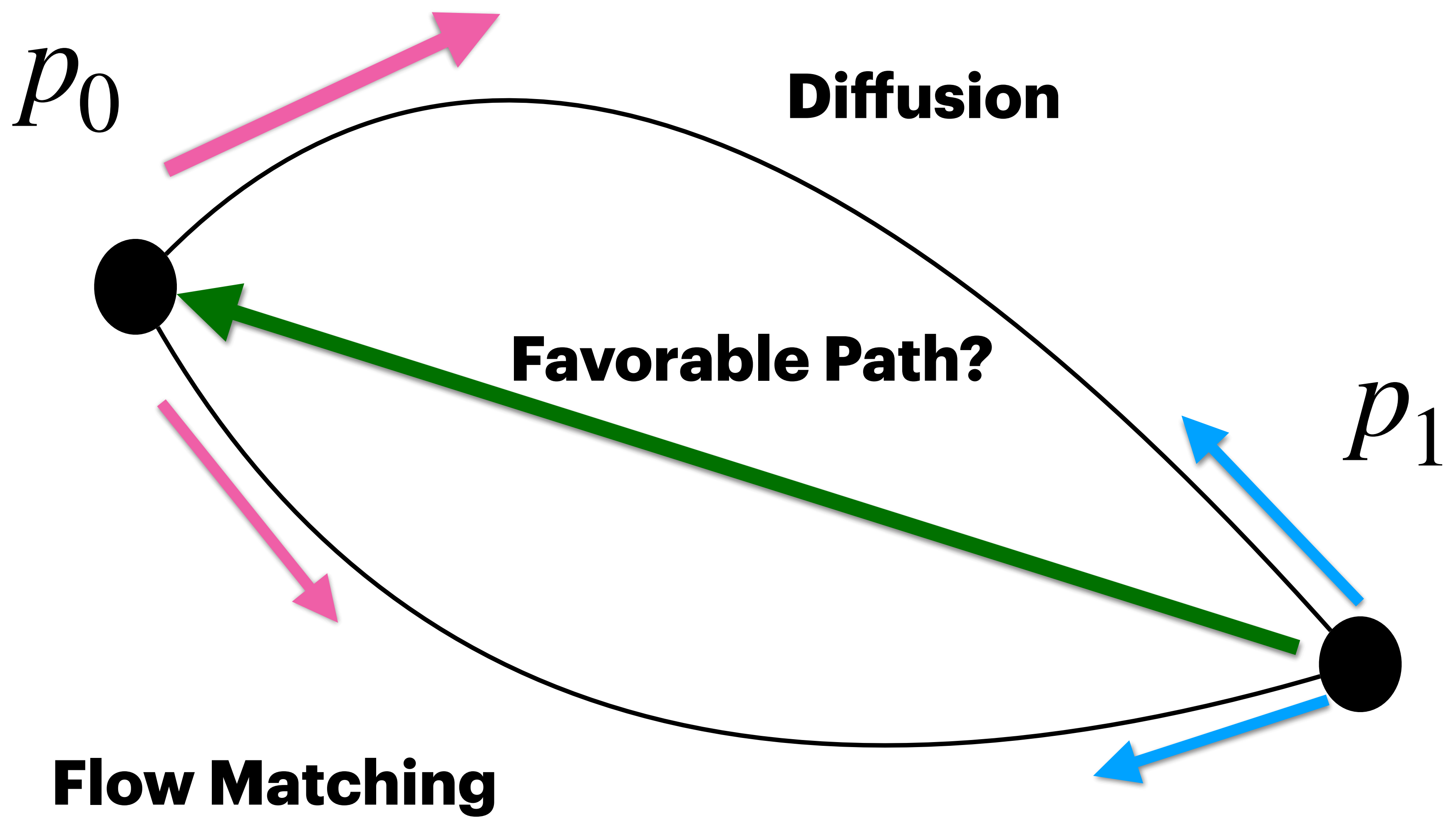
Design Space of Dynamical Generative Modeling

Task:

1. **Generative Modeling:** smooth and straight path For fast sampling.

Design Space and motivations

- Can we incorporate more information of dynamics (i.e Velocity)?
- How to Construct unique path measure which is favorable for fast sampling.



Phase Space Dynamics

$$dx_t = b(x_t, t)dt + g_t dw_t$$

$x_0 \sim p_0$

$x_1 \sim p_1$

- We would like to track the auxiliary velocity variable in the dynamics in order to further utilize them.

Phase Space Dynamics

$$dx_t = v_t dt$$

$$dv_t = a(x_t, v_t, t)dt + g_t dw_t$$

$$\cancel{dx_t = b(x_t, t)dt + g_t dw_t}$$

$x_0 \sim p_0$

$x_1 \sim p_1$

- We use Phase space dynamics (Newtonian Dynamics [1]) in which we have auxiliary velocity variable in the dynamics, similar to Critically Damped Langevin Dynamics ([2],CLD).

[1] https://en.wikipedia.org/wiki/Newtonian_dynamics
[2] Dockhorn, Tim, Arash Vahdat, and Karsten Kreis. "Score-based generative modeling with critically-damped langevin diffusion." *arXiv preprint arXiv:2112.07068* (2021).

Stochastic Optimal Control Phase Space Dynamics

$$dx_t = v_t dt$$
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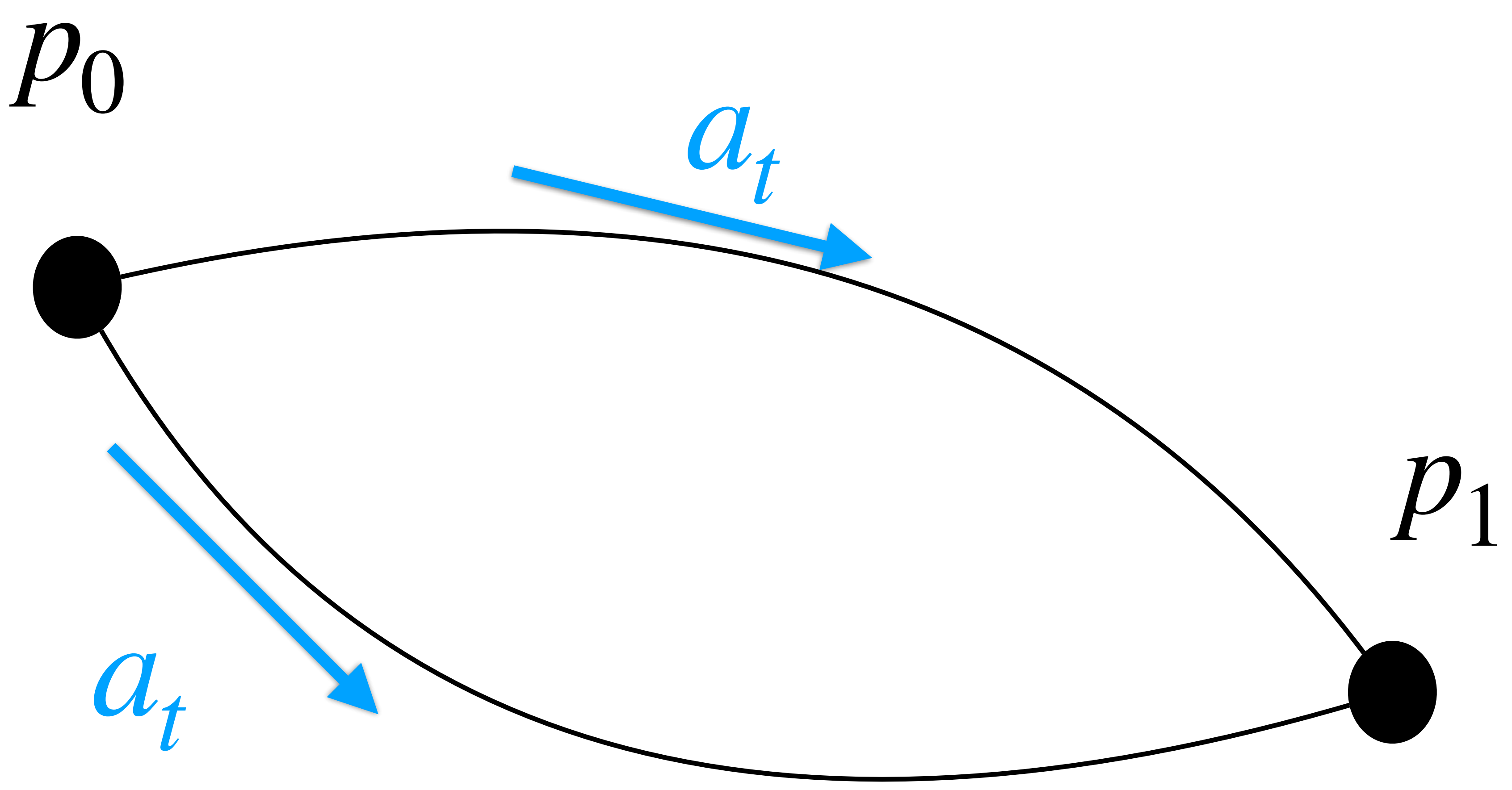

- **Q:**However, <u>The trajectory is still not unique since a_t is not unique .</u> Which trajectories are we looking for?
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Stochastic Optimal Control Phase Space Dynamics

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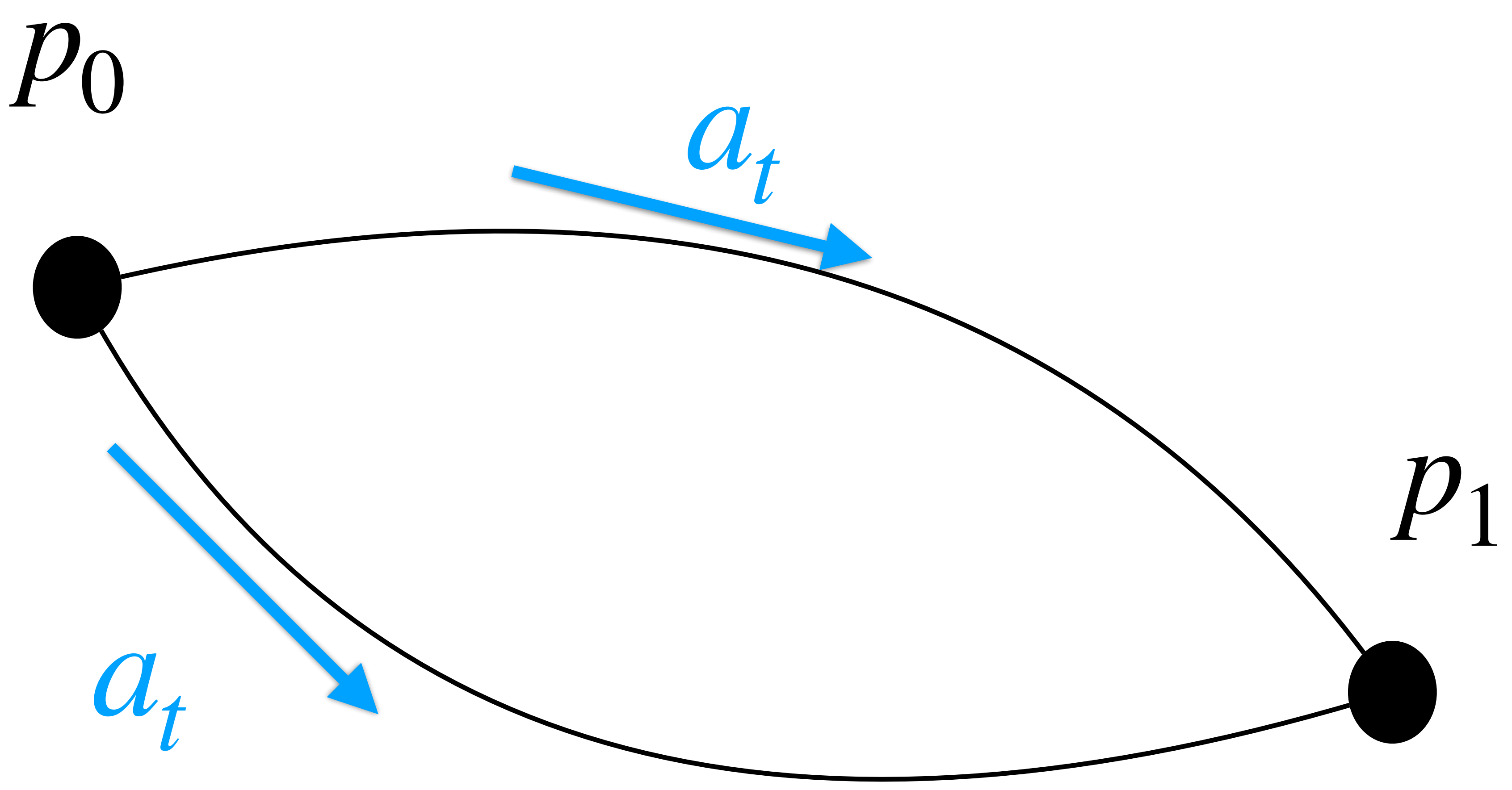

- **Q:**However, <u>The trajectory is still not unique since a_t is not unique .</u> Which trajectories are we looking for?
- **A:**We hope the path is straight and smooth in the position and velocity space! The **sub-optimal** drift term is the **<u>solution of a Stochastic Optimal Control (SOC) Problem</u>**!

$$a^* = argmin_a \mathbb{E}\left[\int_0^1 ||a_t(x_t, v_t, t)||_2^2 dt\right]$$

s.t
$$dx_t = v_t dt$$
$$dv_t = a(x_t, v_t, t)dt + g_t dw_t$$
$$(x_0, x_1) \sim p_0 \otimes p_1$$

Stochastic Optimal Control Phase Space Dynamics

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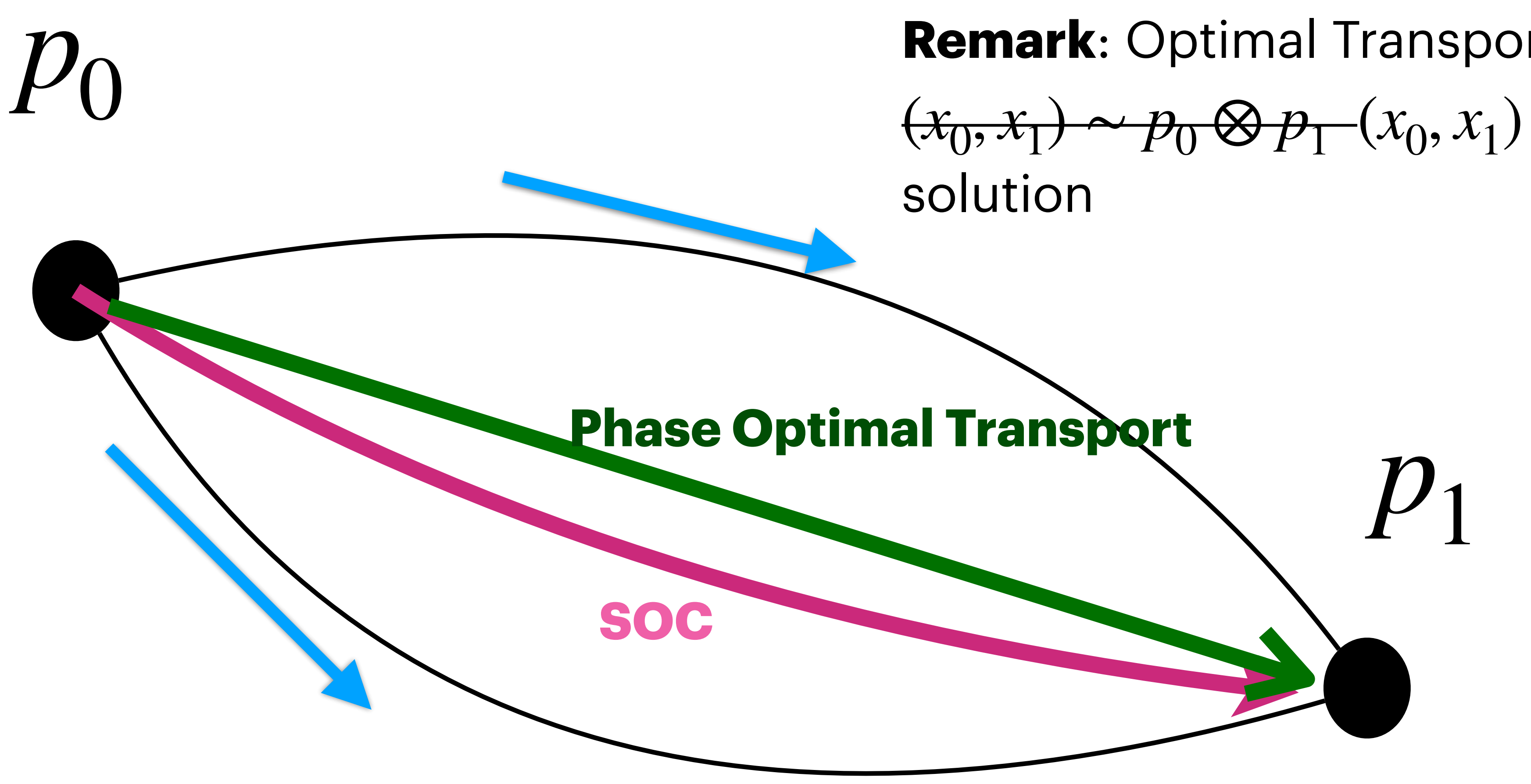

Remark: Optimal Transport needs correct pairing $\cancel{(x_0, x_1) \sim p_0 \otimes p_1}$ $(x_0, x_1) \sim \Pi^{OT}(p_0, p_1)$ + SOC solution

$$a^* = g_t^2 P_{11}\left[\frac{x_1 - x_t}{1 - t} - v_t\right]$$

$$P_{11} := \frac{-4}{g_t^2(t-1)}$$

Stochastic Optimal Control Phase Space Dynamics

$x_0 \sim p_0$  $x_1 \sim p_1$

$$\begin{bmatrix} \mathrm{d}\mathbf{x}_t \\ \mathrm{d}\mathbf{v}_t \end{bmatrix} = \begin{bmatrix} \mathbf{v}_t \\ \mathbf{F}_t \end{bmatrix} \mathrm{d}t + \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & g_t \end{bmatrix} \mathrm{d}\mathbf{w}_t \quad \text{s.t} \quad \mathbf{m}_0 := \begin{bmatrix} \mathbf{x}_0 \\ \mathbf{v}_0 \end{bmatrix} \sim \mathcal{N}(\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0),$$

$$\text{Bridge Matching SDE} : \mathbf{F}_t := \mathbf{F}_t^b(\mathbf{m}_t, t) \equiv \mathbf{a}_t^*(\mathbf{m}_t, t),$$

$$\text{Probablistic ODE} : \mathbf{F}_t := \mathbf{F}_t^p(\mathbf{m}_t, t) \equiv \mathbf{a}_t^*(\mathbf{m}_t, t) - \frac{1}{2} g_t^2 \nabla_{\mathbf{v}} \log p(\mathbf{m}, t)$$

Quality

Speed

- **Training:** One can regress F_t using neural network to construct the SDE or ODE to make the bridge between two distributions.

$$L = \mathbb{E}_t \mathbb{E}_{x_0} \mathbb{E}_{x_t} || F_t^\theta(x_t, v_t, t) - F_t ||_2^2$$

Wait, why it is better?

Design Space of Dynamical Generative Modeling

Task:

1. **Generative Modeling:** smooth and straight path For fast sampling.

2. Design Space and motivations

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- Construct unique path measure which is favorable for fast sampling.

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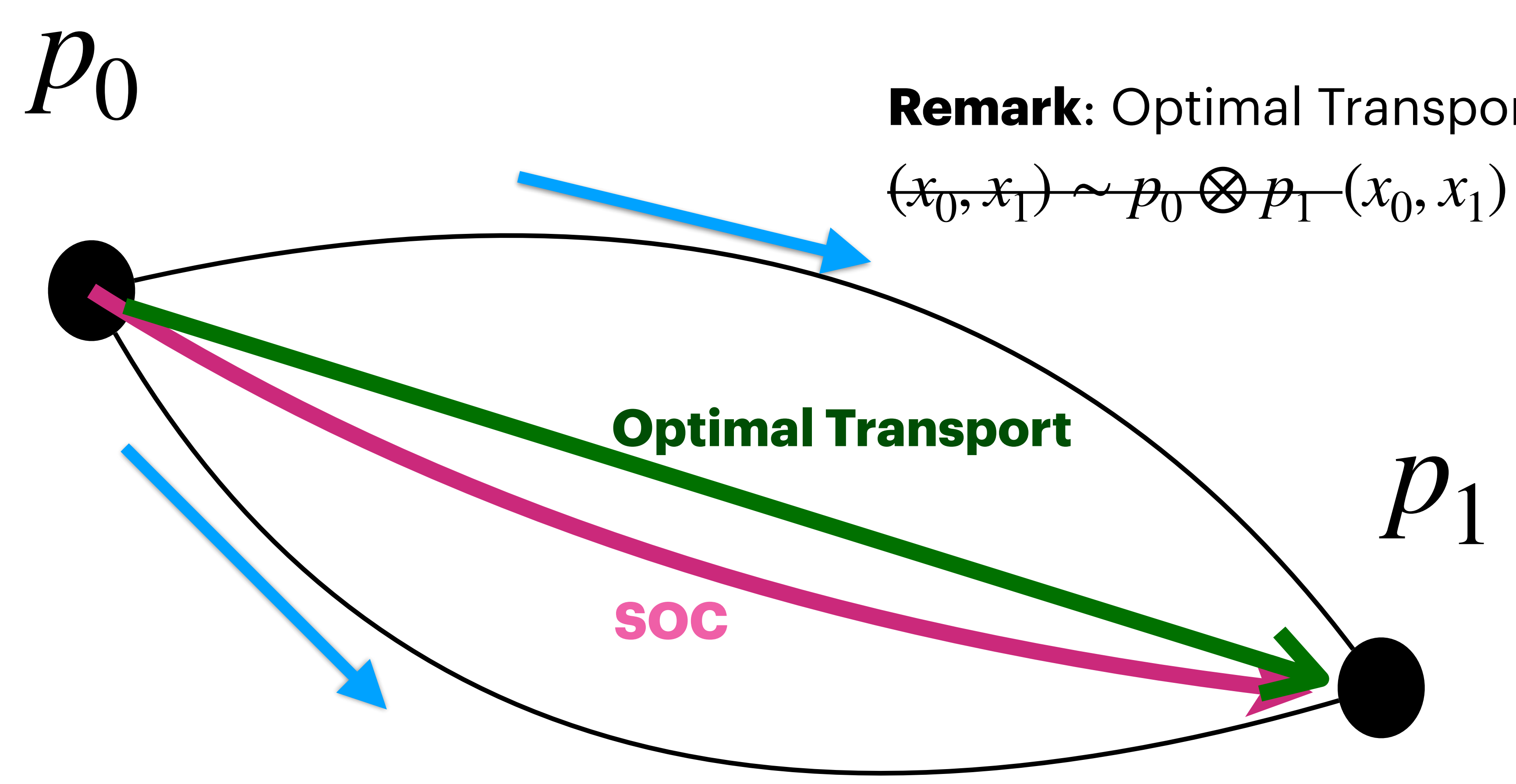
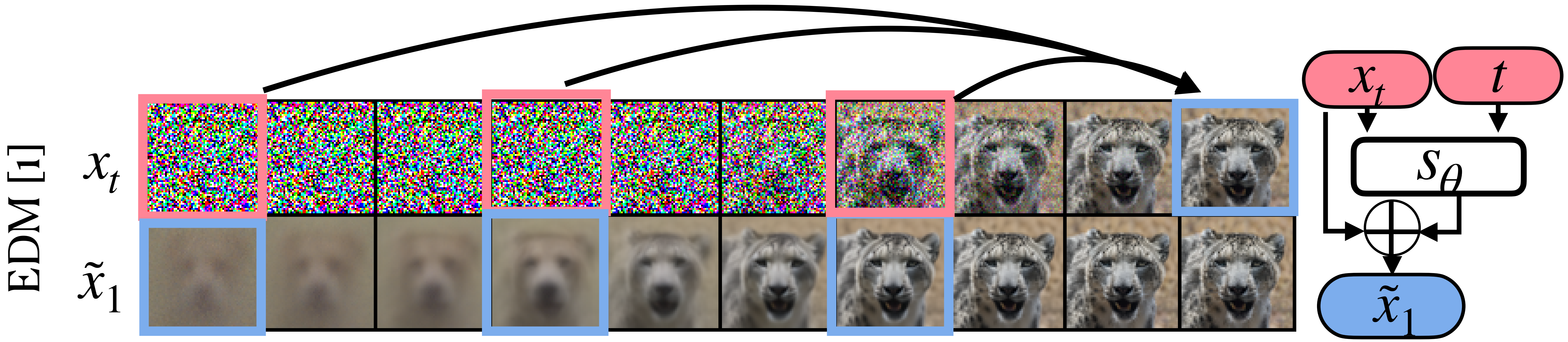


Sampling Hop

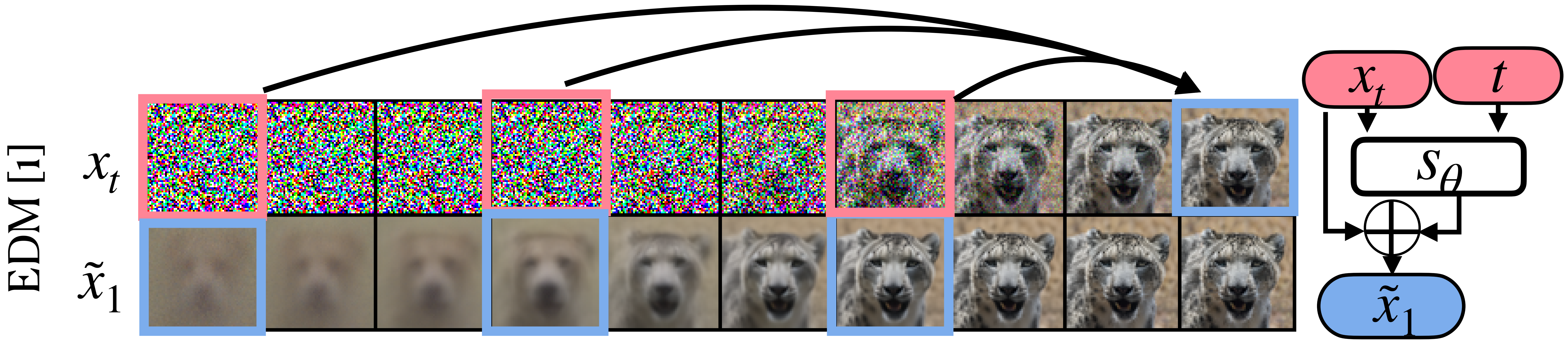
With additional information of the dynamics



[1]Karras, Tero, et al. "Elucidating the design space of diffusion-based generative models."

Sampling Hop

With additional information of the dynamics



CLD[2]

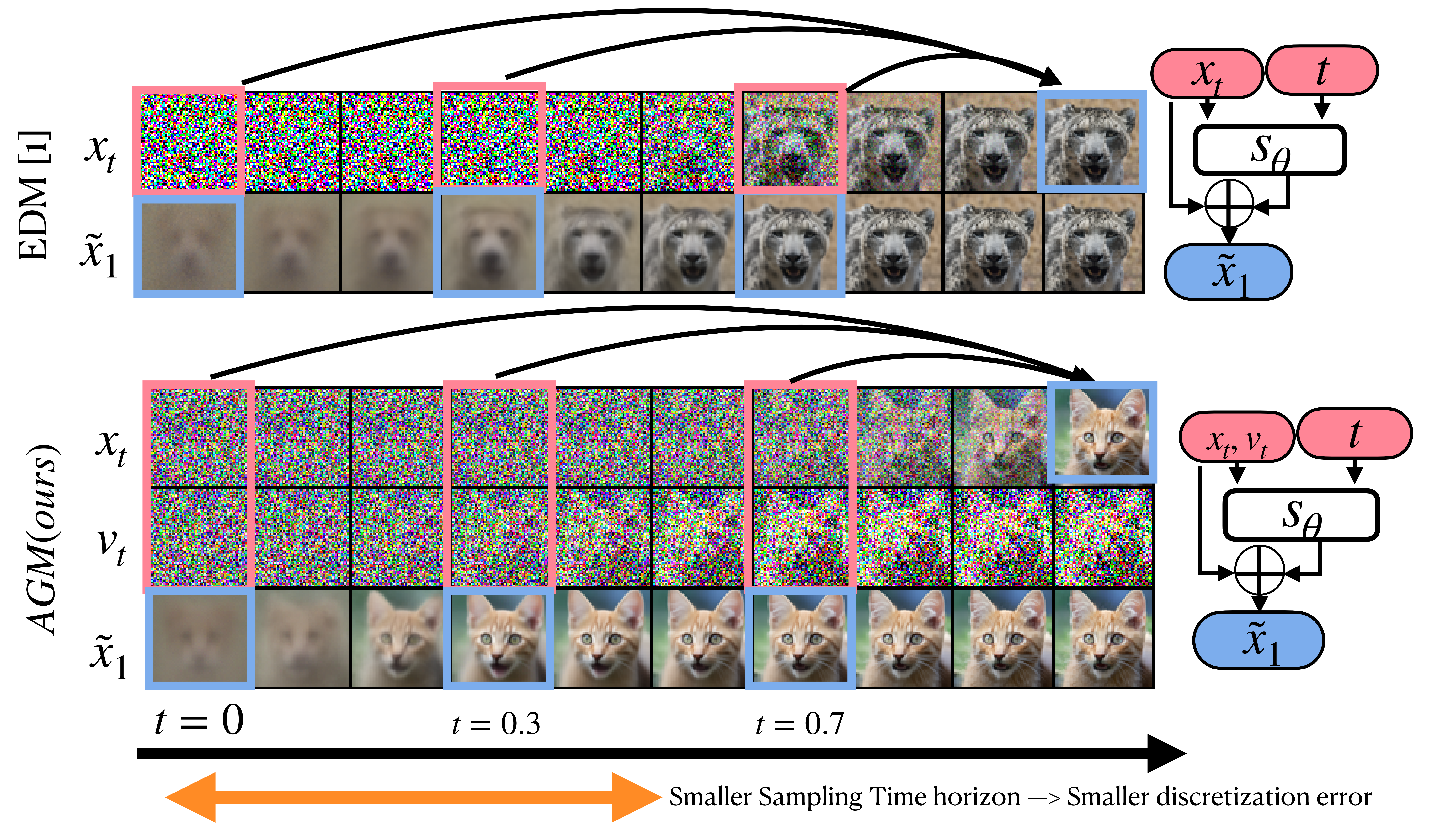
Regressing $\nabla_v \log p(x, v, t)$ ✖→ Predict $\tilde{x}_1$

[1]Karras, Tero, et al. "Elucidating the design space of diffusion-based generative models."

[2]Dockhron et al. Critically Damped Langevin Dynamics

Sampling Hop

With additional information of the dynamics



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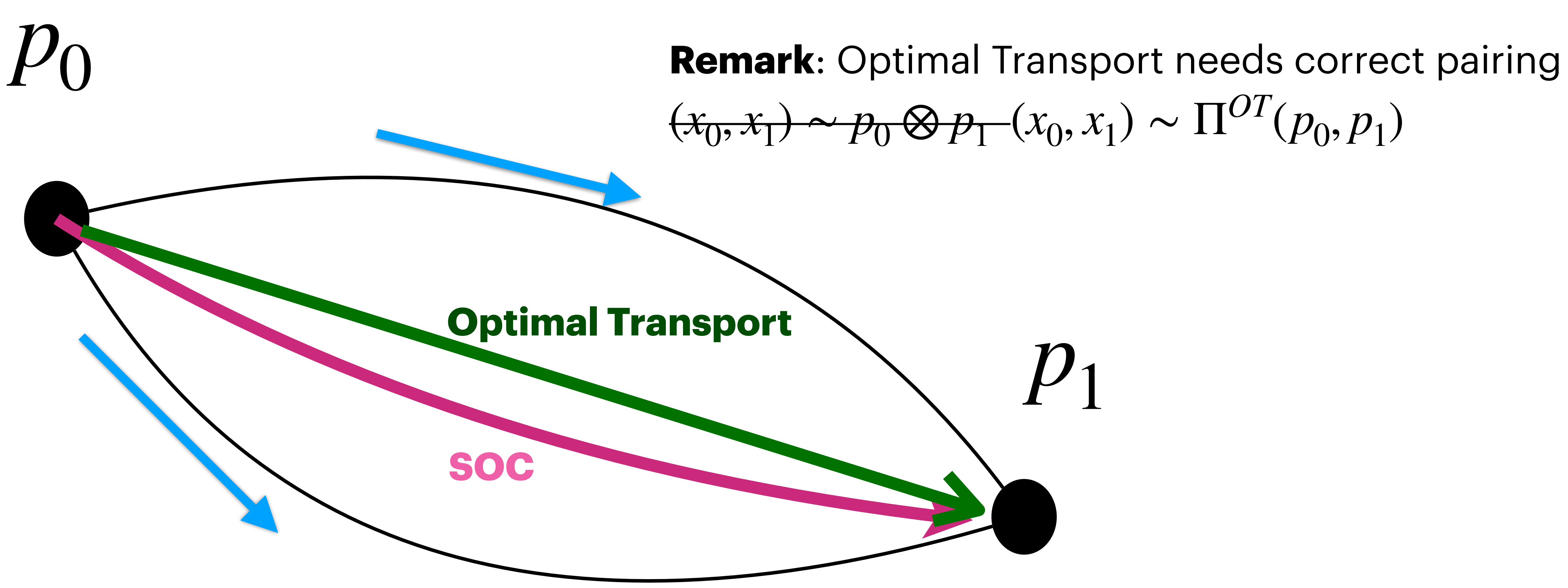
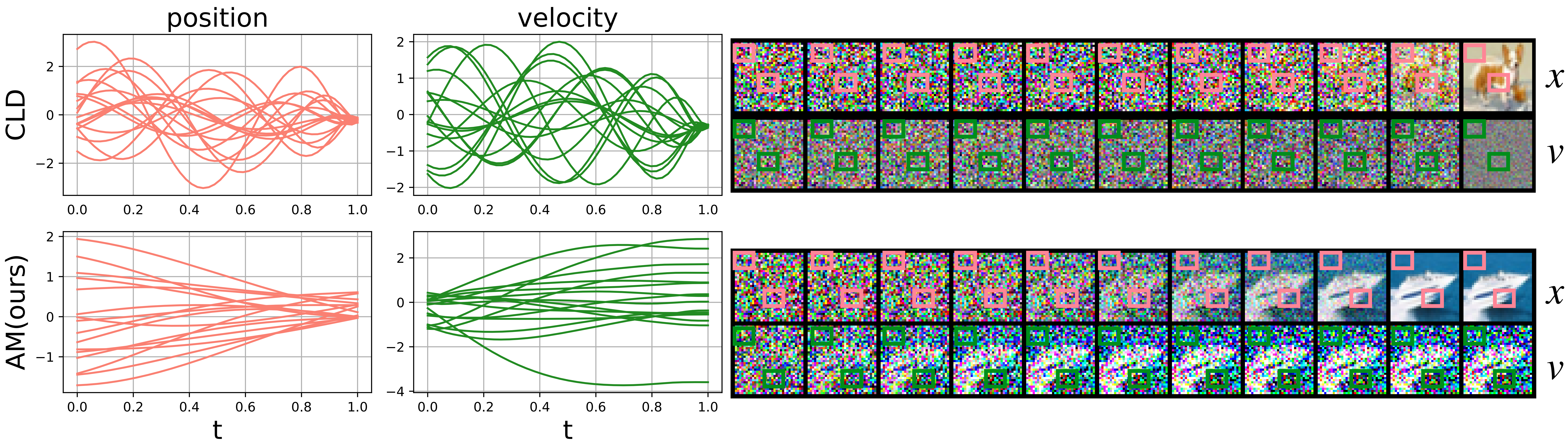
- Construct unique path measure which is favorable for sampling



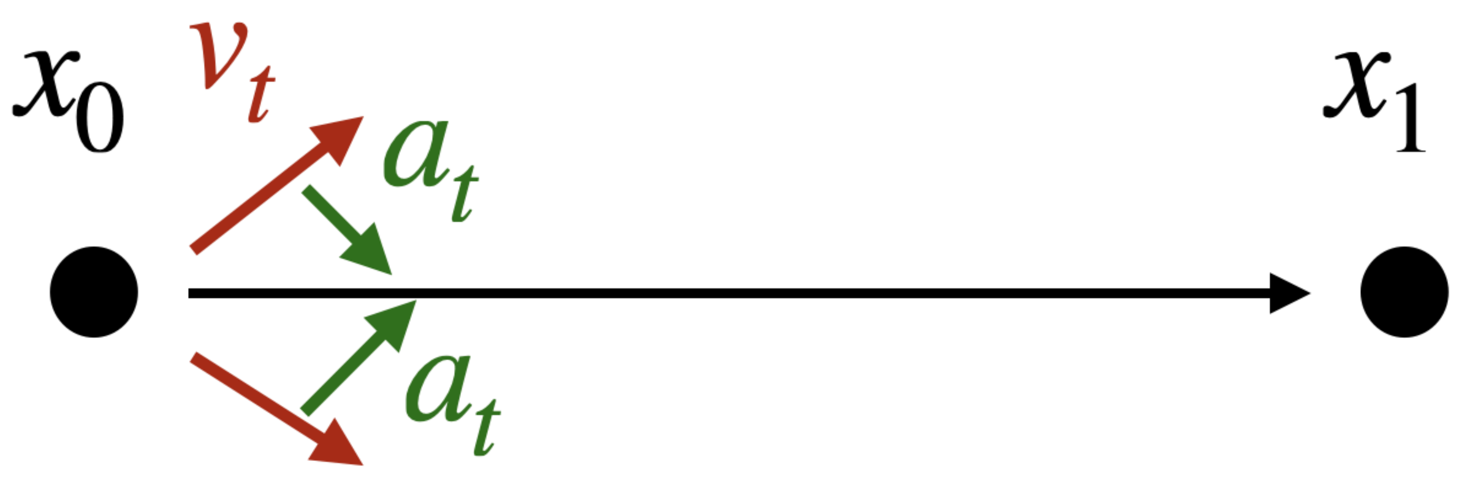
Stochastic Optimal Control

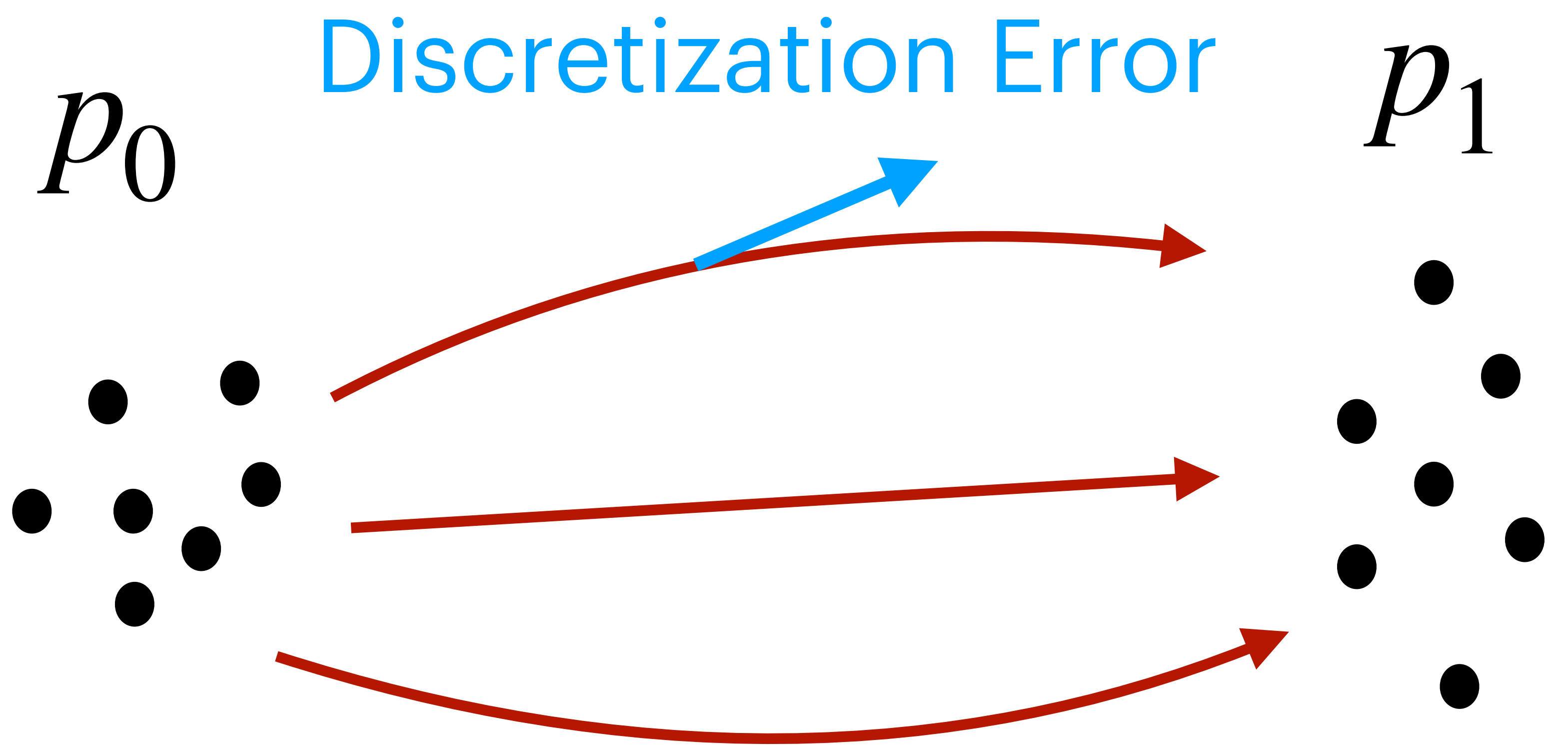
Induces Smoother and Straighter Trajectories

Trajectories of random sampled pixels compared with Critically Damped Langevin Dynamics.

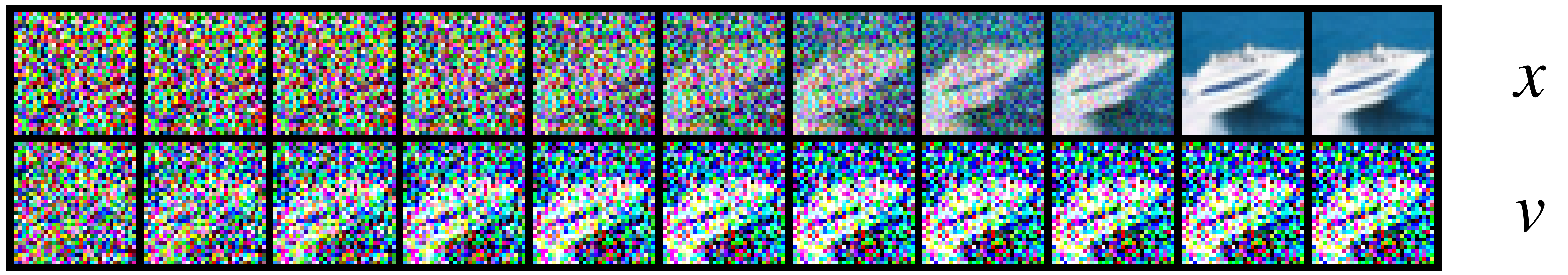


Stable Velocity Field

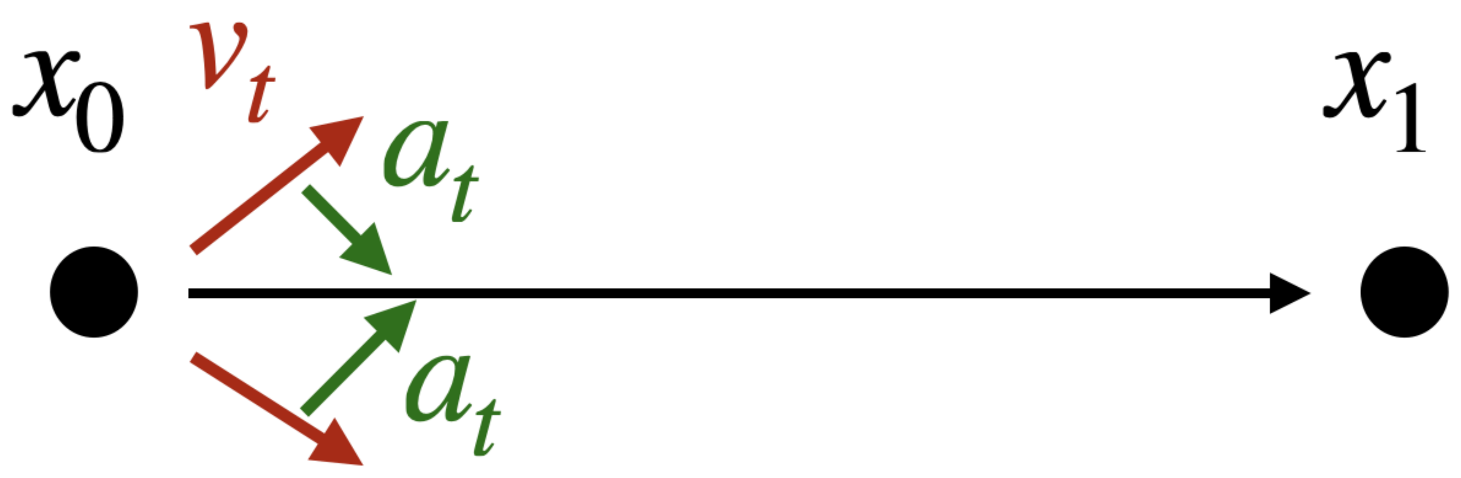


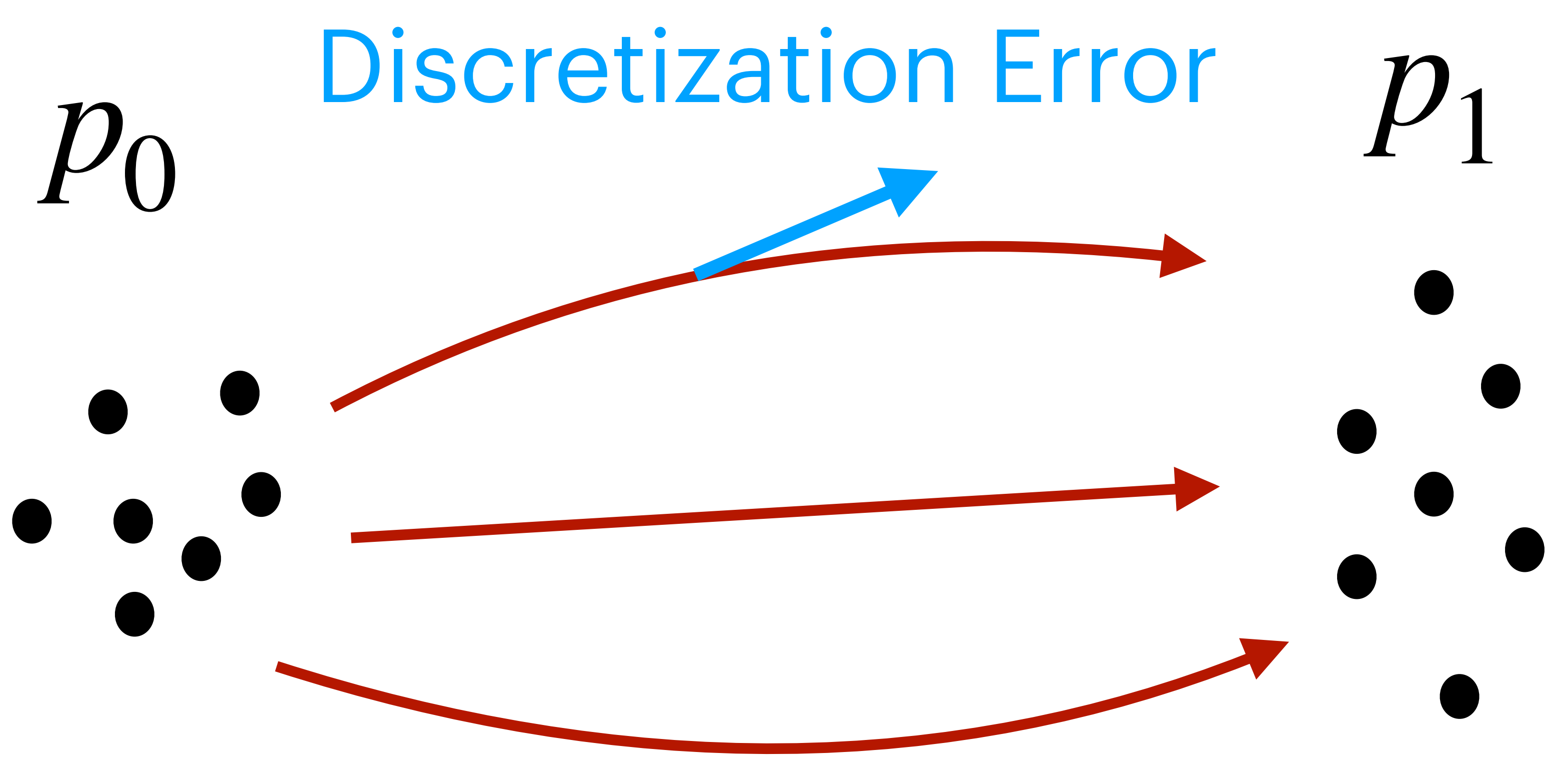


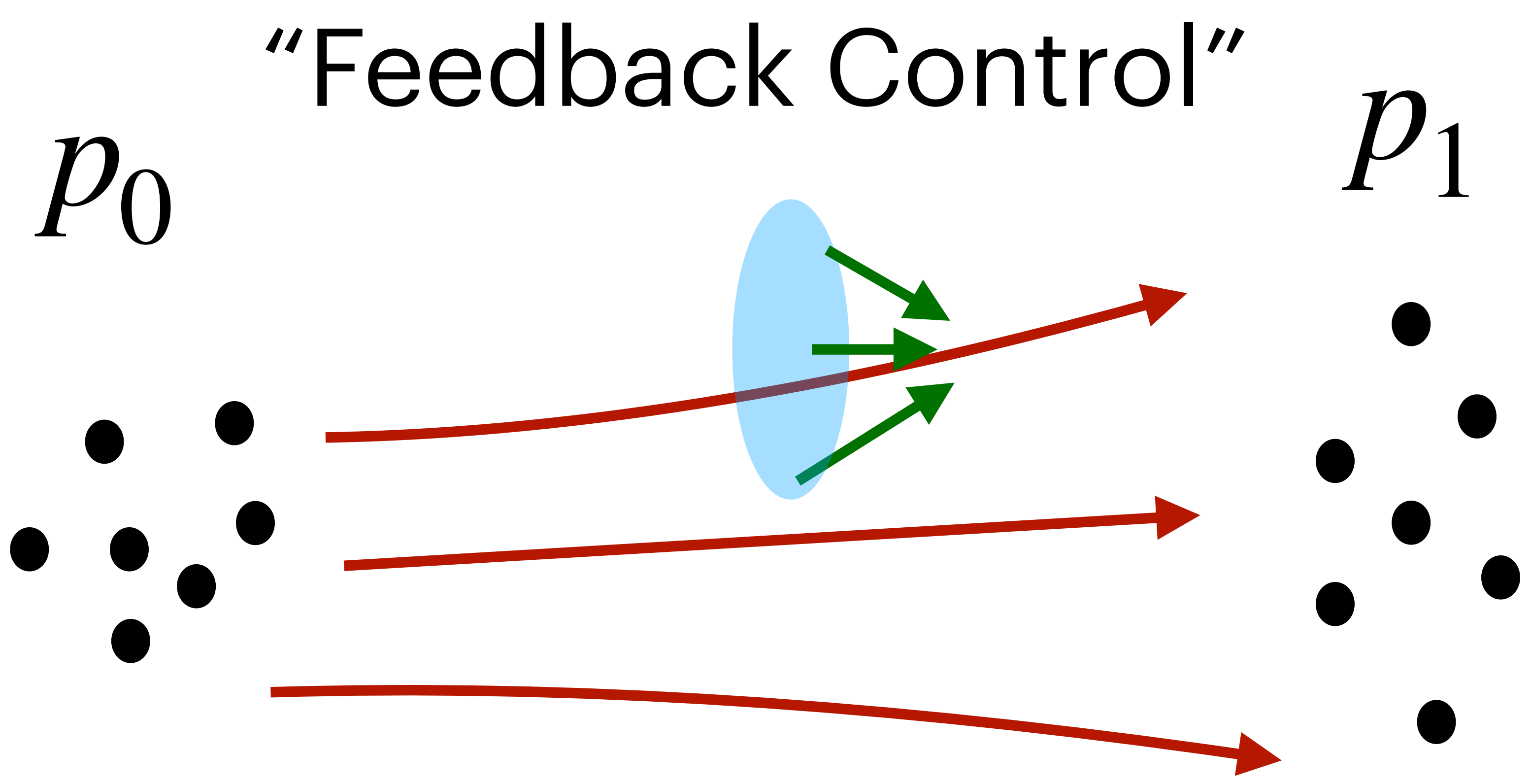
1. During training, both velocity and position are perturbed.
2. The variance of velocity is large which has high tolerance to discretization error.

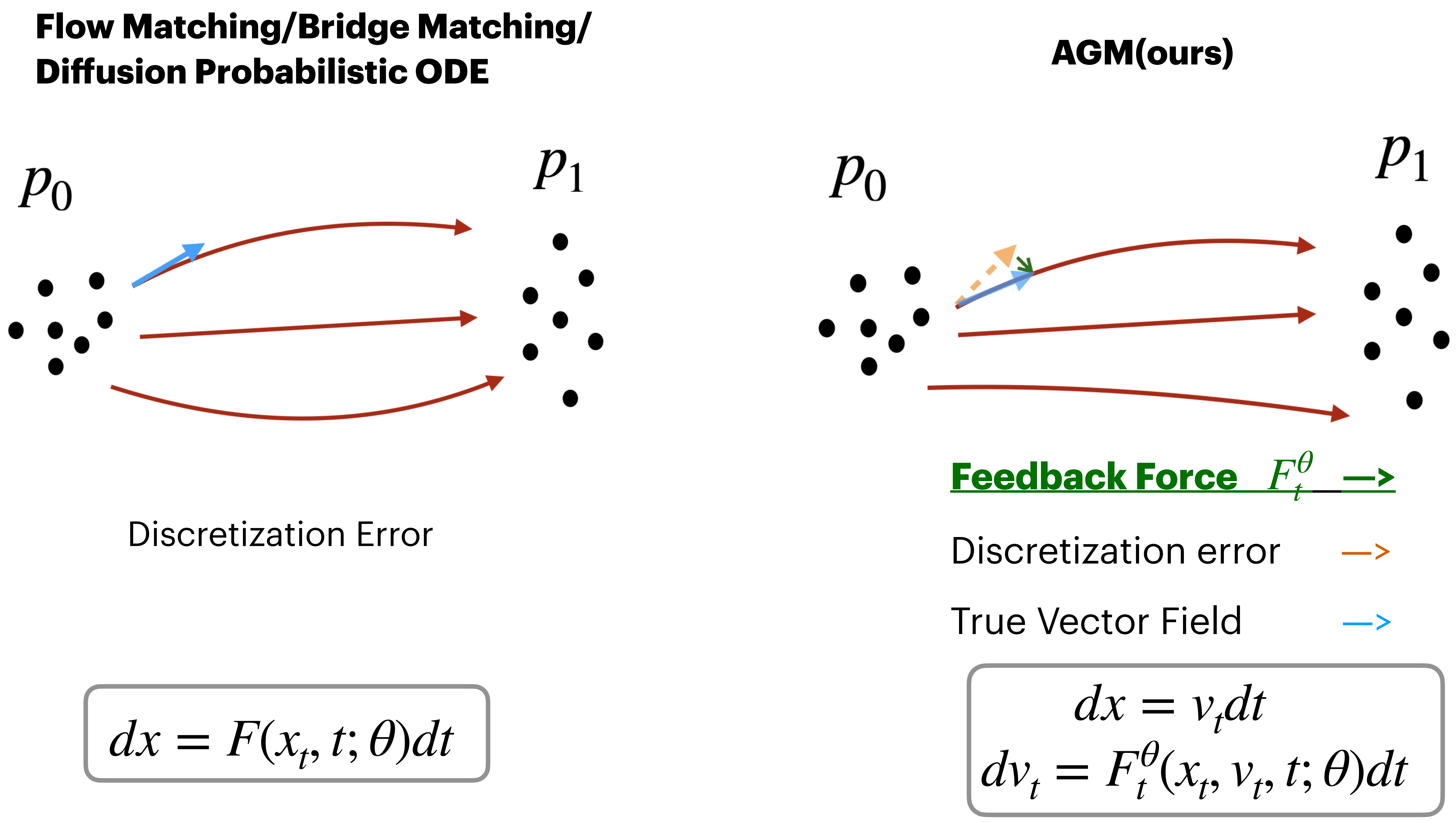


Stable Velocity Field

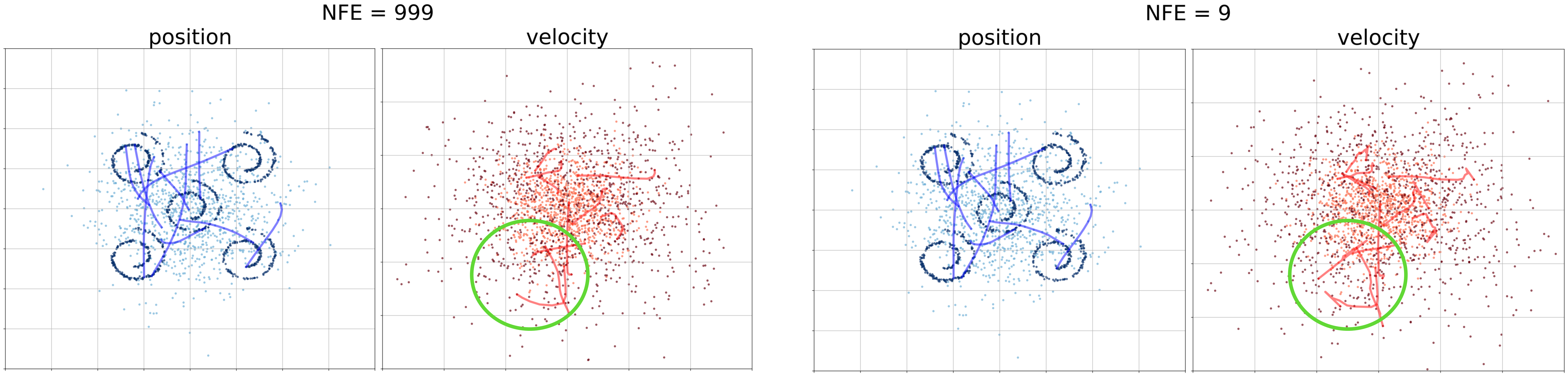







Flow Matching/Bridge Matching/
Diffusion Probabilistic ODE
p_0
p_1
Discretization Error
$dx = F(x_t, t; \theta)dt$
AGM(ours)
p_0
p_1
Feedback Force F_t^θ
Discretization error
True Vector Field
$dx = v_t dt$
$dv_t = F_t^\theta(x_t, v_t, t; \theta)dt$

FeedBack Force



1. When NFE is 100 times less, AGM is not accurately solving the ODE (see green circle).
2. Due to Force Feed Back Control, the position trajectory will not change and keep straight.

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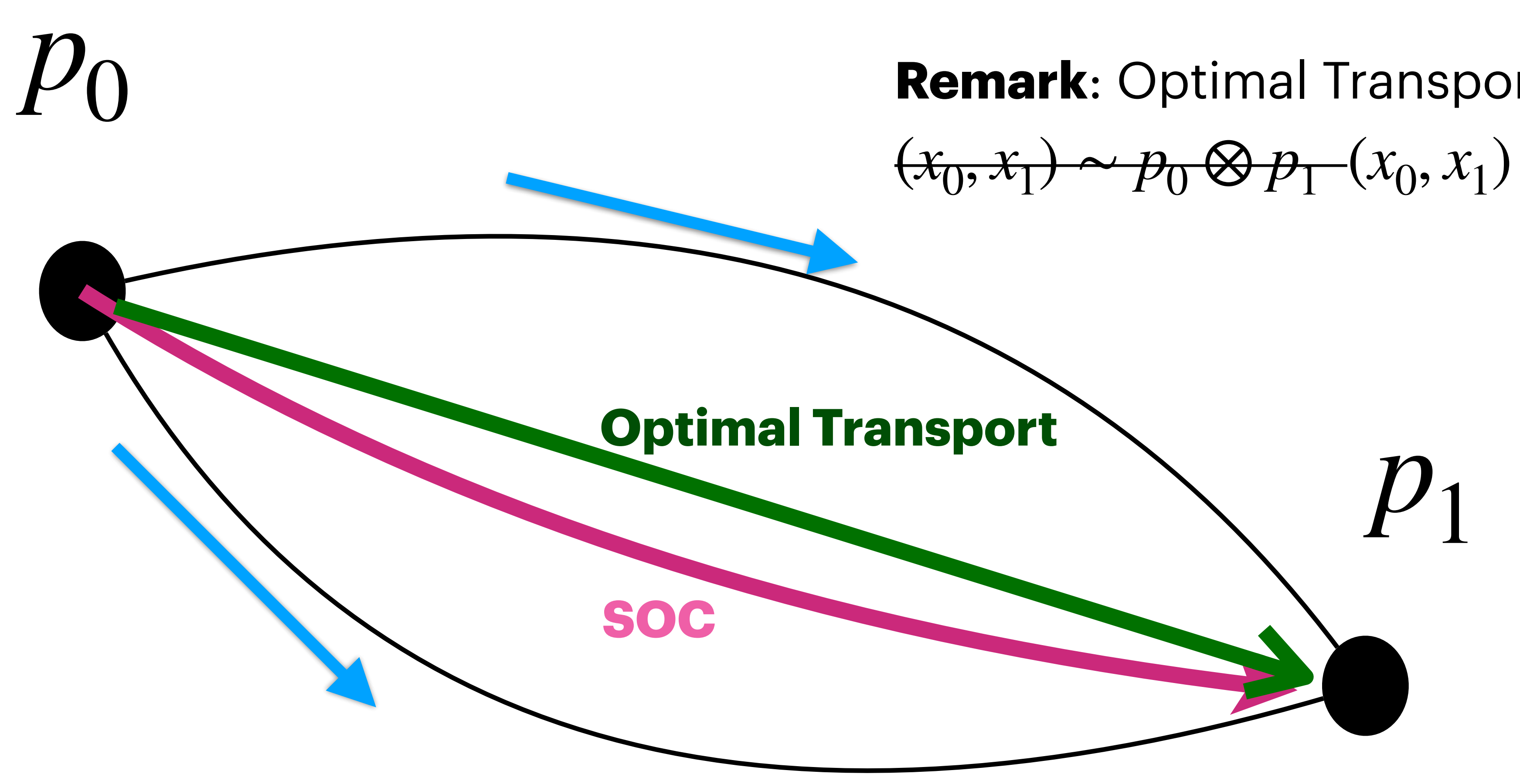
1. **Generative Modeling:** smooth and straight path For fast sampling.

Remark: Optimal Transport needs correct pairing
$\cancel{(x_0, x_1) \sim p_0 \otimes p_1}\ (x_0, x_1) \sim \Pi^{OT}(p_0, p_1)$



2. Design Space and motivations

- Let model incorporate <u>more information</u> of dynamics (i.e Velocity).
- Construct <u>unique path measure</u> which is <u>favorable for sampling</u>

} **That's it?**

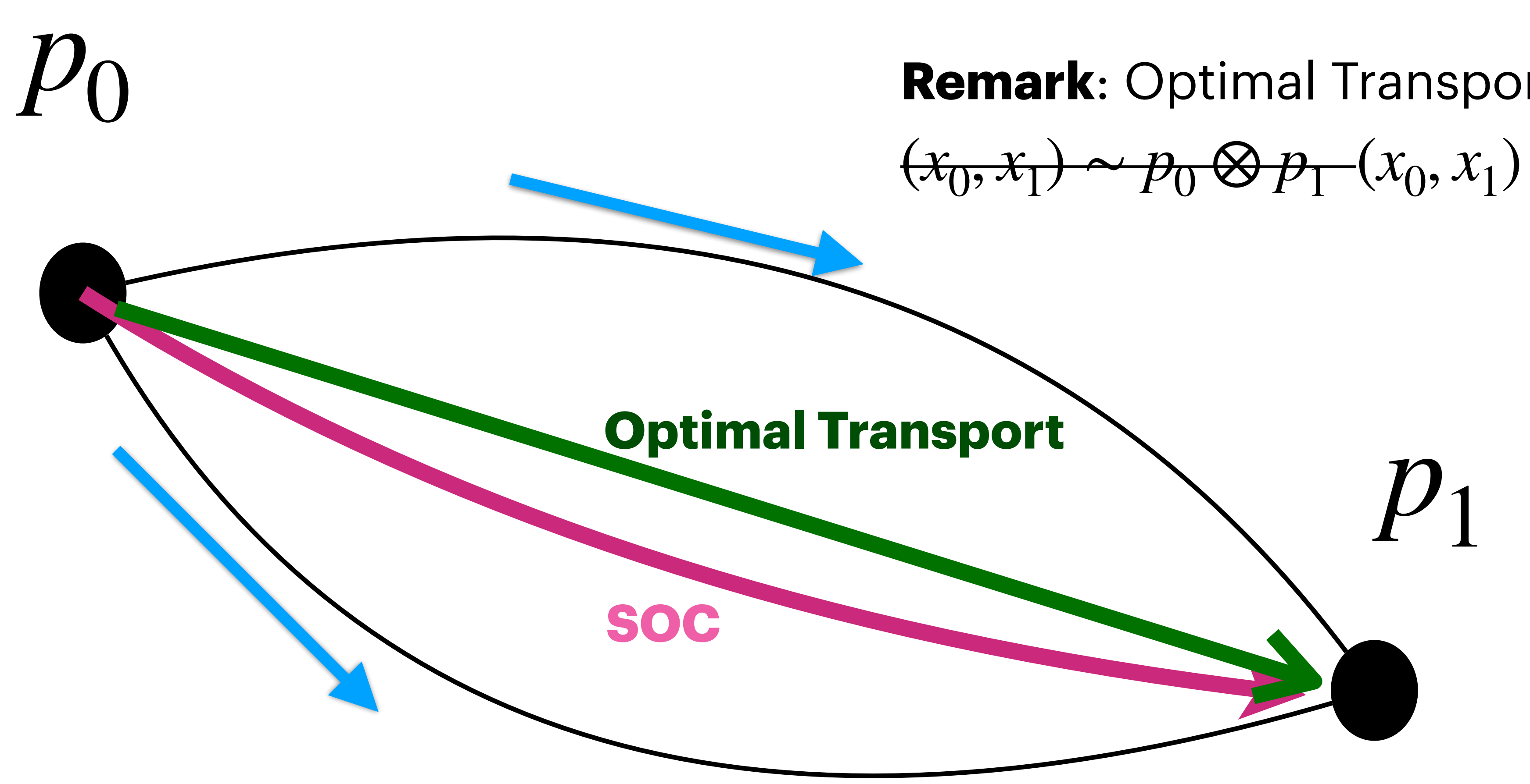
Design Space of Dynamical Generative Modeling

Task:

1. **Generative Modeling:** smooth and straight path For fast sampling.

Remark: Optimal Transport needs correct pairing

$\cancel{(x_0, x_1) \sim p_0 \otimes p_1} (x_0, x_1) \sim \Pi^{OT}(p_0, p_1)$



2. Design Space and motivations

- Let model incorporate more information of dynamics (i.e Velocity).
- Construct unique path measure which is favorable for sampling

That's it? No!

Delay Error in Momentum System

1. We find that there will be <u>Delay Error</u> When conducting sampling (propagating momentum dynamics.)

Euler Discretization:

When $t = t$

$$x_{t+\delta_t} = x_t + v_t \cdot \delta_t$$

$$v_{t+\delta_t} = v_t + F_t^\theta(x_t, v_t, t) \cdot \delta_t$$

When $t = t + \delta_t$

$$x_{t+2\delta_t} = x_{t+\delta_t} + v_{t+\delta_t} \cdot \delta_t$$

$$v_{t+2\delta_t} = v_{t+\delta_t} + F_{t+\delta_t}^\theta(x_{t+\delta_t}, v_{t+\delta_t}, t + \delta_t) \cdot \delta_{t+\delta_t}$$

Learnt Force term F_t^θ cannot influence the position until next timestep. It is obvious that such <u>error will be amplified when interval δ_t is large</u>.

Delay Error in Momentum System

Euler Discretization:

When $t = t$

$$x_{t+\delta_t} = x_t + v_t \cdot \delta_t$$

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Such system is well-known under-actuated system in the control/robotics domain, in which the control/Force cannot be injected into full channel.

Delay Error in Momentum System

Exponential Integrator:

Given System: $$dx_t = (\boxed{A(t)}x_t + \boxed{B(t)}F_t)dt$$

The solution is: $$x(t) = \Phi(t,0)x_0 + \int_0^t \Phi(t,\tau)B(t)F_\tau d\tau$$

Where: $\Phi(\cdot,\cdot)$ is the transition kernel of uncontrolled system.

Maybe Unknown Fact:

DDIM[1] is <u>*EXACTLY*</u> same as Exponential Integrator [2] in continuous limit.

[1] Song, Jiaming, Chenlin Meng, and Stefano Ermon. "Denoising diffusion implicit models." *arXiv preprint arXiv:2010.02502* (2020).
[2]Qinsheng Zhang et al. fast sampling of Diffusion Models with Exponential Integrator

Delay Error in Momentum System

Exponential Integrator:

$$\begin{bmatrix} \mathbf{x}_{t_{i+1}} \\ \mathbf{v}_{t_{i+1}} \end{bmatrix} = \Phi(t_{i+1}, t_i) \begin{bmatrix} \mathbf{x}_t \\ \mathbf{v}_t \end{bmatrix} + \sum_{j=0}^{w} \begin{bmatrix} \int_{t_i}^{t_{i+1}} (t_{i+1} - \tau)\, \mathbf{z}_\tau \cdot \mathbf{M}_{i,j}(\tau) \mathrm{d}\tau \cdot \mathbf{s}_t^\theta(\mathbf{m}_{t_{i-j}}, t_{i-j})) \\ \int_{t_i}^{t_{i+1}} \mathbf{z}_\tau \cdot \mathbf{M}_{i,j}(\tau) \mathrm{d}\tau \cdot \mathbf{s}_t^\theta(\mathbf{m}_{t_{i-j}}, t_{i-j}) \end{bmatrix}$$

$$\text{Where } \mathbf{M}_{i,j}(\tau) = \prod_{k \neq j} \left(\frac{\tau - t_{i-k}}{t_{i-j} - t_{i-k}} \right), \quad \text{and} \quad \Phi(t, s) = \begin{bmatrix} 1 & t - s \\ 0 & 1 \end{bmatrix}.$$

Where we reparamterized: $F_t^\theta := s_t^\theta \cdot z_t$, and z_t is the normalizer which normalizes the output of neural network s_t^θ to standard variance.

Delay Error in Momentum System

Exponential Integrator:

Delay issue closed :)

$$\begin{bmatrix} \mathbf{x}_{t_{i+1}} \\ \mathbf{v}_{t_{i+1}} \end{bmatrix} = \Phi(t_{i+1}, t_i) \begin{bmatrix} \mathbf{x}_t \\ \mathbf{v}_t \end{bmatrix} + \sum_{j=0}^{w} \begin{bmatrix} \int_{t_i}^{t_{i+1}} (t_{i+1} - \tau)\, \mathbf{z}_\tau \cdot \mathbf{M}_{i,j}(\tau) \mathrm{d}\tau \, \boxed{\mathbf{s}_t^\theta(\mathbf{m}_{t_{i-j}}, t_{i-j}))} \\ \int_{t_i}^{t_{i+1}} \mathbf{z}_\tau \cdot \mathbf{M}_{i,j}(\tau) \mathrm{d}\tau \, \boxed{\mathbf{s}_t^\theta(\mathbf{m}_{t_{i-j}}, t_{i-j})} \end{bmatrix}$$

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Acceleration Generative Model

Components

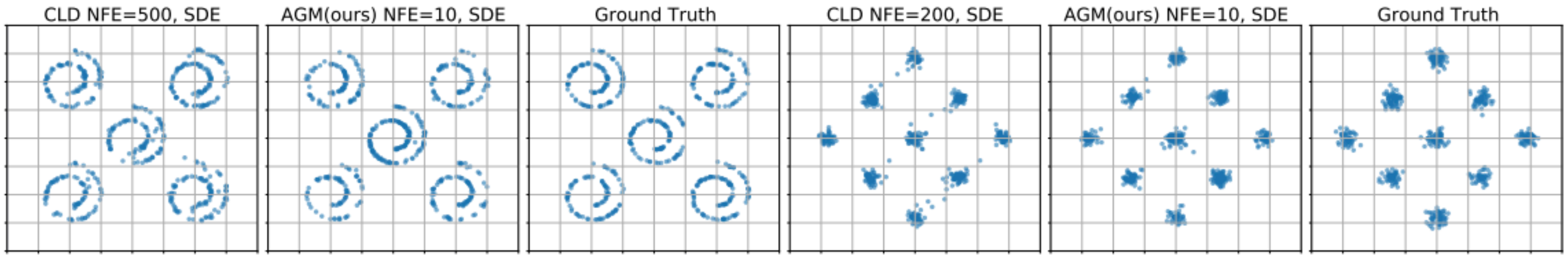
1. Stochastic Phase Space Dynamics
2. Stochastic Optimal Control
3. Exponential Integrator

Algorithm Design

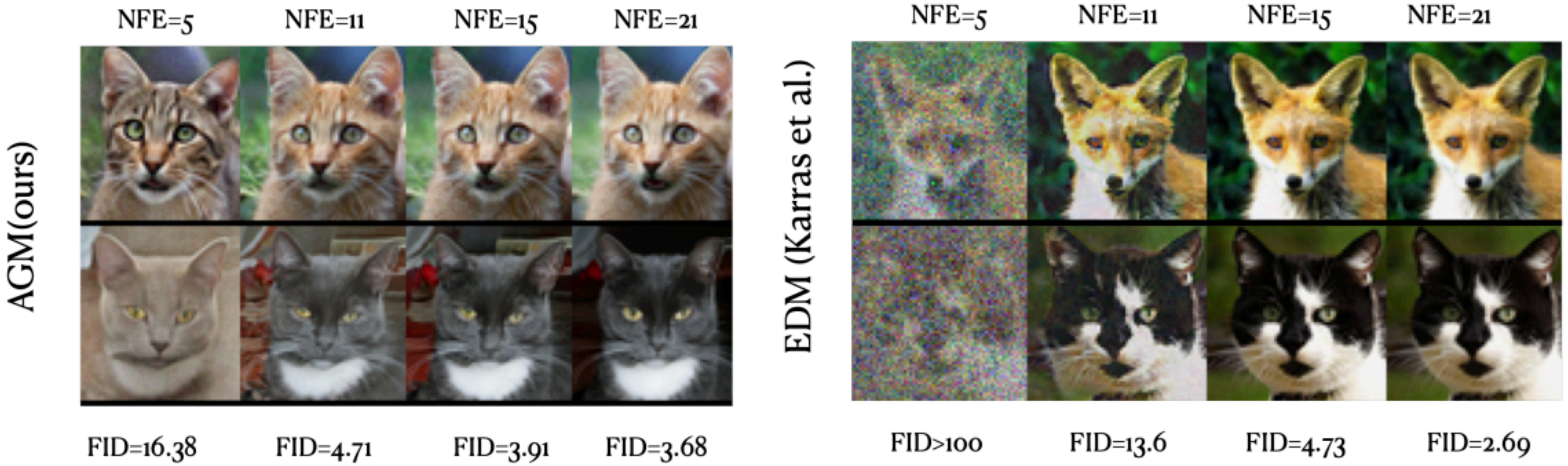
1. Sampling-Hop
2. Straighten Trajectories
3. Resolve delay issue

Results

Compare with CLD[1]:



Compare with EDM [2]:



[1]Dockhorn, Tim, Arash Vahdat, and Karsten Kreis. "Score-based generative modeling with critically-damped langevin diffusion."
[2]Karras, Tero, et al. "Elucidating the design space of diffusion-based generative models."

Results

Position

t=0.0

Velocity

t=0.0

Predicted x_1

t=0.0

Unconditional Cifar10

Dynamics Order	Model Name	NFE↓ 5	10	20
1st order dynamics	EDM (Karras et al., 2022)	> 100	15.78	**2.23**
	VP+EI (Zhang & Chen, 2022)	15.37	**4.17**	3.03
	DDIM (Song et al., 2020a)	26.91	11.14	3.50
	Analytic-DPM(Bao et al., 2022)	51.47	14.06	6.74
2nd order dynamics	CLD+EI (Zhang et al., 2022)	N/A	13.41	3.39
	AGM-ODE(ours)	**11.93**	4.60	2.60

Unconditional Imagenet

Model	NFE↓	FID↓
FM-OT(Lipman et al., 2022)	138	14.45
MFM(Pooladian et al., 2023)	132	11.82
MFM(Pooladian et al., 2023)	40	12.97
AGM-ODE(ours)	40	10.97
AGM-ODE(ours)	30	11.09
AGM-ODE(ours)	20	12.55

Results

Position

t=0.0

Velocity

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Predicted x_1

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Unconditional Cifar10

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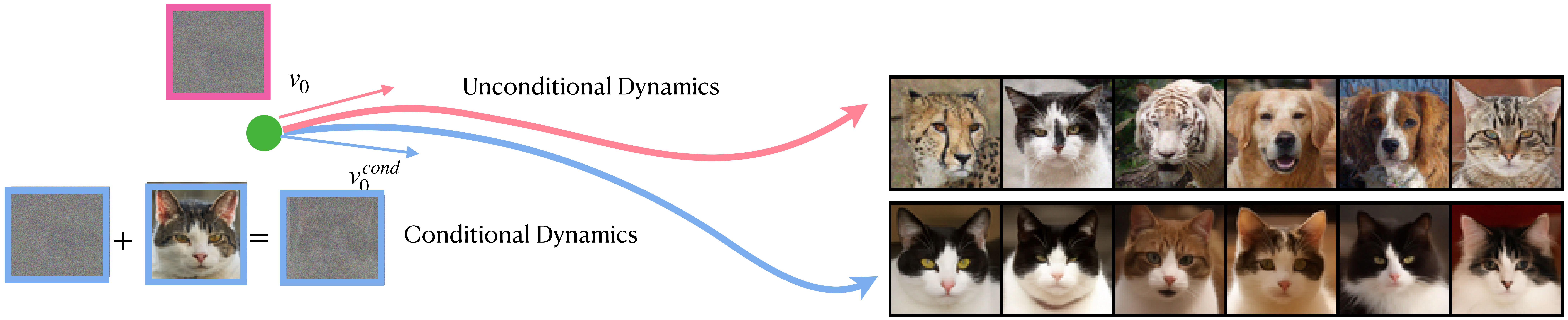
As a dynamical generative model, it can be further improved by:

1. OT pairing
2. Distillation

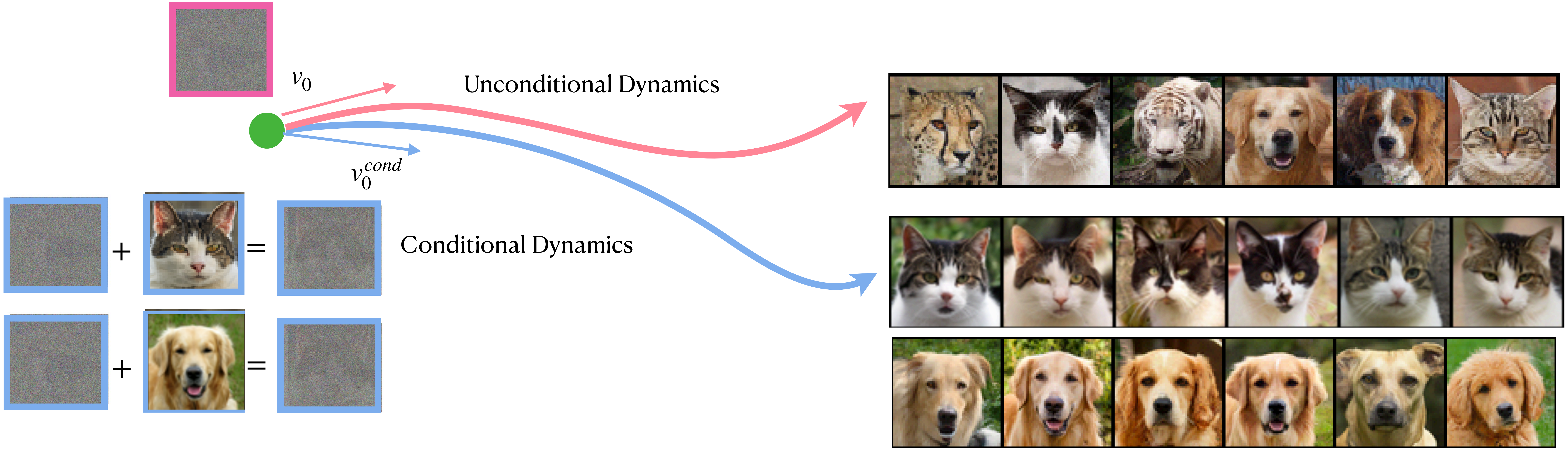
One more Thing :)

Stroke Based Conditional Generation

By leveraging velocity Space



1. Velocity has explicitly physical meaning as momentum.
2. One can guide the generation path by only changing initial auxiliary velocity.
3. The model does not need fine tuning or further training.



1. Velocity has explicitly physical meaning as momentum.
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Agenda

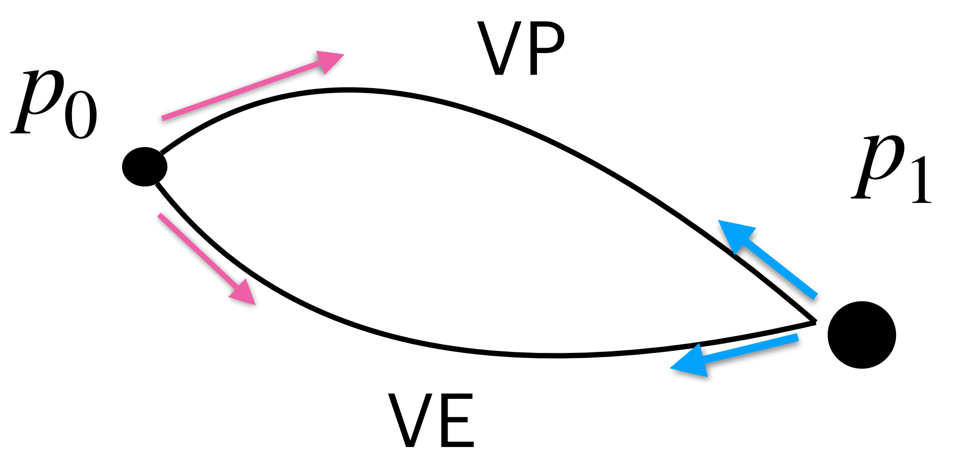
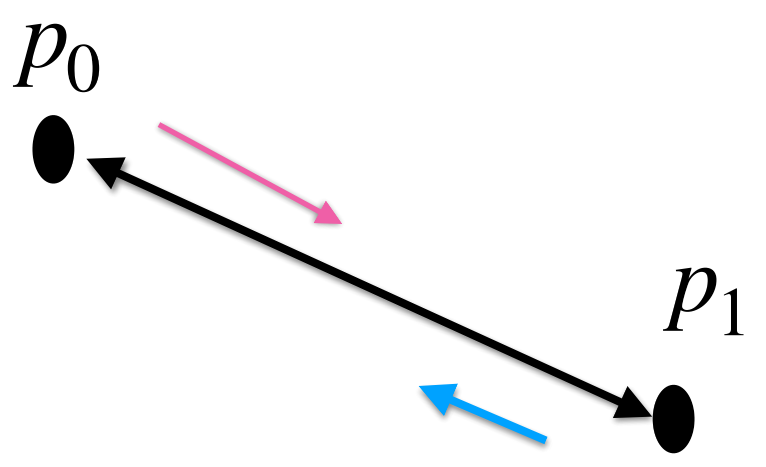
- Gentle Introduction.
- Generative Modeling with Phase Stochastic Bridges
- **Trajectory Inference: momentum Schrödinger Bridge for Biology**
- Future Directions
- Q&A

Multi-marginal momentum Schrödinger Bridge

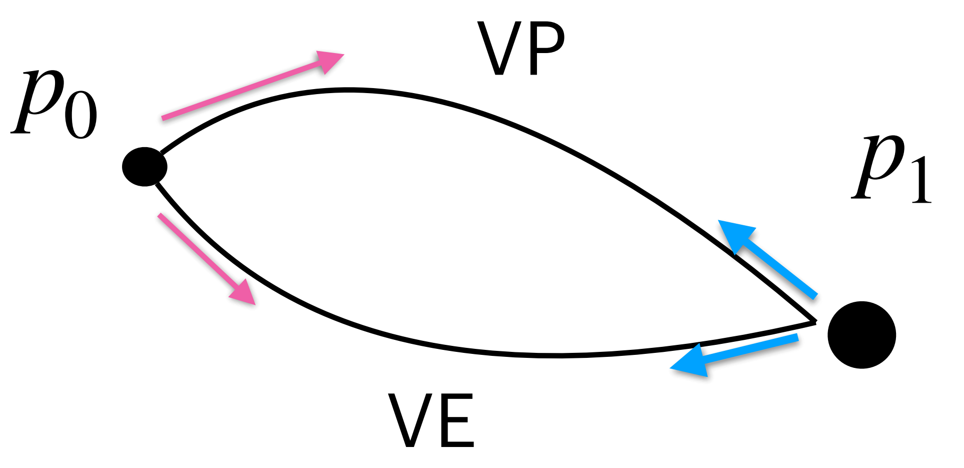
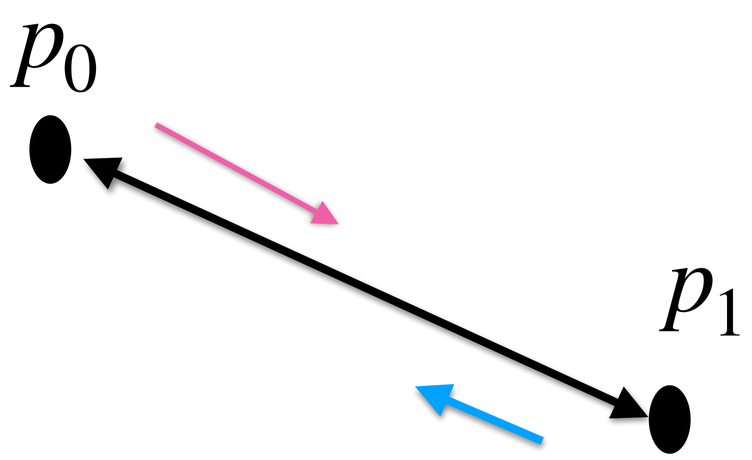
Comparisons

	Diffusion Model	Schrödinger Bridge	**Momentum Schrödinger Bridge**
Path Measure			
Boundaries/ Constraints			
Pairing			

Comparisons

	Diffusion Model	Schrödinger Bridge	**Momentum Schrödinger Bridge**
Path Measure			
Boundaries/ Constraints			
Pairing			

Comparisons

	Diffusion Model	Schrödinger Bridge	**Momentum Schrödinger Bridge**
Path Measure			
Boundaries/ Constraints	p_0  p_1 	p_0  p_1 	
Pairing			

Comparisons

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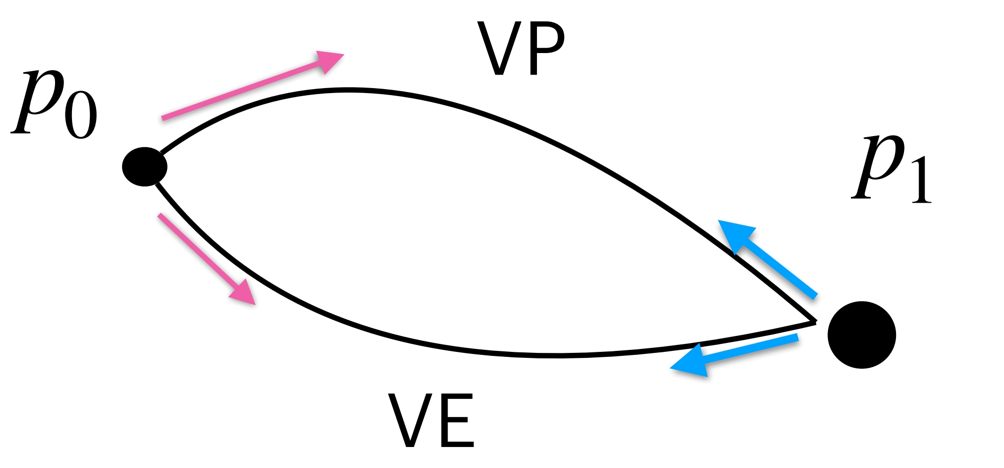
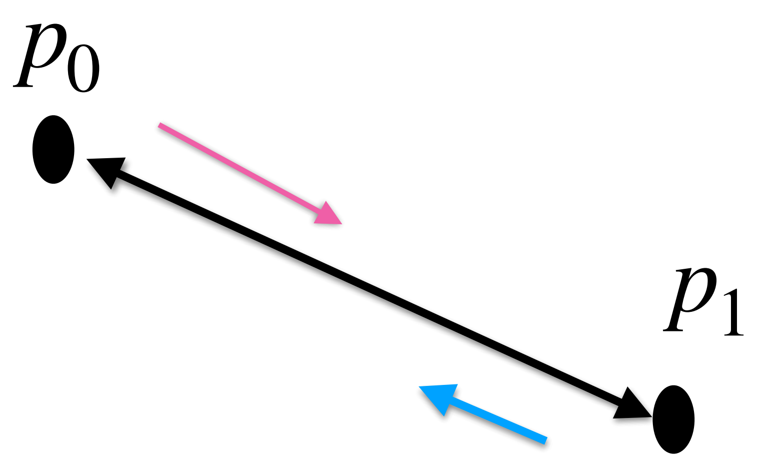
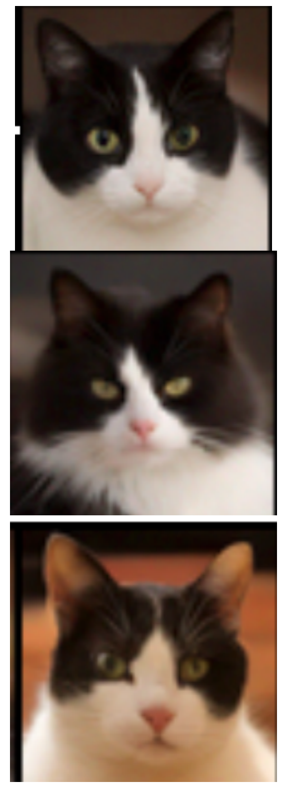
Path Measure			
Boundaries/ Constraints	p_0  p_1 	p_0  p_1 	
Pairing	✗	 Stochastic Pairing 	

Comparisons

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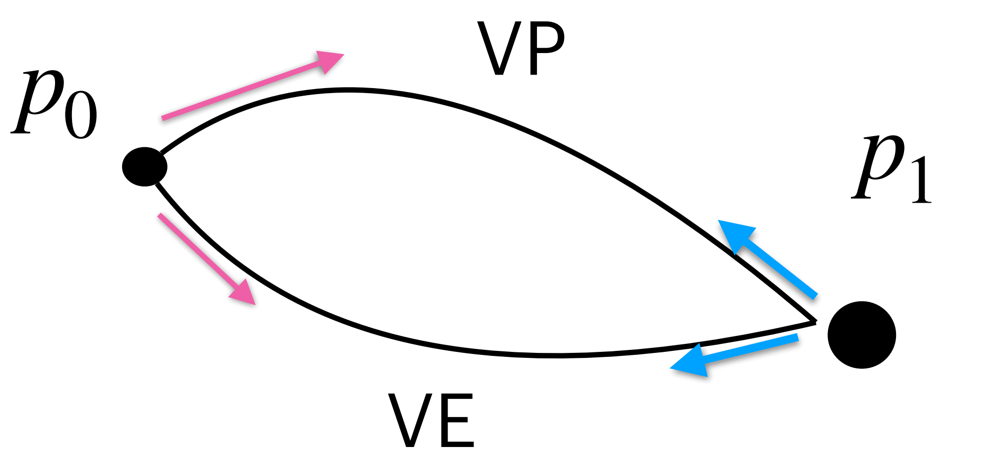
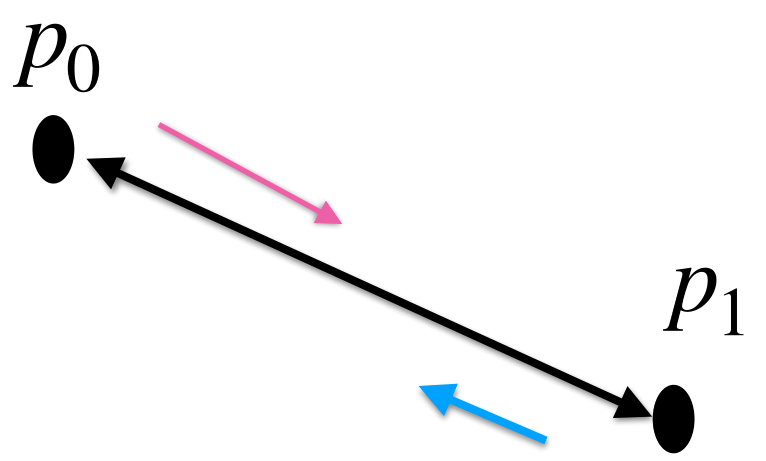
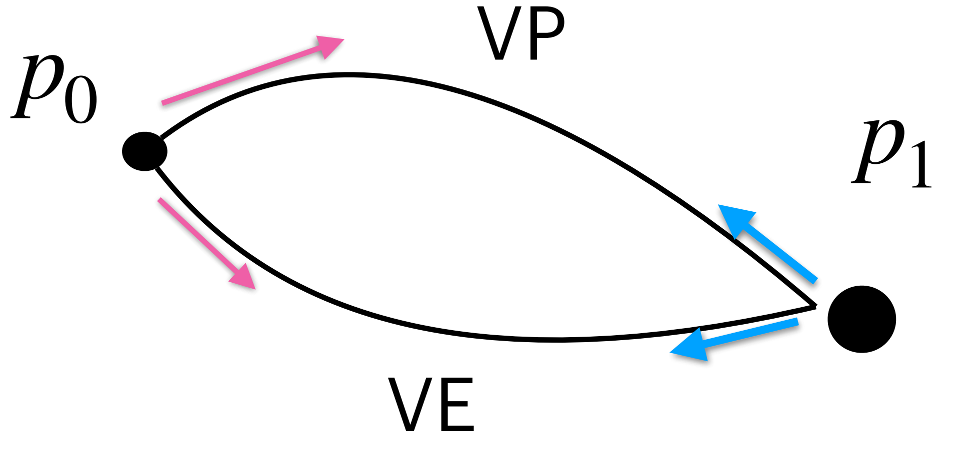
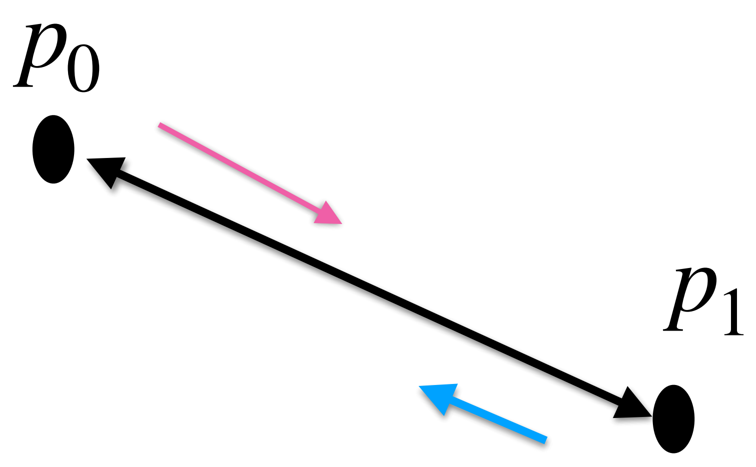
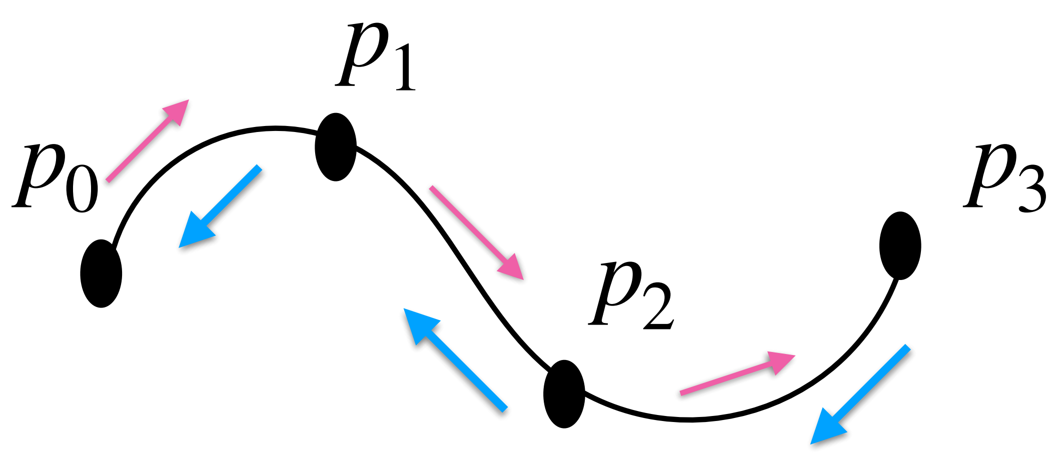
Path Measure			
Boundaries/ Constraints	p_0  p_1 	p_0  p_1 	
Pairing	Conditional Generation Predefined pairing	Automatically find pairing	

Comparisons

	Diffusion Model	Schrödinger Bridge	**Momentum Schrödinger Bridge**
Path Measure			
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Comparisons

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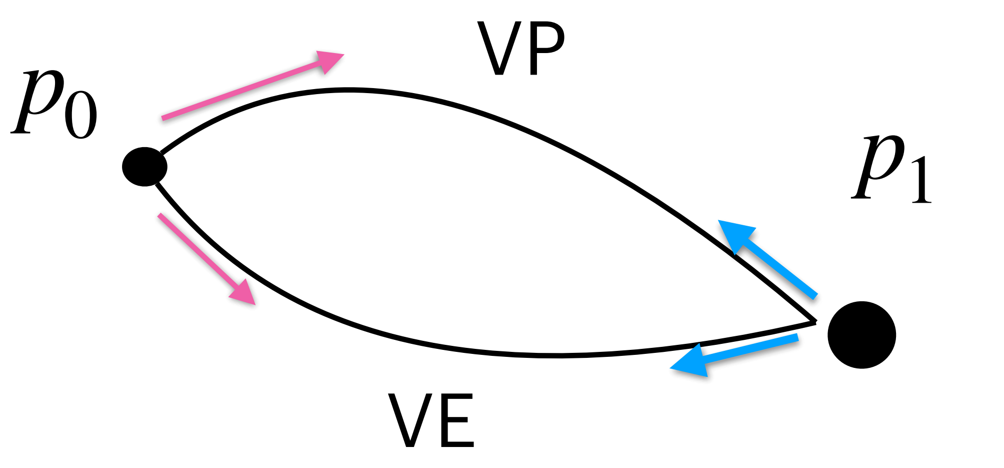
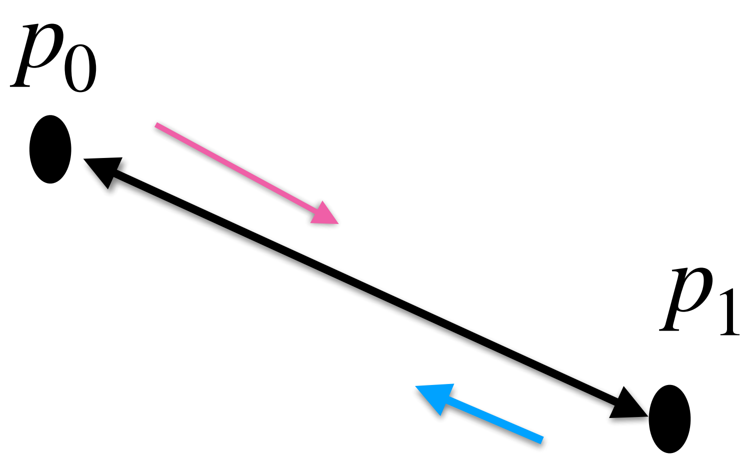
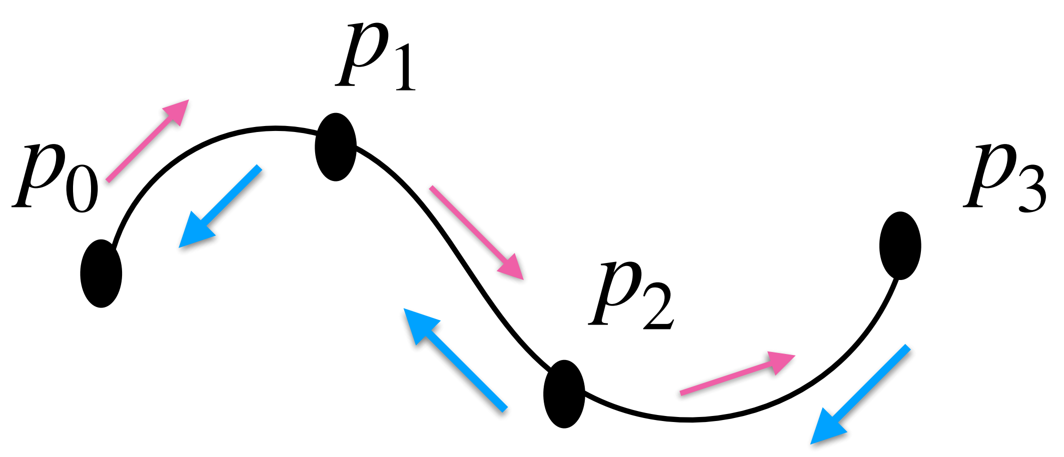
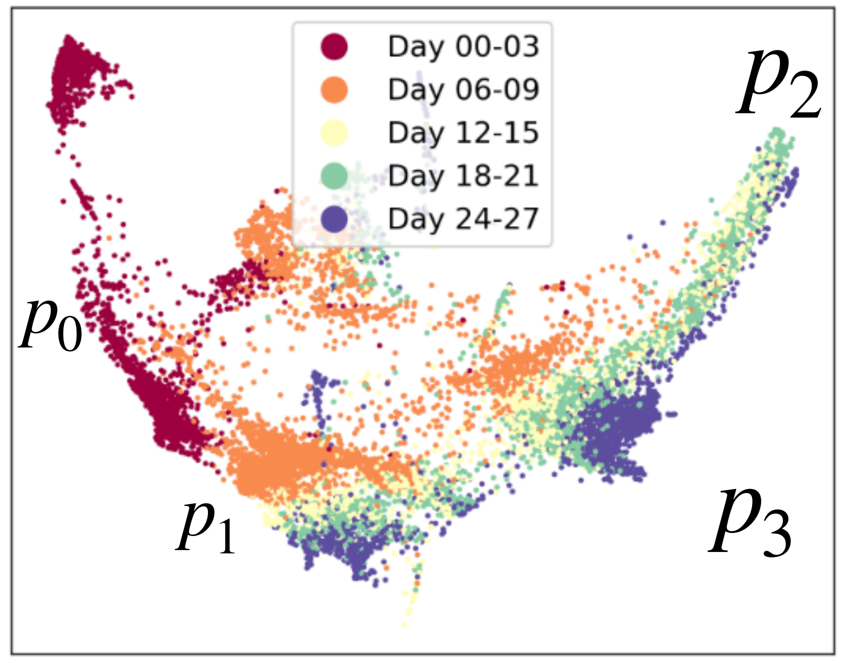
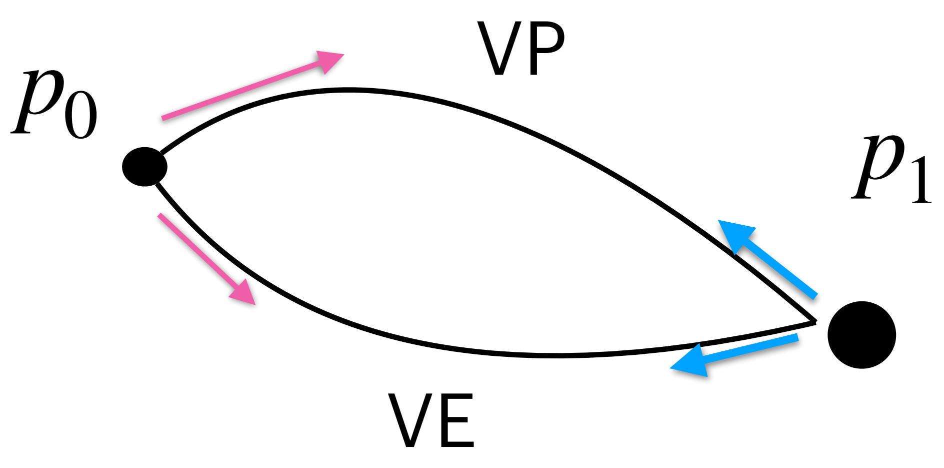
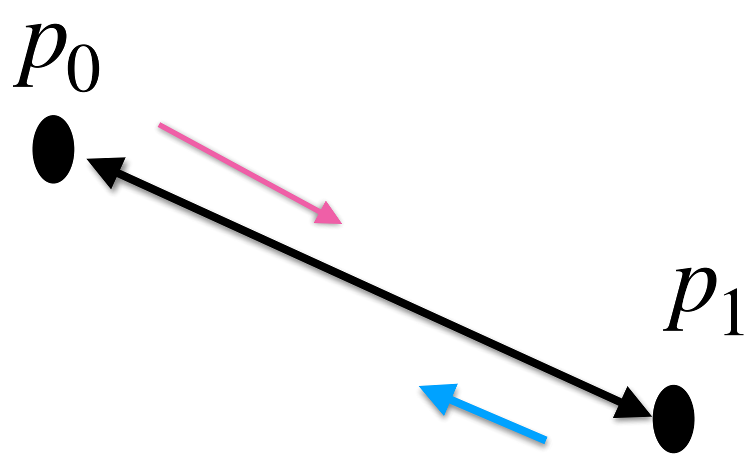
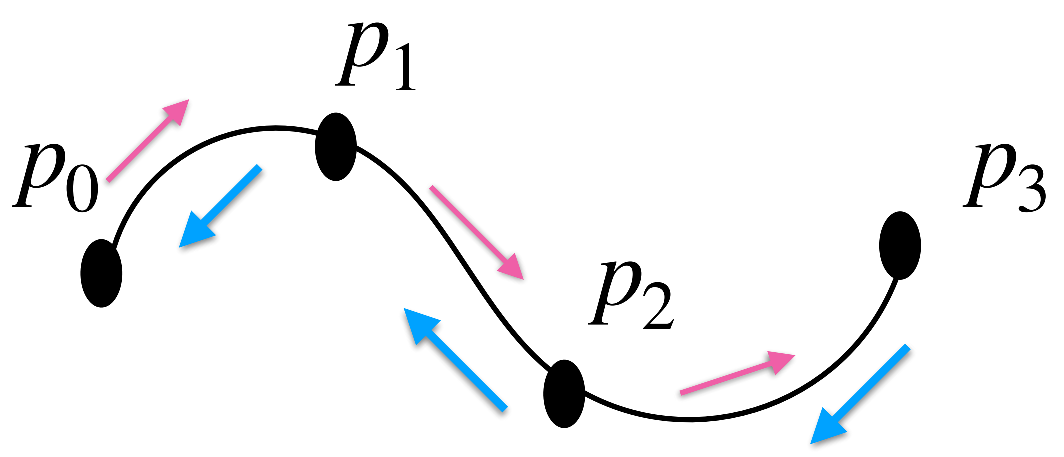
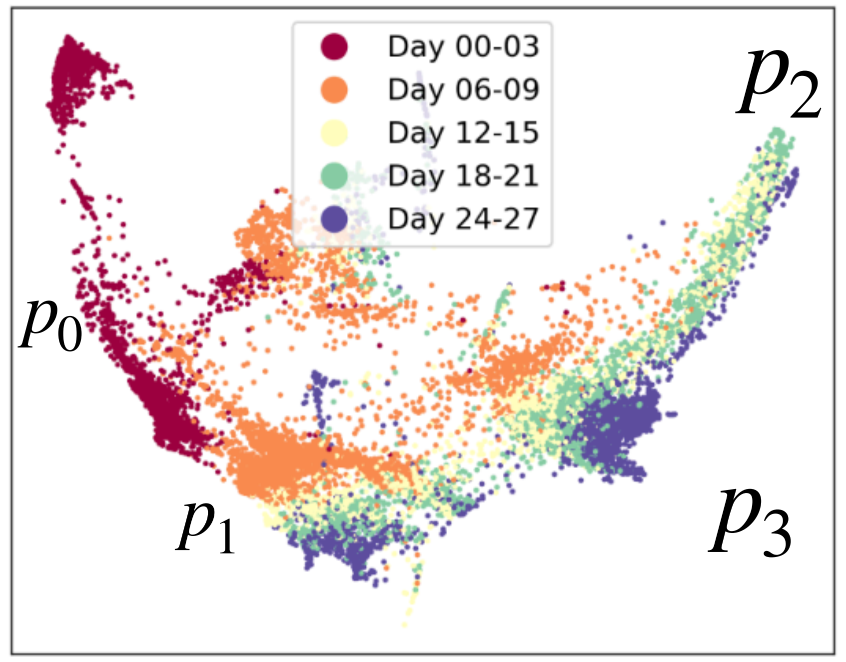
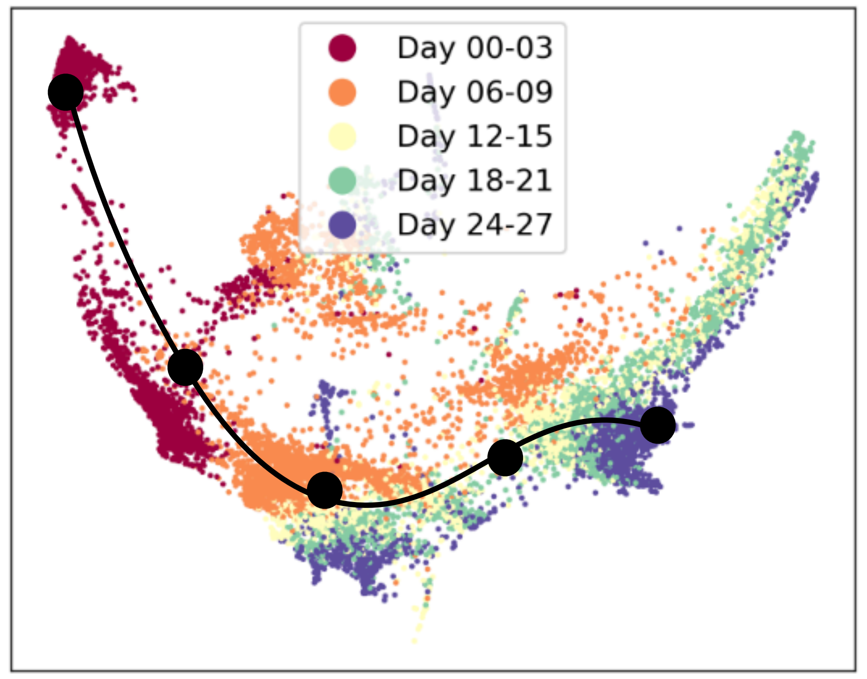
Path Measure			
Boundaries/ Constraints	p_0  p_1 	p_0  p_1 	
Pairing	Conditional Generation Predefined pairing	Automatically find pairing	

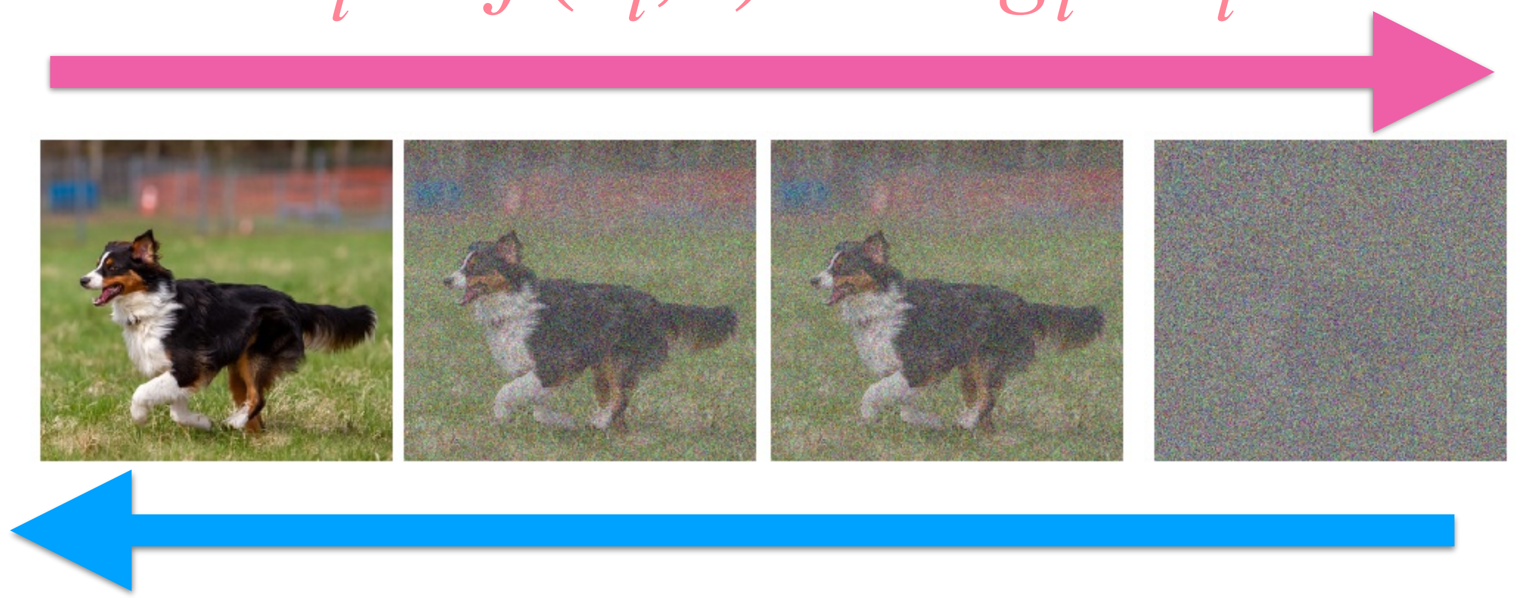
Comparisons

	Diffusion Model	Schrödinger Bridge	**Momentum Schrödinger Bridge**
Path Measure			
Boundaries/ Constraints	p_0  p_1 	p_0  p_1 	
Pairing	Conditional Generation Predefined pairing	Automatically find pairing	

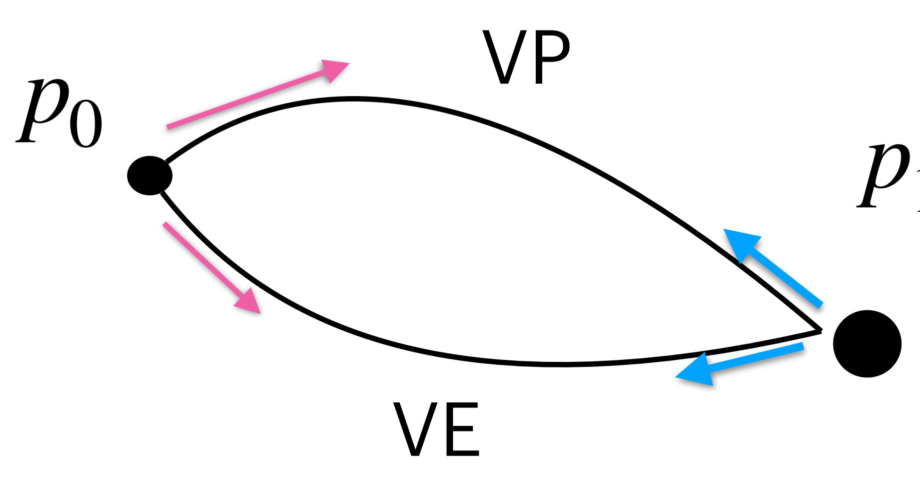
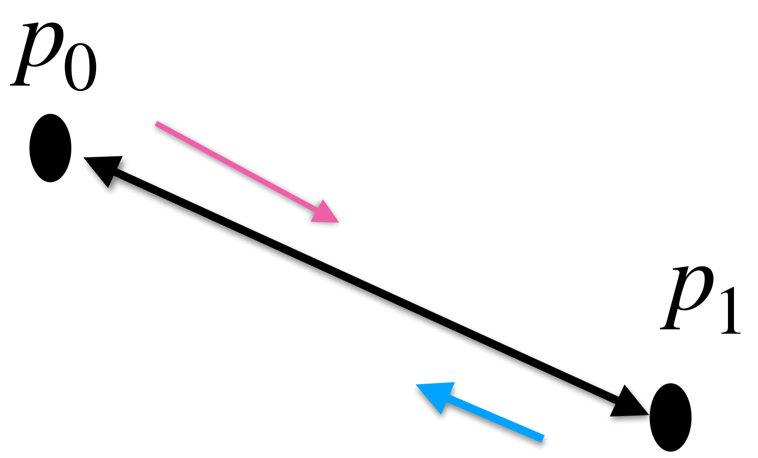
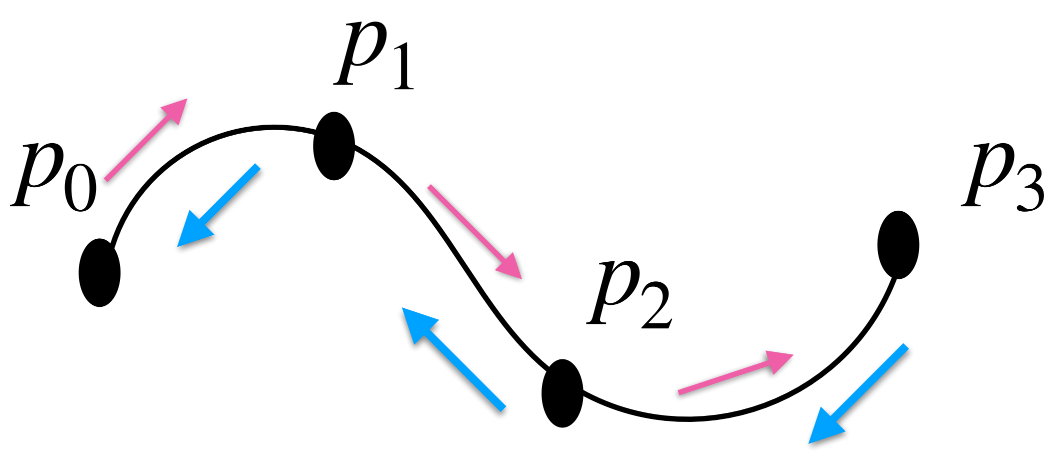
Lets go slightly deeper

Training

$$dx_t = f(x_t, t)dt + g_t dw_t$$

$x_0 \sim p_0$  $x_1 \sim p_1$

$$dx_t = b(x_t, t)dt + g_t dw_t$$

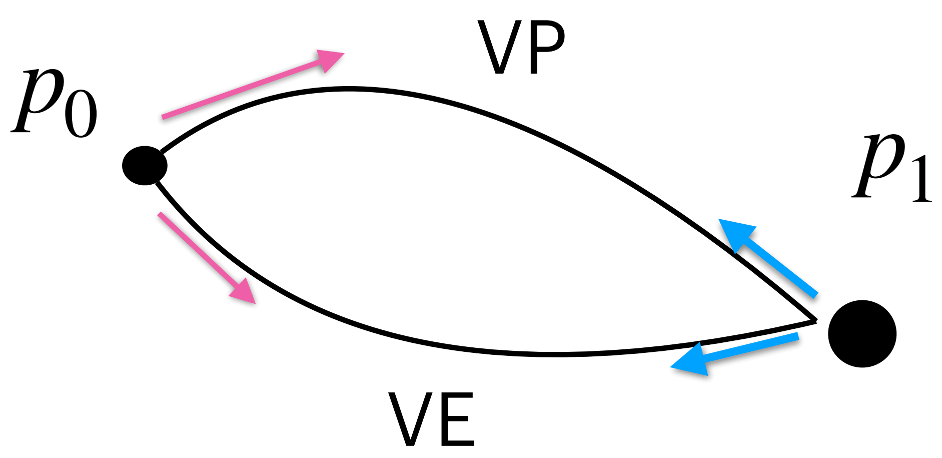
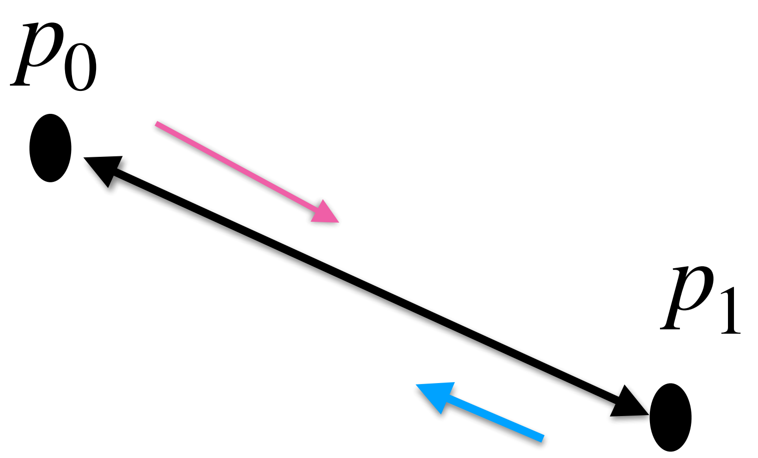
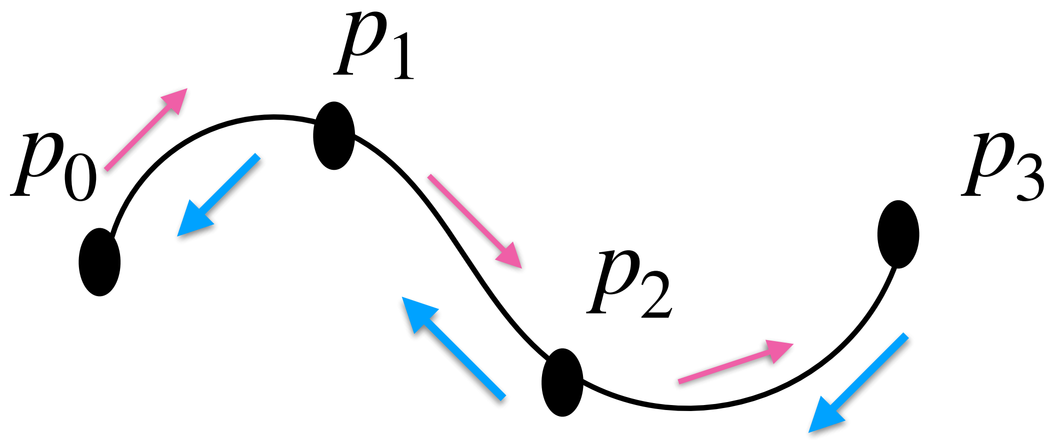
	Diffusion Model	Schrödinger Bridge	**Momentum Schrödinger Bridge**
Path Measure			
Training			

Training

$\mu \quad dx_t = f(x_t, t)dt + g_t dw_t$

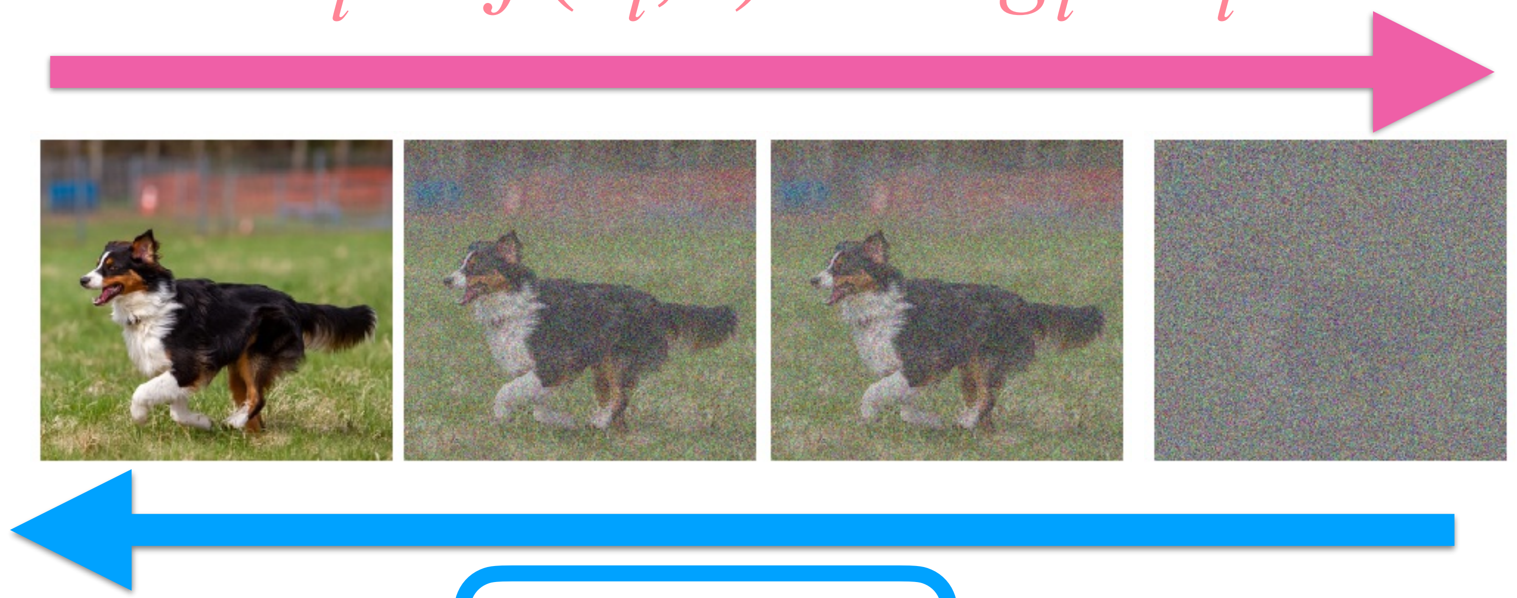
$x_0 \sim p_0$  $x_1 \sim p_1$

$\nu^\theta \quad dx_t = \boxed{b(x_t, t; \theta)dt} + g_t dw_t$

	Diffusion Model	Schrödinger Bridge	**Momentum Schrödinger Bridge**
Path Measure			
Training			

Training

μ $\quad dx_t = f(x_t, t)dt + g_t dw_t$

$x_0 \sim p_0$  $x_1 \sim p_1$

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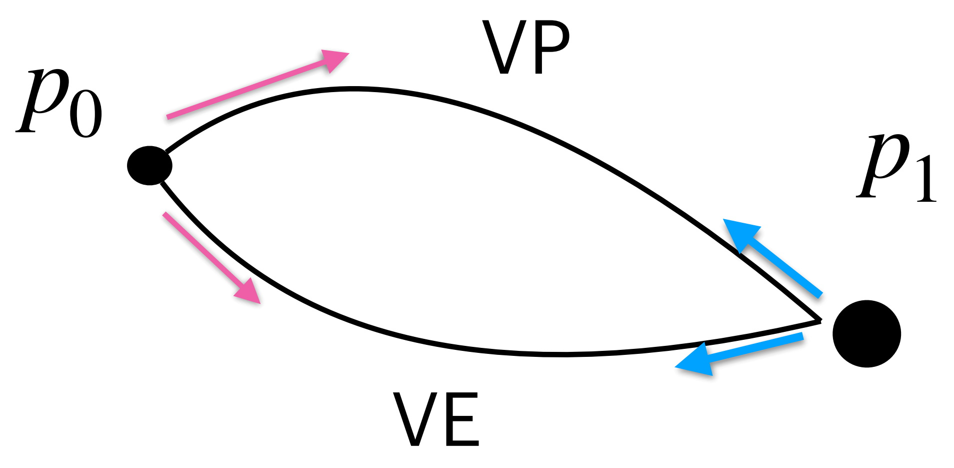
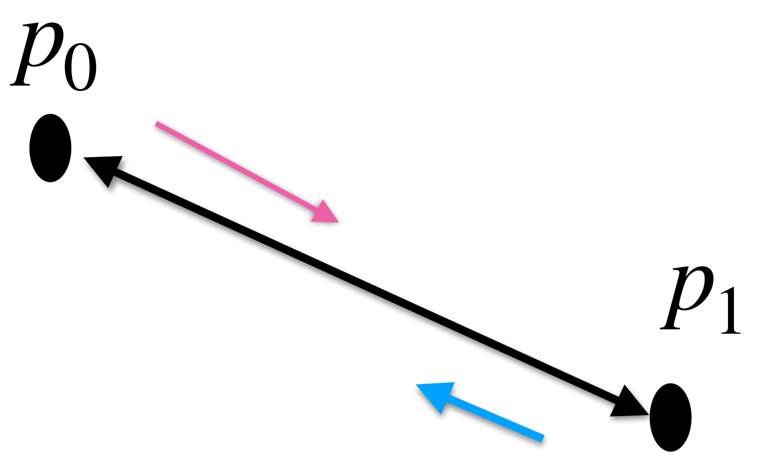
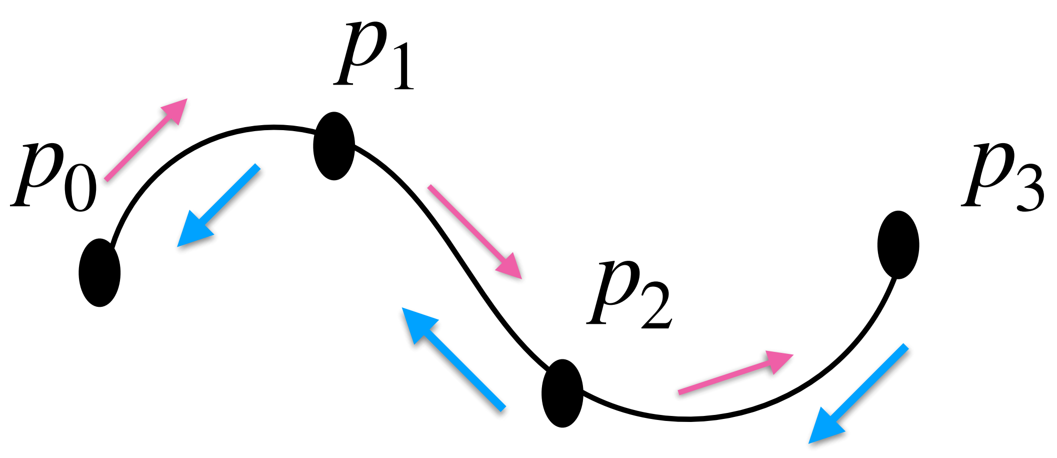
Path Measure			
Training	$\min_\theta KL(\mu \,\|\|\, \nu^\theta)$		

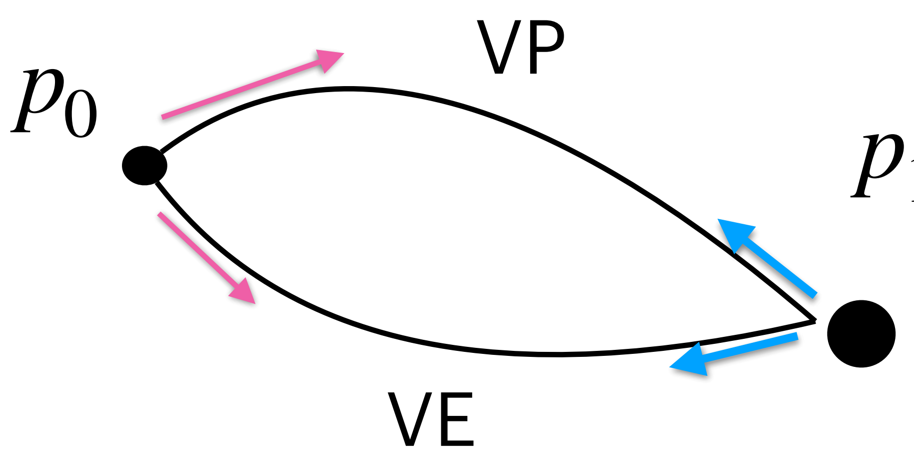
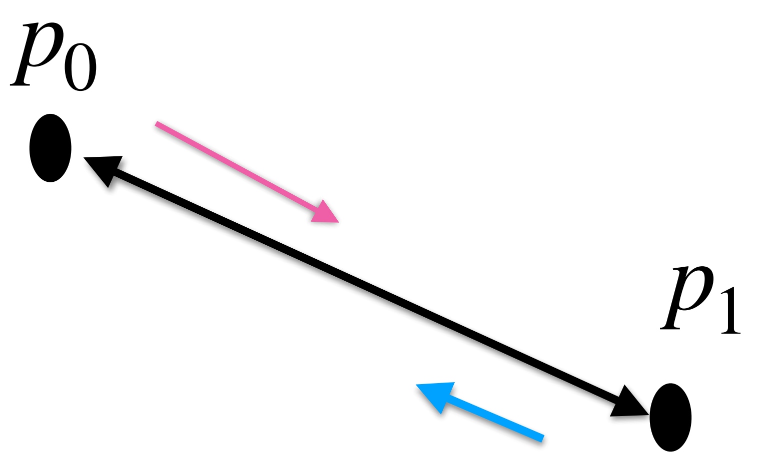
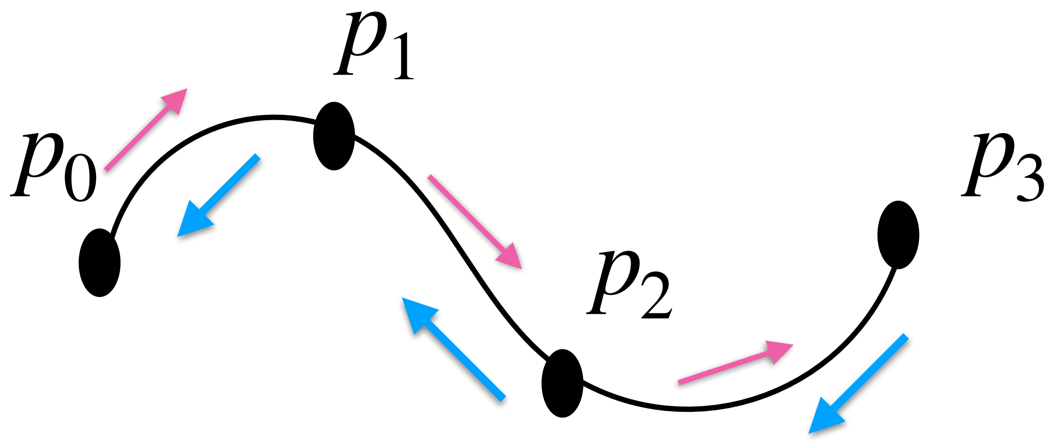
Training

$\mu \quad dx_t = f(x_t, t)dt + g_t dw_t$

$x_0 \sim p_0$

$x_1 \sim p_1$

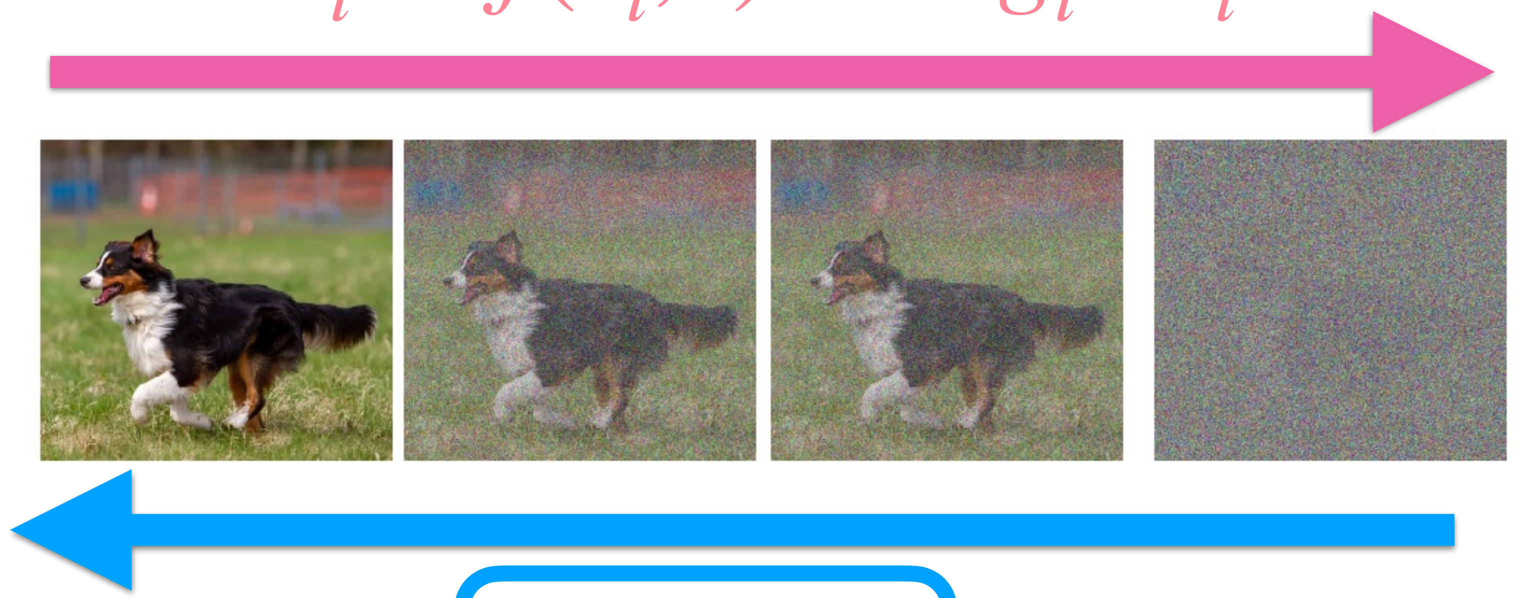
$\nu^\theta \quad dx_t = \boxed{b(x_t, t; \theta)dt} + g_t dw_t$

	Diffusion Model	Schrödinger Bridge	**Momentum Schrödinger Bridge**
Path Measure			
Training	**Denoising Score Matching**		

Training

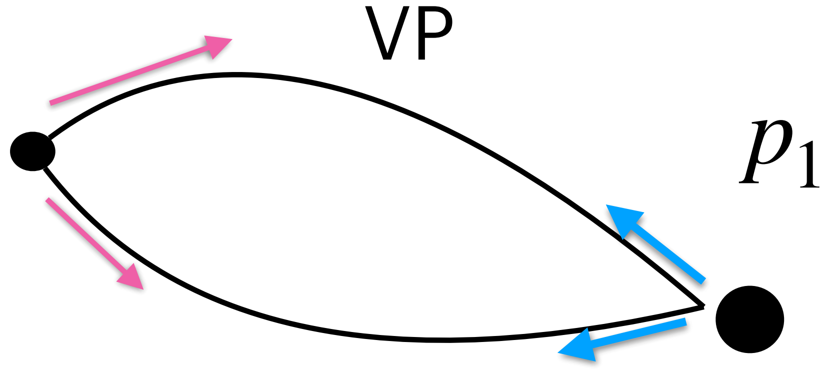
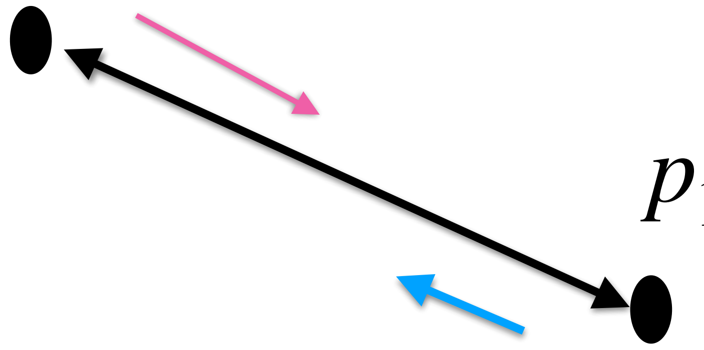
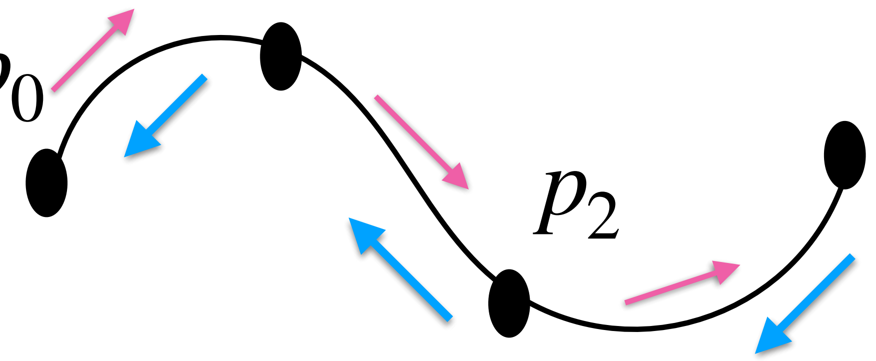
$\mu \quad dx_t = f(x_t, t)dt + g_t dw_t$

$x_0 \sim p_0$

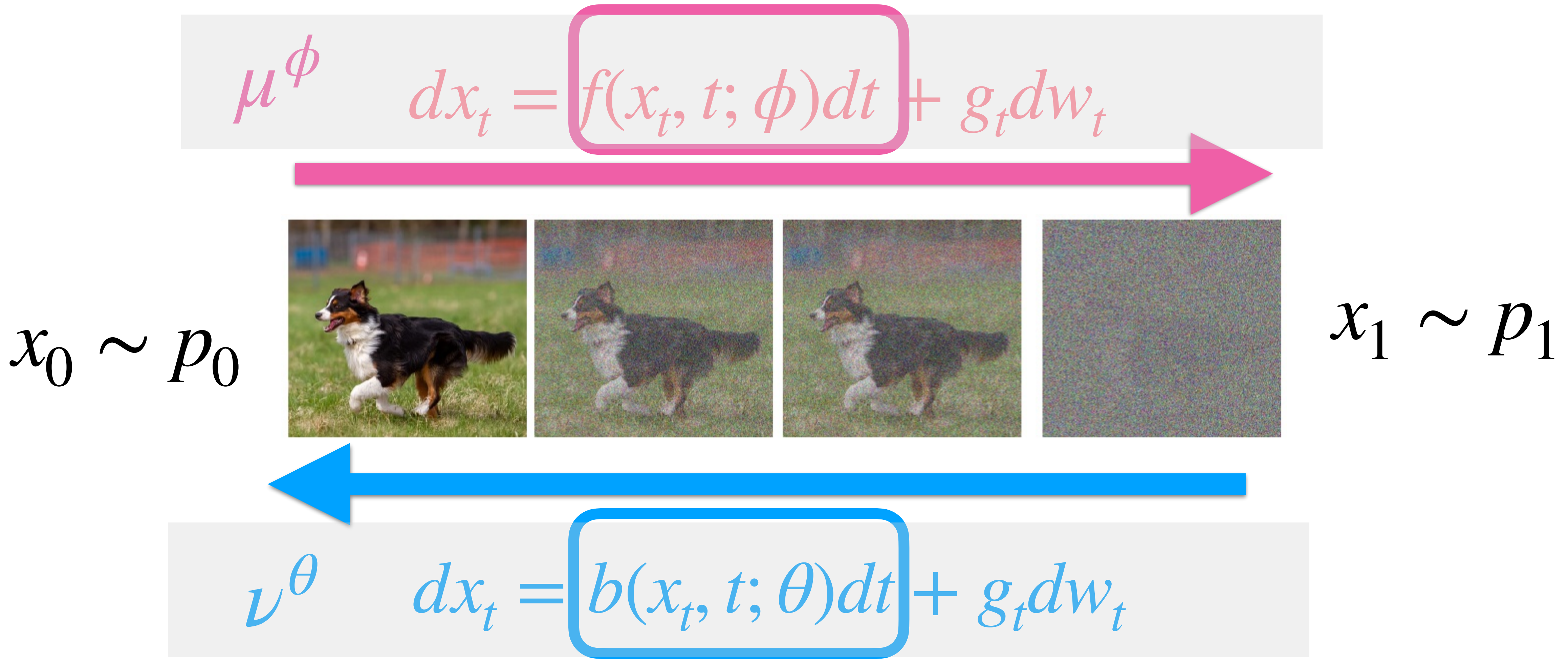


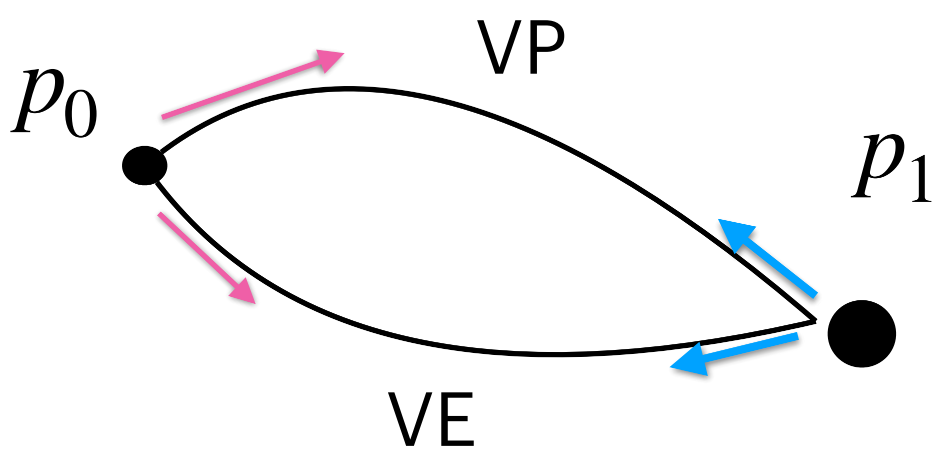
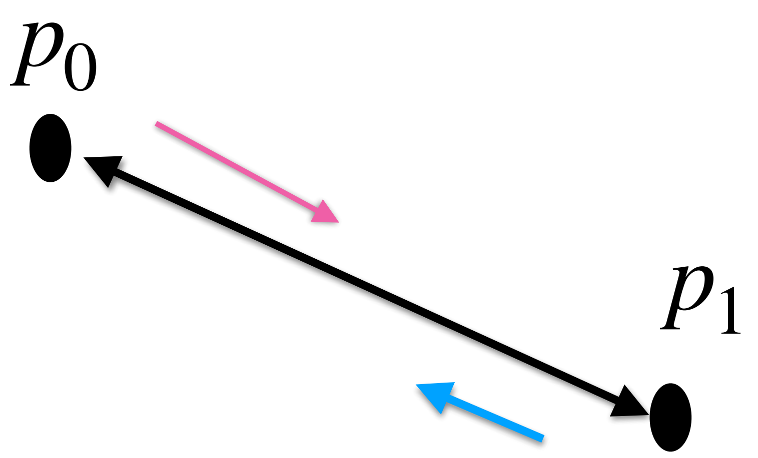
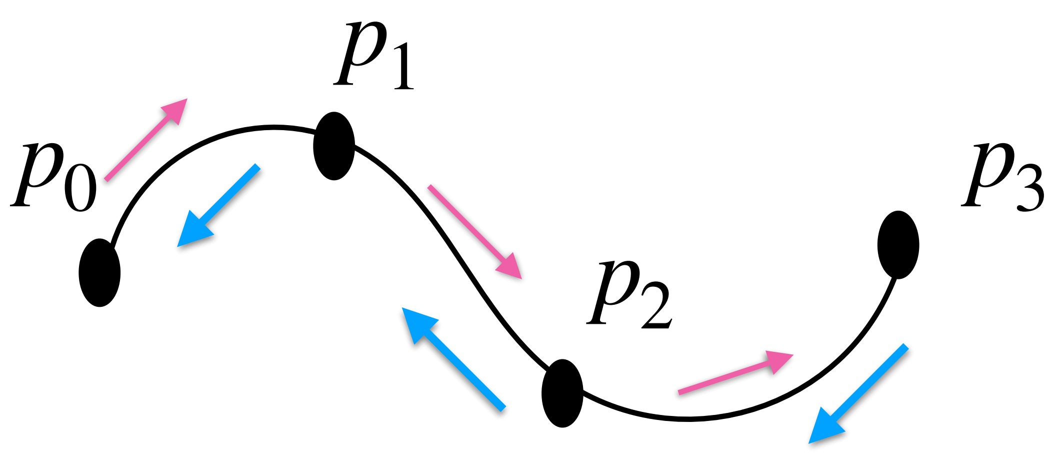
$x_1 \sim p_1$

$\nu^\theta \quad dx_t = \boxed{b(x_t, t; \theta)dt} + g_t dw_t$

	Diffusion Model	Schrödinger Bridge	**Momentum Schrödinger Bridge**
Path Measure			
Training	$\min_\theta KL(\mu \,\|\| \nu^\theta)$ $\nu \in \left\{ \int \pi_{0,1} dx_0 = p_1 \right\}$		

Training



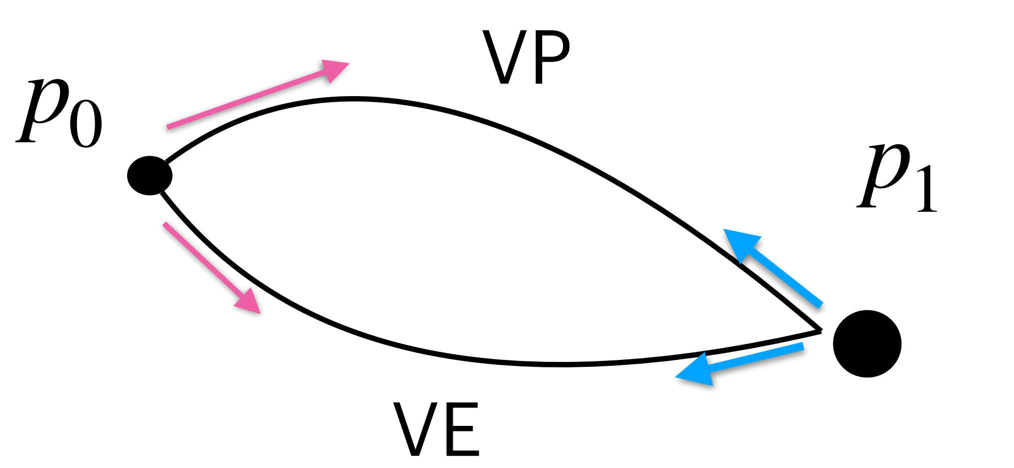
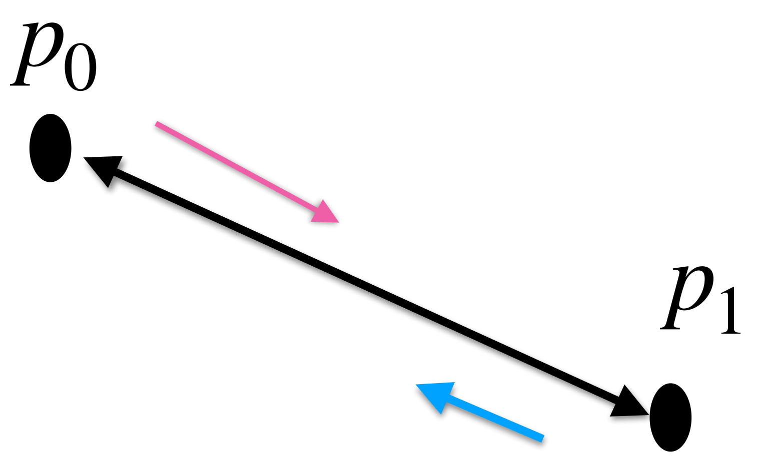
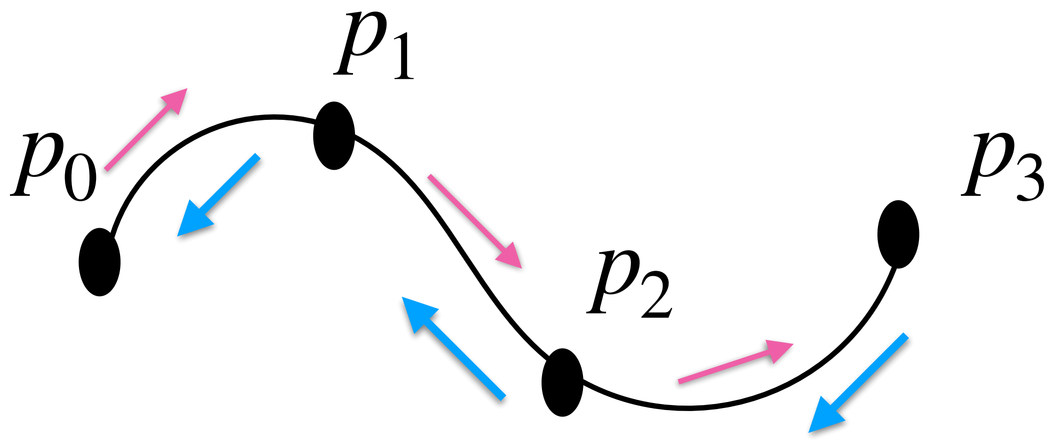
	Diffusion Model	Schrödinger Bridge	**Momentum Schrödinger Bridge**
Path Measure			
Training	**Denoising Score Matching**		

Training

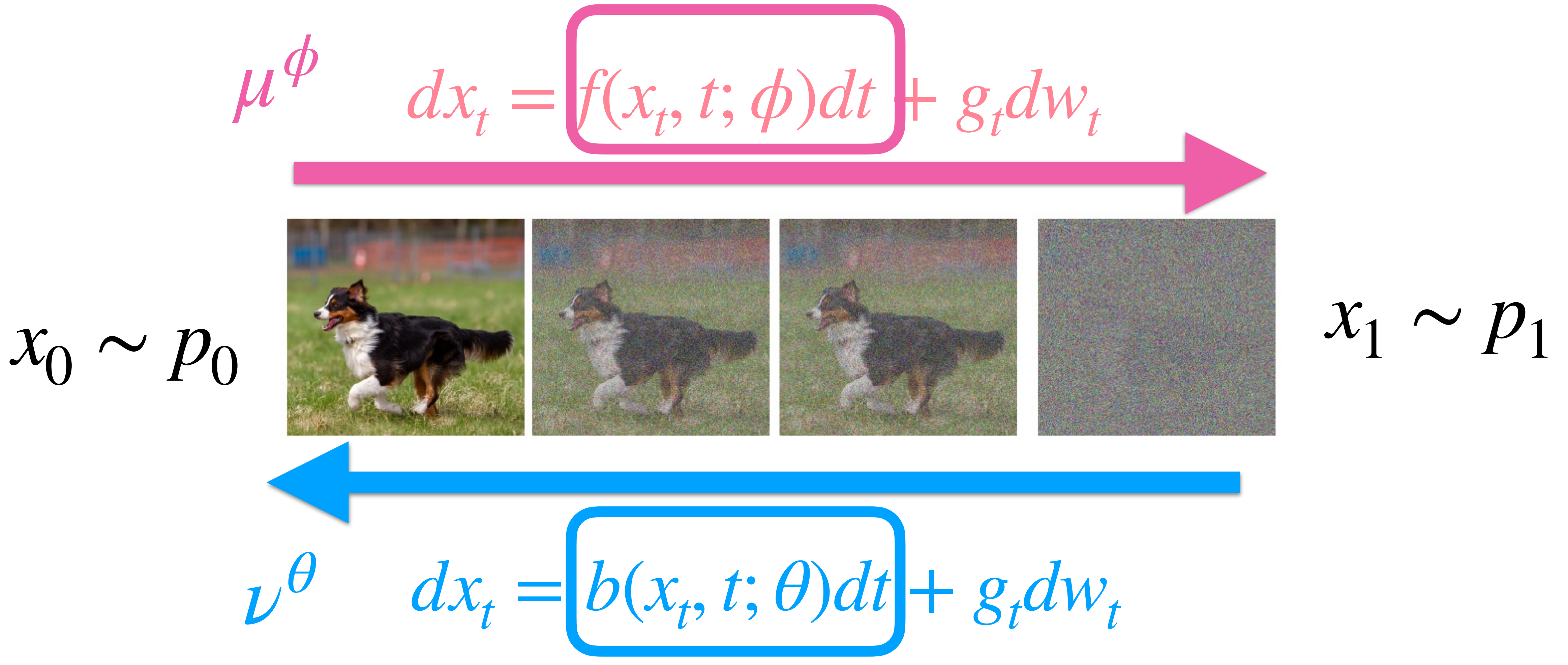
μ^{ϕ} $\quad dx_t = \boxed{f(x_t, t; \phi)dt} + g_t dw_t$

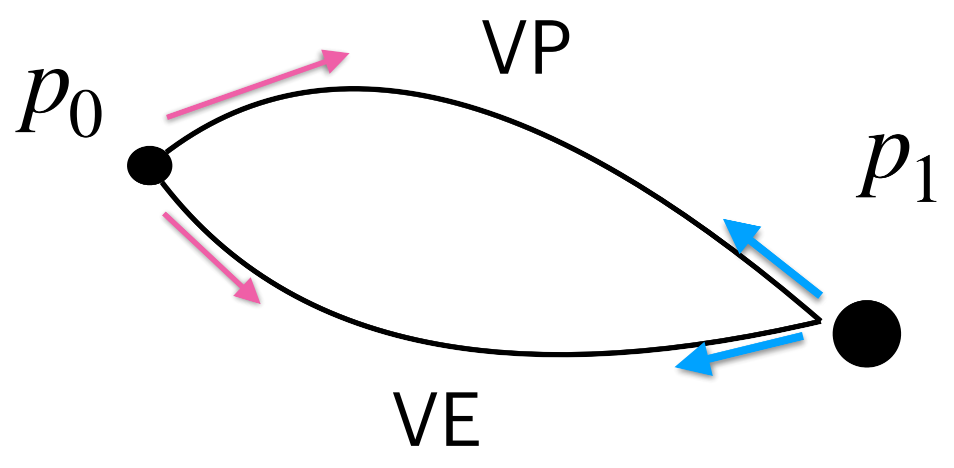
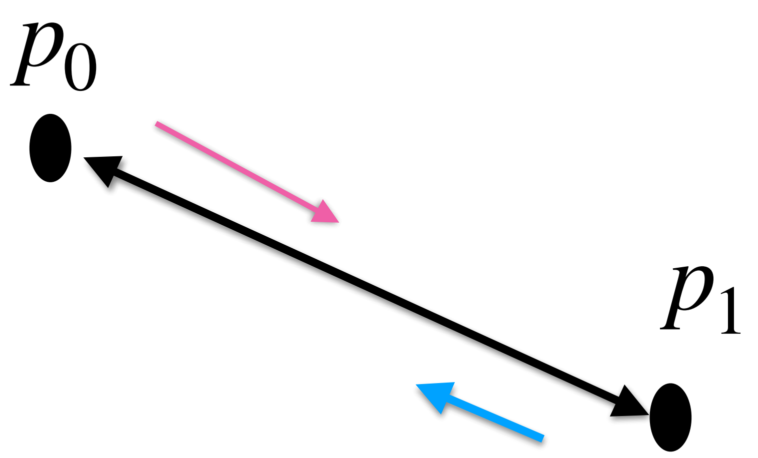
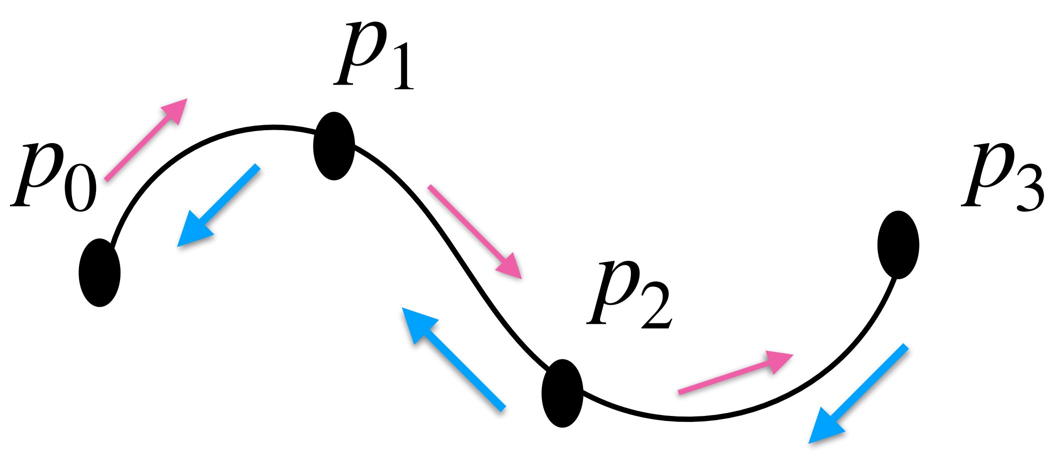
$x_0 \sim p_0$  $x_1 \sim p_1$

ν^{θ} $\quad dx_t = \boxed{b(x_t, t; \theta)dt} + g_t dw_t$

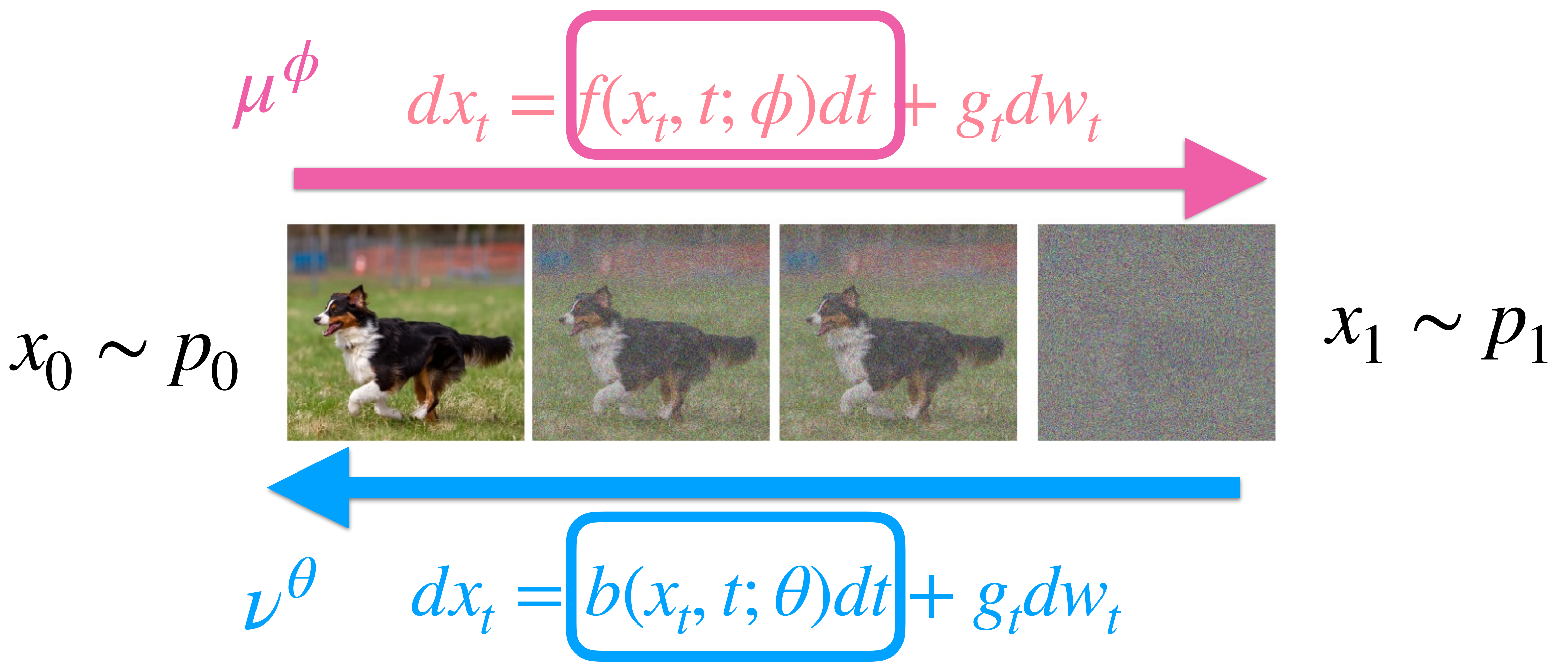
	Diffusion Model	Schrödinger Bridge	**Momentum Schrödinger Bridge**
Path Measure			
Training	**Denoising Score Matching**	$\min_{\theta} KL(\mu^{\phi} \| \| \nu^{\theta}) \quad \nu \in \left\{ \int \pi_{0,1} dx_0 = p_1 \right\}$ $\min_{\phi} KL(\nu^{\theta} \| \| \mu^{\phi}) \quad \mu \in \left\{ \int \pi_{0,1} dx_1 = p_0 \right\}$	

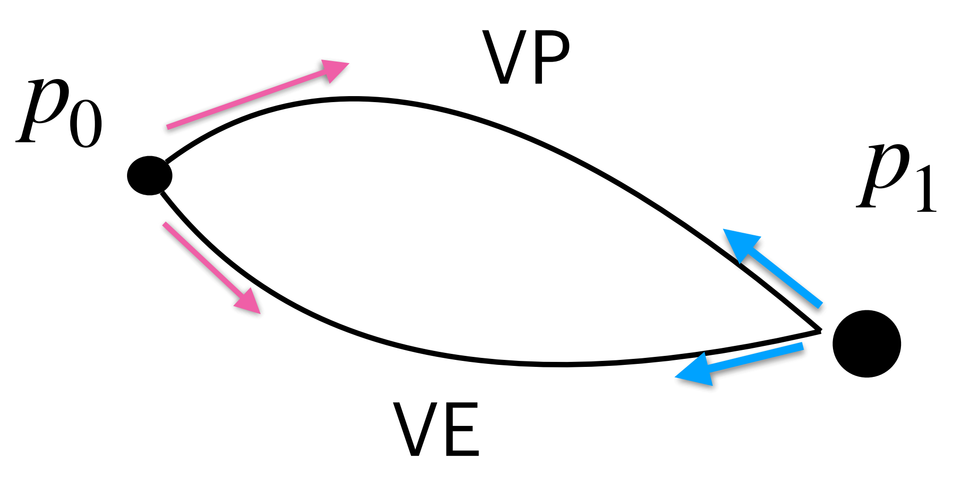
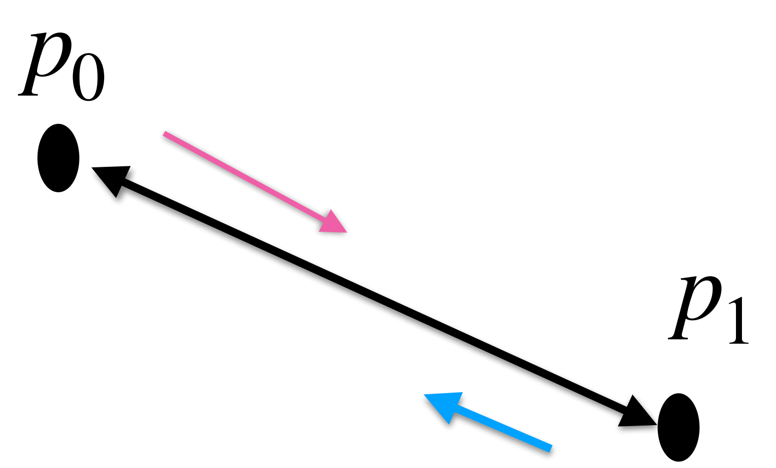
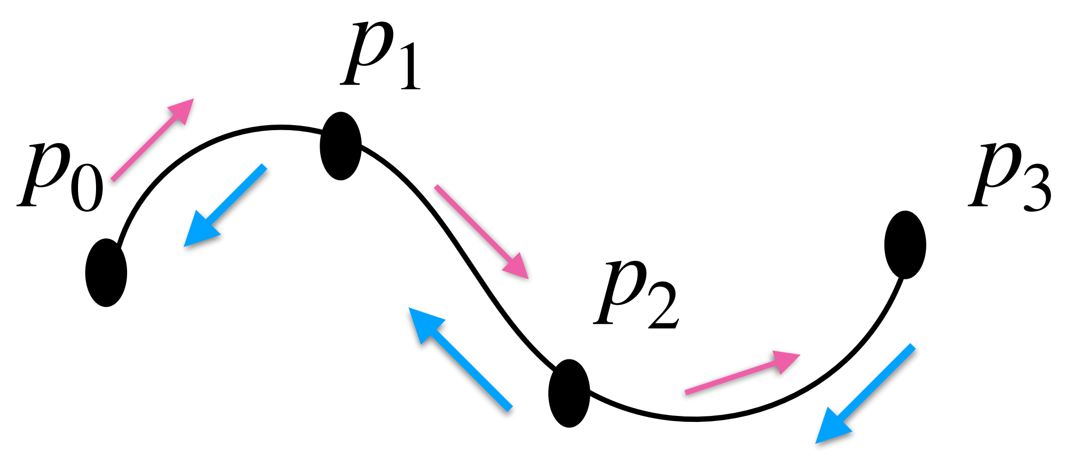
Training



	Diffusion Model	Schrödinger Bridge	**Momentum Schrödinger Bridge**
Path Measure			
Training	**Denoising Score Matching**	$\min_\theta KL(\mu^\phi \| \| \nu^\theta)$ $\nu \in \left\{ \int \pi_{0,1} dx_0 = p_1 \right\}$ $\min_\phi KL(\nu^\theta \| \| \mu^\phi)$ $\mu \in \left\{ \int \pi_{0,1} dx_1 = p_0 \right\}$	

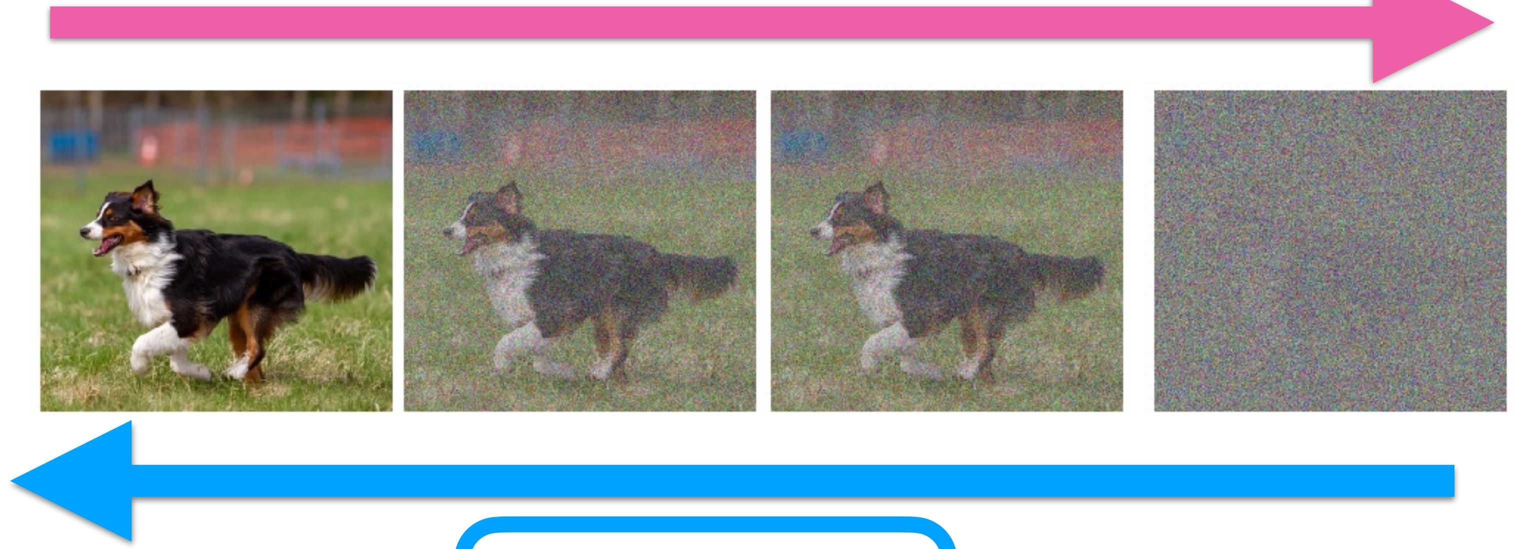
Training



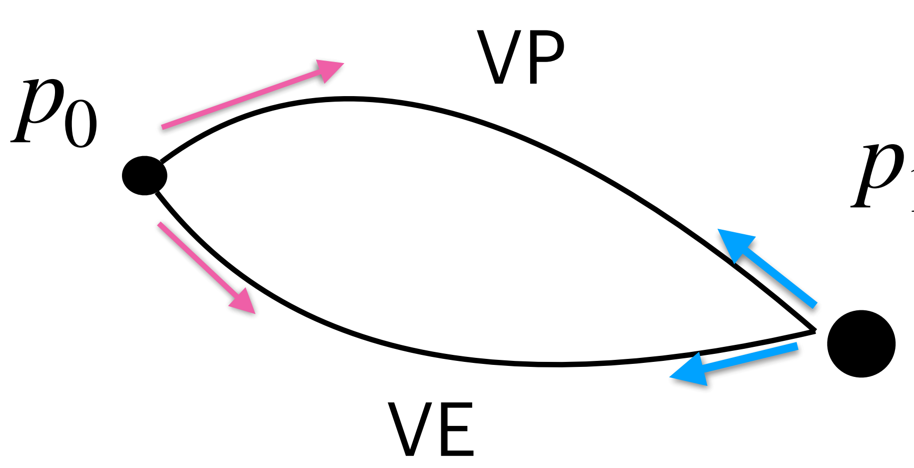
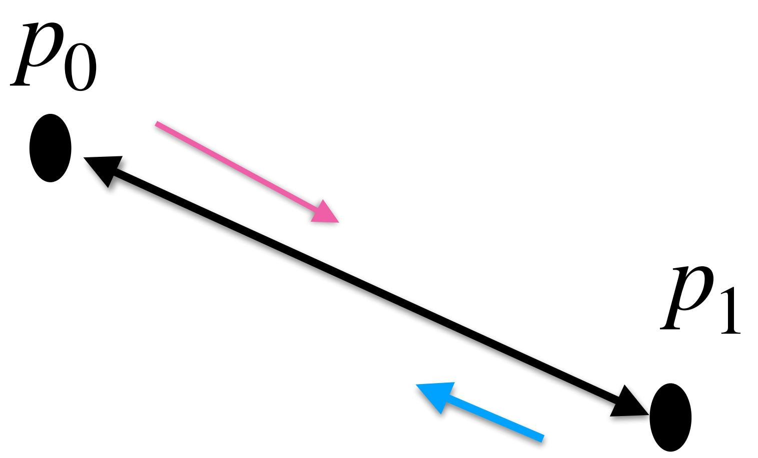
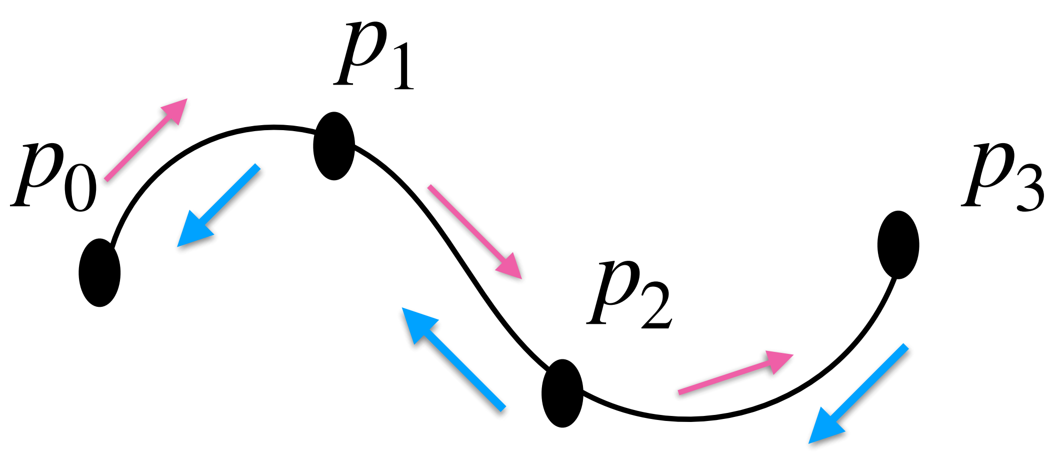
	Diffusion Model	Schrödinger Bridge	**Momentum Schrödinger Bridge**
Path Measure			
Training	**Denoising Score Matching**	**Iterative Proportional Fitting**	

Training

μ^{ϕ} $\quad dx_t = \boxed{f(x_t, t; \phi)dt} + g_t dw_t$

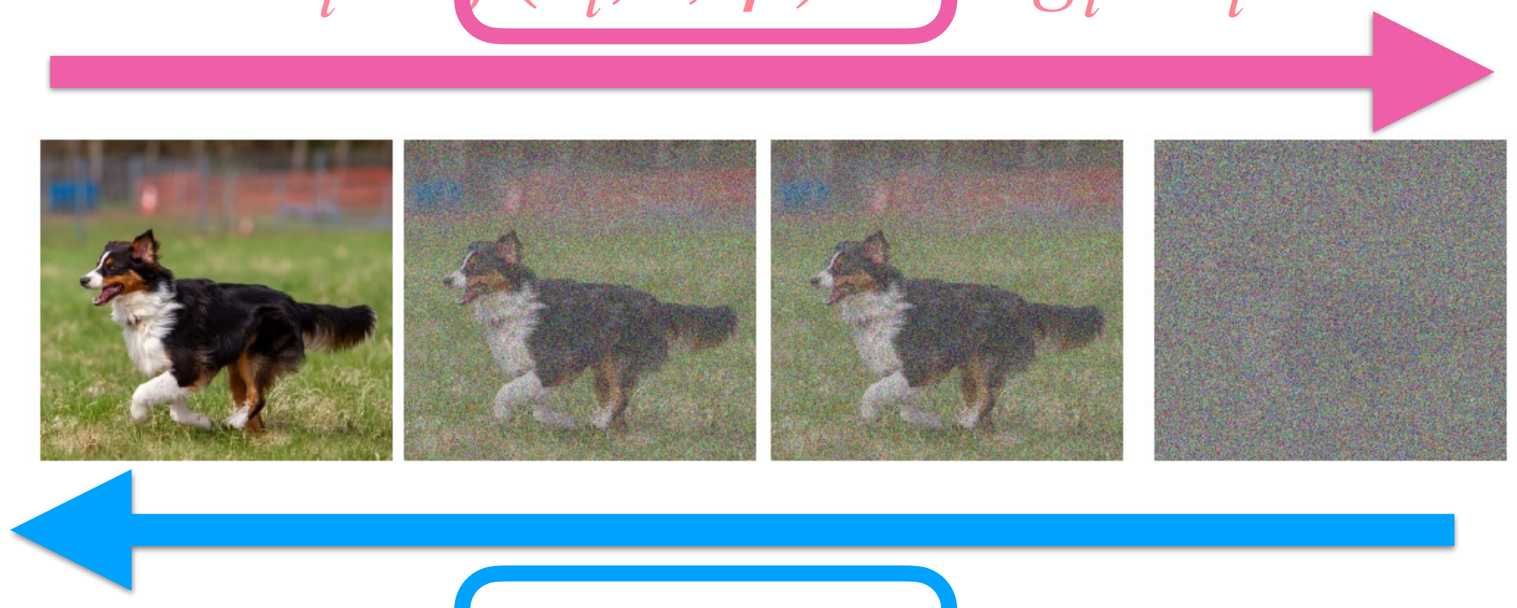
$x_0 \sim p_0$  $x_1 \sim p_1$

ν^{θ} $\quad dx_t = \boxed{b(x_t, t; \theta)dt} + g_t dw_t$

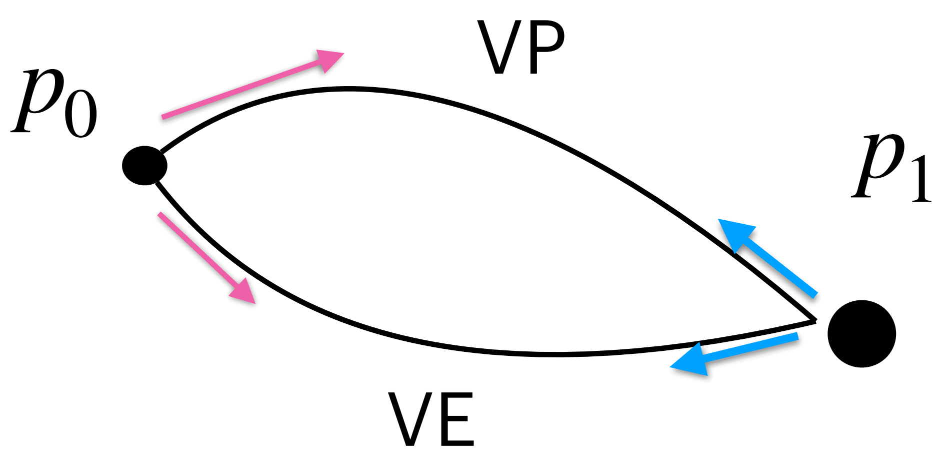
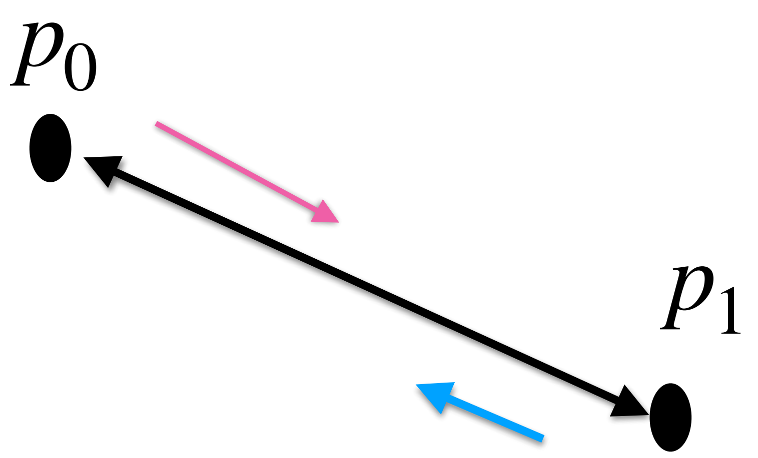
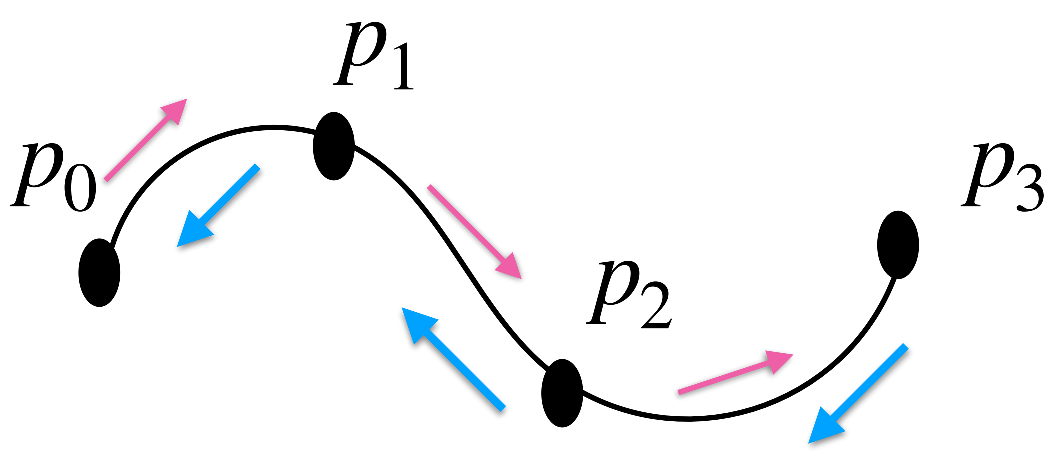
	Diffusion Model	Schrödinger Bridge	**Momentum Schrödinger Bridge**
Path Measure			
Training	**Denoising Score Matching**	$\min_{f} \int_0^T \int \lvert\lvert f_t \rvert\rvert_2^2 dxdt$ $\min_{b} \int_0^T \int \lvert\lvert b_t \rvert\rvert_2^2 dxdt$	

Training

μ^{ϕ} $\quad dx_t = \boxed{f(x_t, t; \phi)dt} + g_t dw_t$

$x_0 \sim p_0$  $x_1 \sim p_1$

ν^{θ} $\quad dx_t = \boxed{b(x_t, t; \theta)dt} + g_t dw_t$

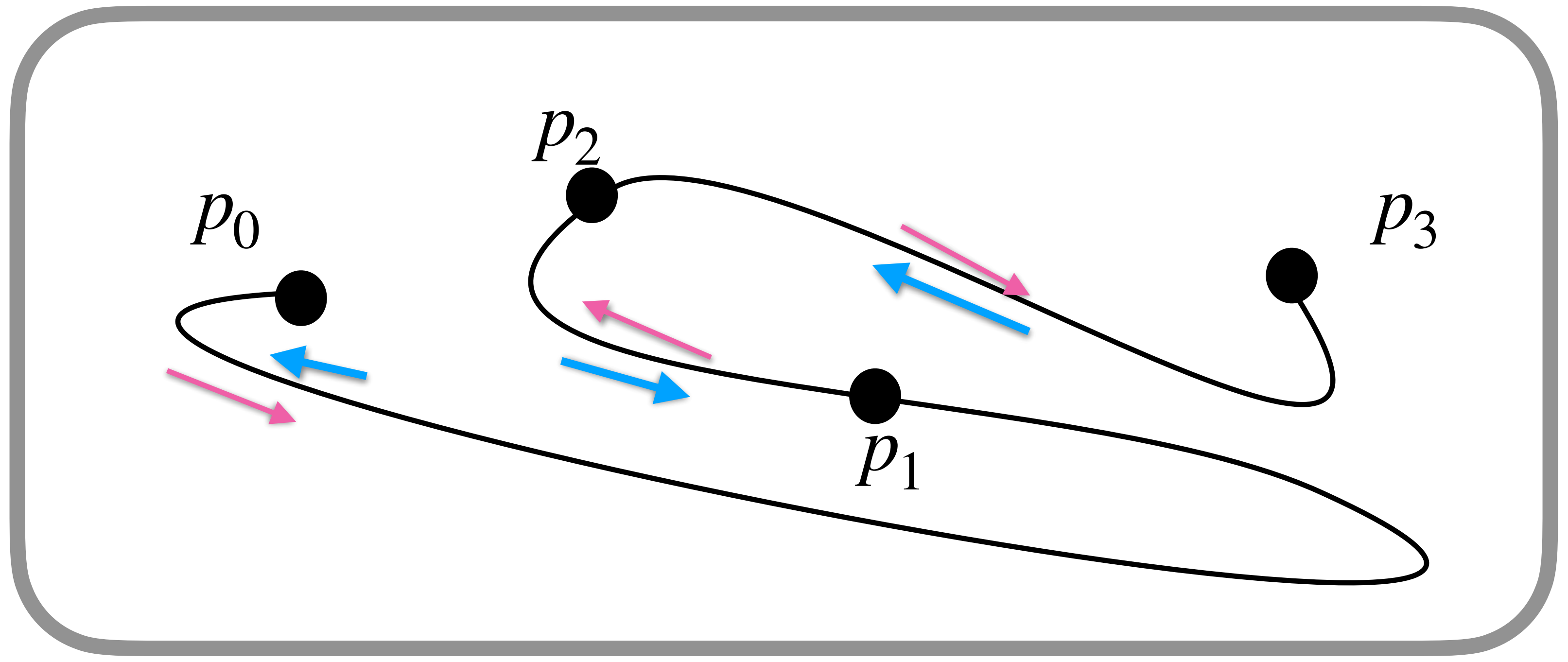
	Diffusion Model	Schrödinger Bridge	**Momentum Schrödinger Bridge**
Path Measure			
Training	**Denoising Score Matching**	**Iterative Proportional Fitting**	**?**

Problem Formulation

Requirements:

1. Preserve the boundaries marginals. — Maximizing likelihood.

$$dx_t = f_t dt + g_t dw_t \quad s.t \quad x_i \sim p_i$$



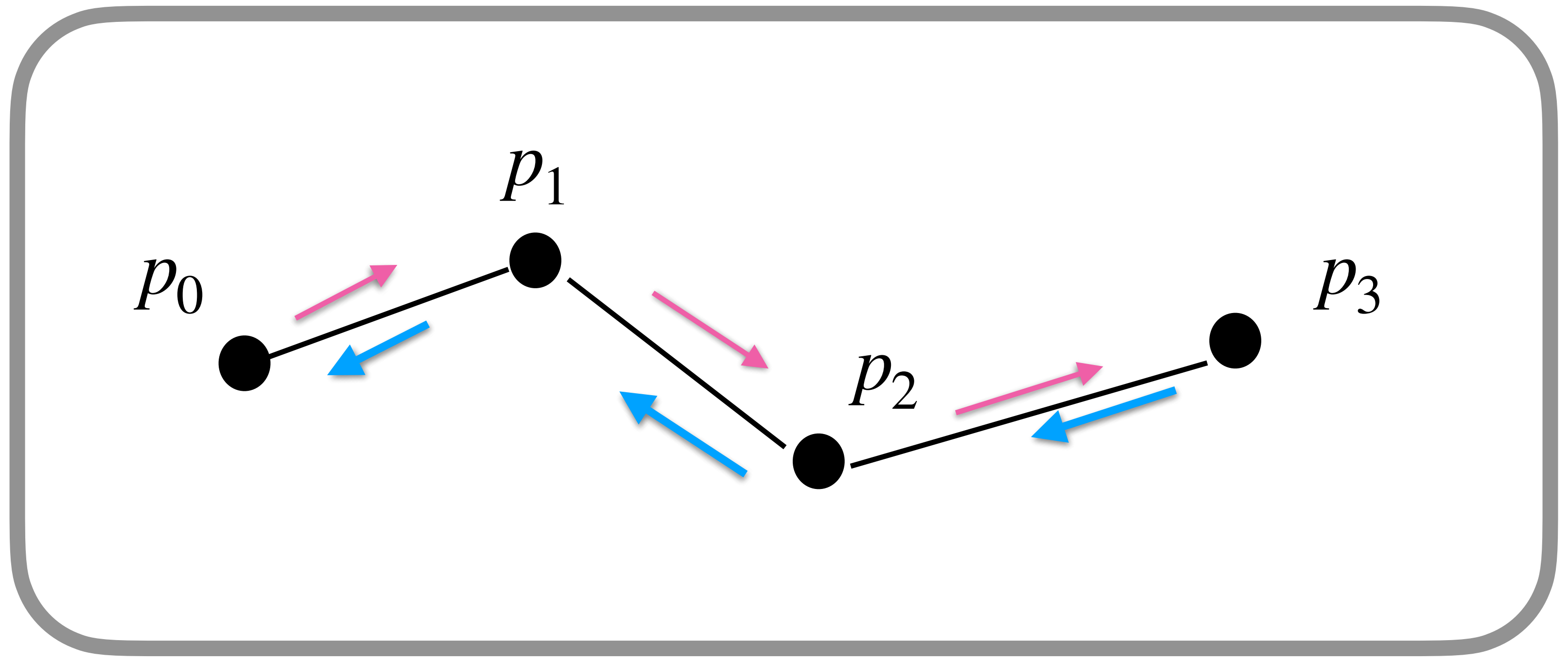
Arbitrary Path with good likelihood

Problem Formulation

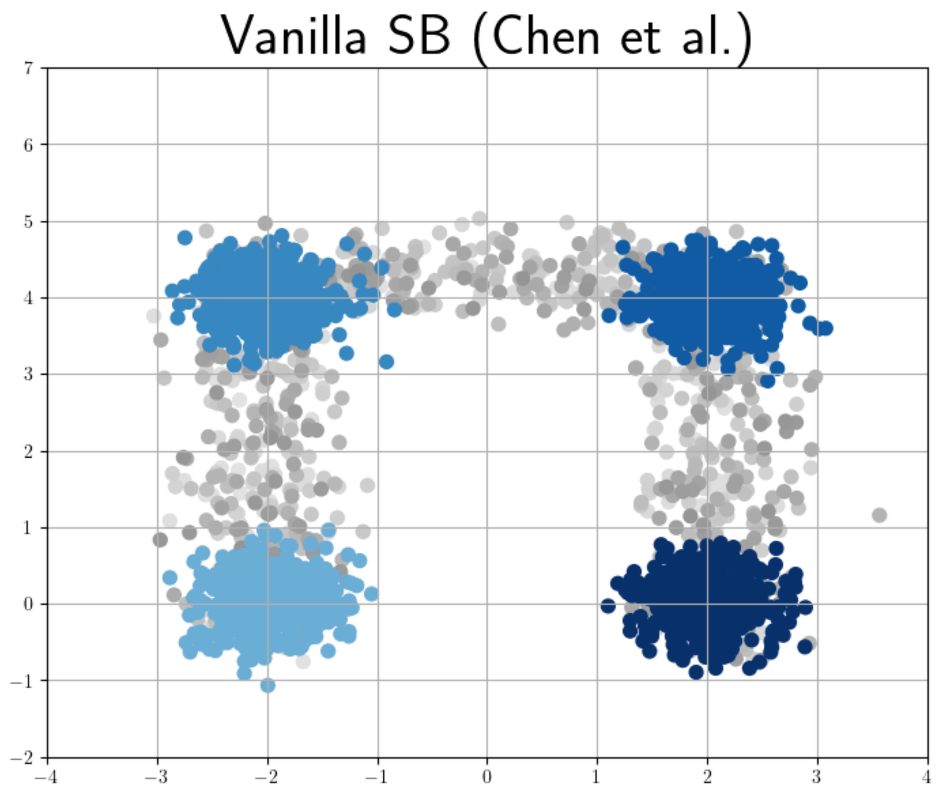
Requirements:

1. Preserve the boundaries marginals. — Maximizing likelihood.
2. Optimality Structure — Schrödinger Bridge

$$\min_{f_t} \int_0^T \int ||f_t||_2^2 \, dx dt \quad dx_t = f_t dt + g_t dw_t \quad s.t \quad x_i \sim p_i$$



Zig-Zag Like Path

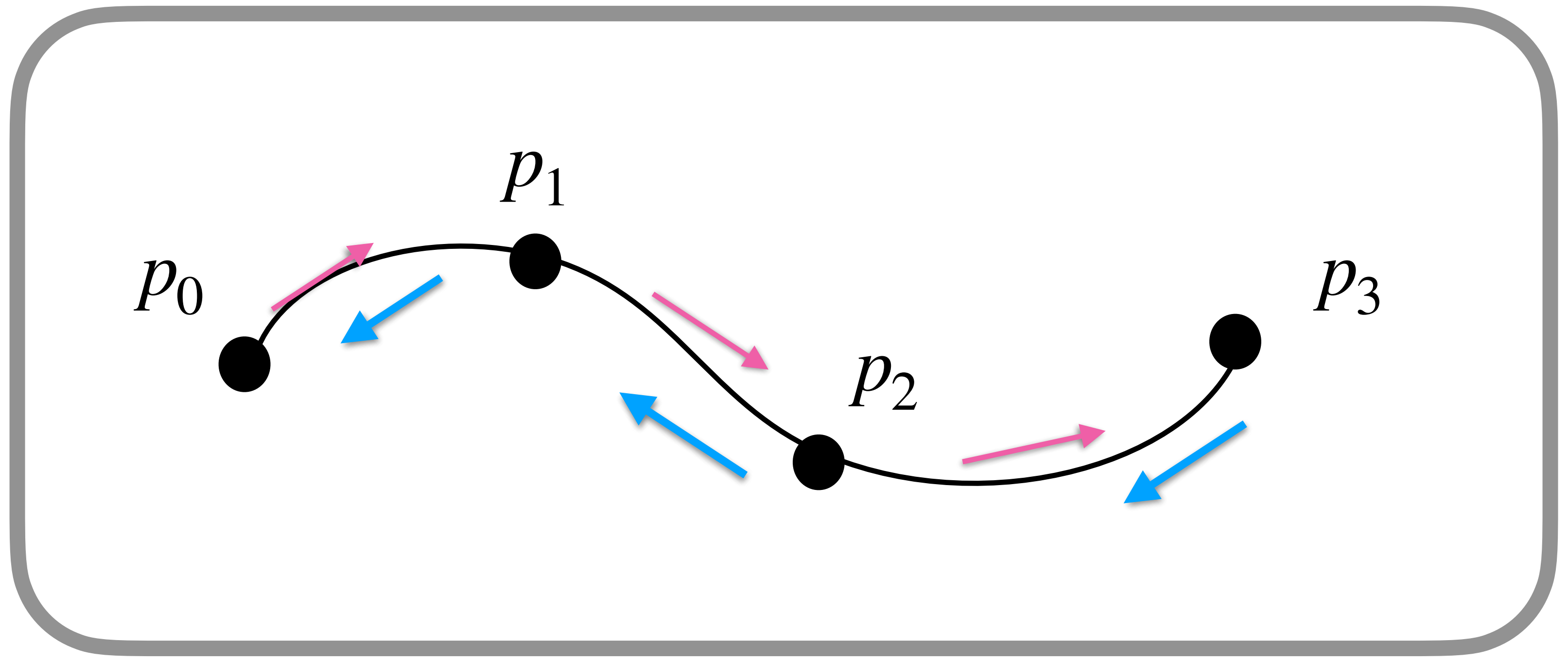


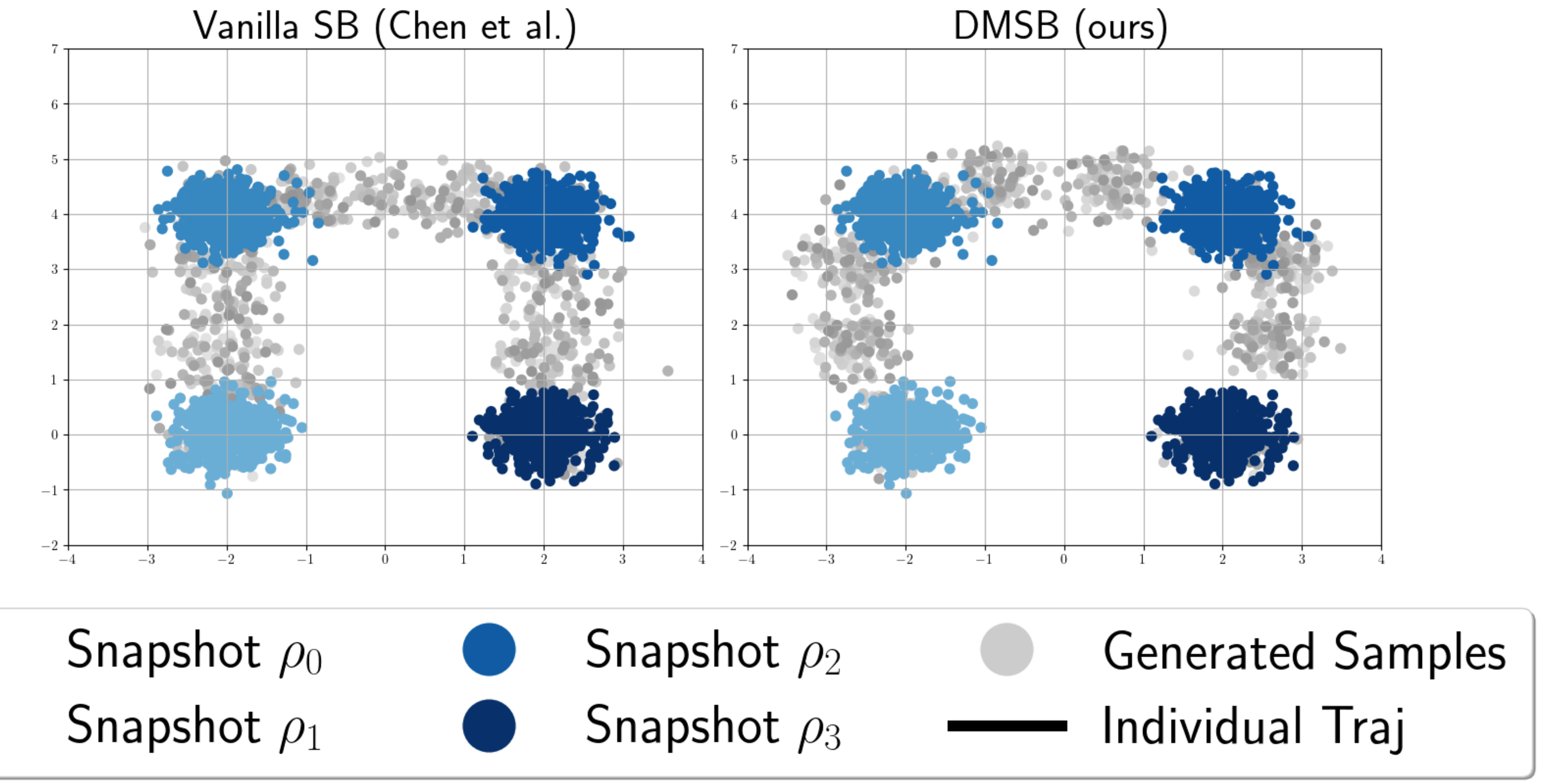
Problem Formulation

Requirement:

1. Preserve the boundaries marginals. — Maximizing likelihood.
2. Optimality Structure — Schrödinger Bridge
3. Smoothest Interpolants in density space — momentum Schrödinger Bridge (by product: pairing)

$$\min_{z_t} \int_0^T \int ||z_t||_2^2 dxdt \quad \begin{aligned} dx_t &= v_t dt \\ dv_t &= z_t dt + g_t dw_t \end{aligned} \quad s.t \quad x_i \sim p_i$$



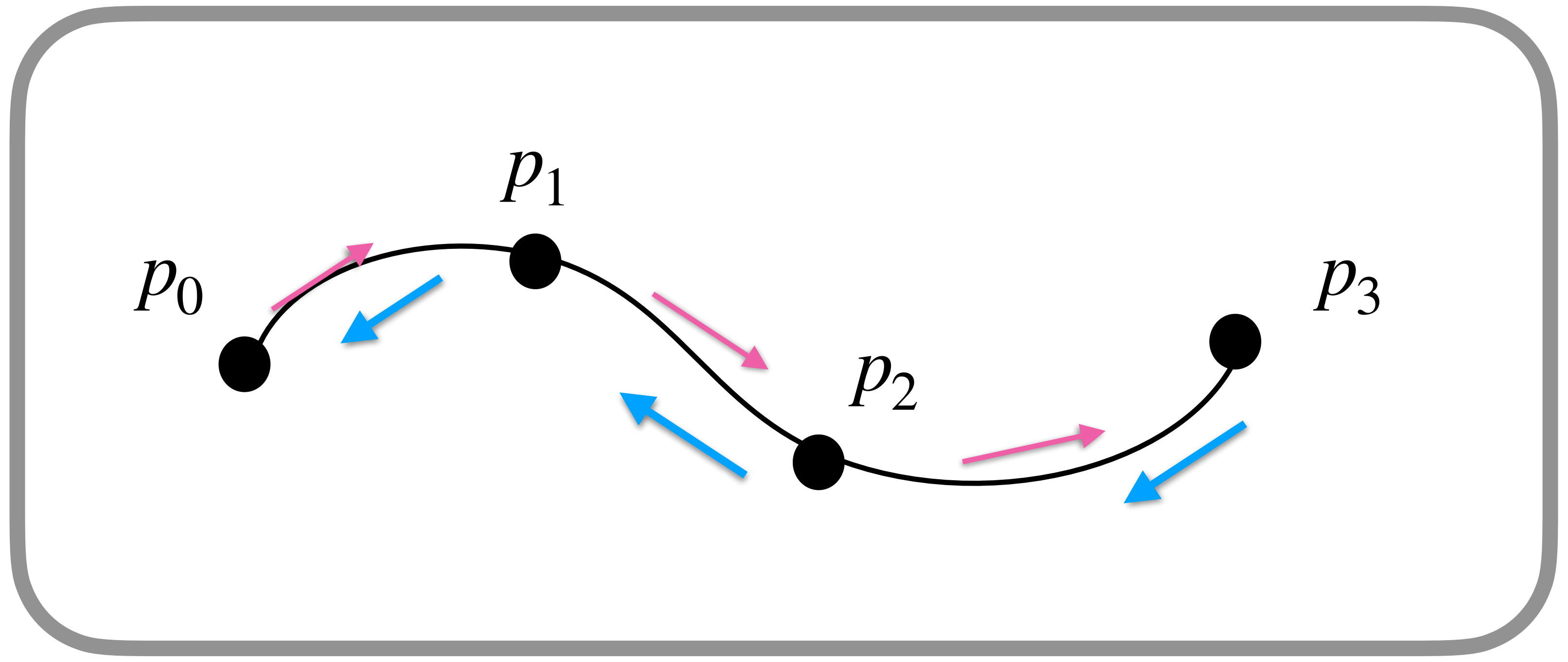


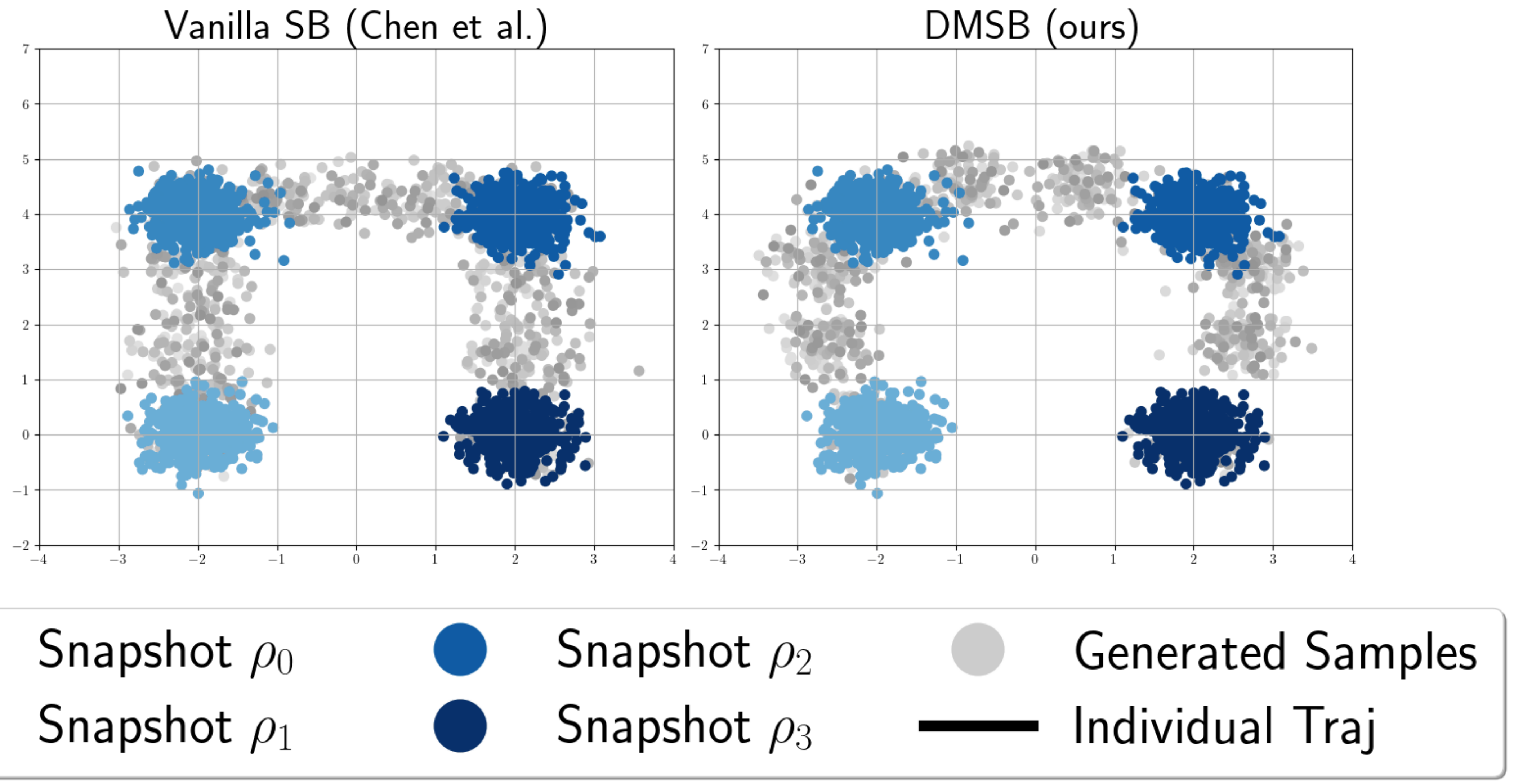
Problem Formulation

Requirement:

1. Preserve the boundaries marginals. — Maximizing likelihood.
2. Optimality Structure — Schrödinger Bridge
3. Smoothest Interpolants in density space — momentum Schrödinger Bridge (by product: pairing)

$$\cancel{\min_{z_t} \int_0^T \int ||z_t||_2^2 dx dt} \quad \begin{array}{l} \cancel{dx_t = v_t dt} \\ \cancel{dv_t = z_t dt + g_t dw_t} \end{array} \quad s.t \quad x_i \sim p_i$$



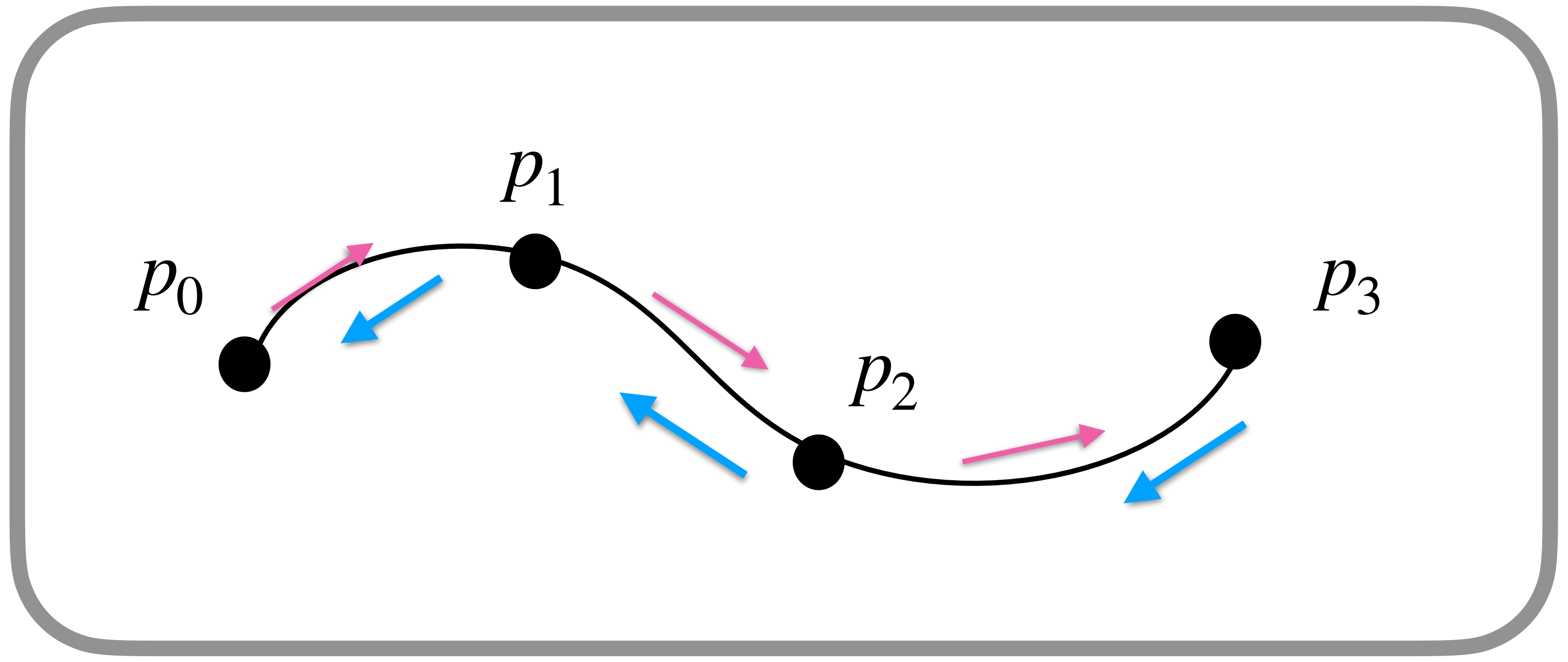


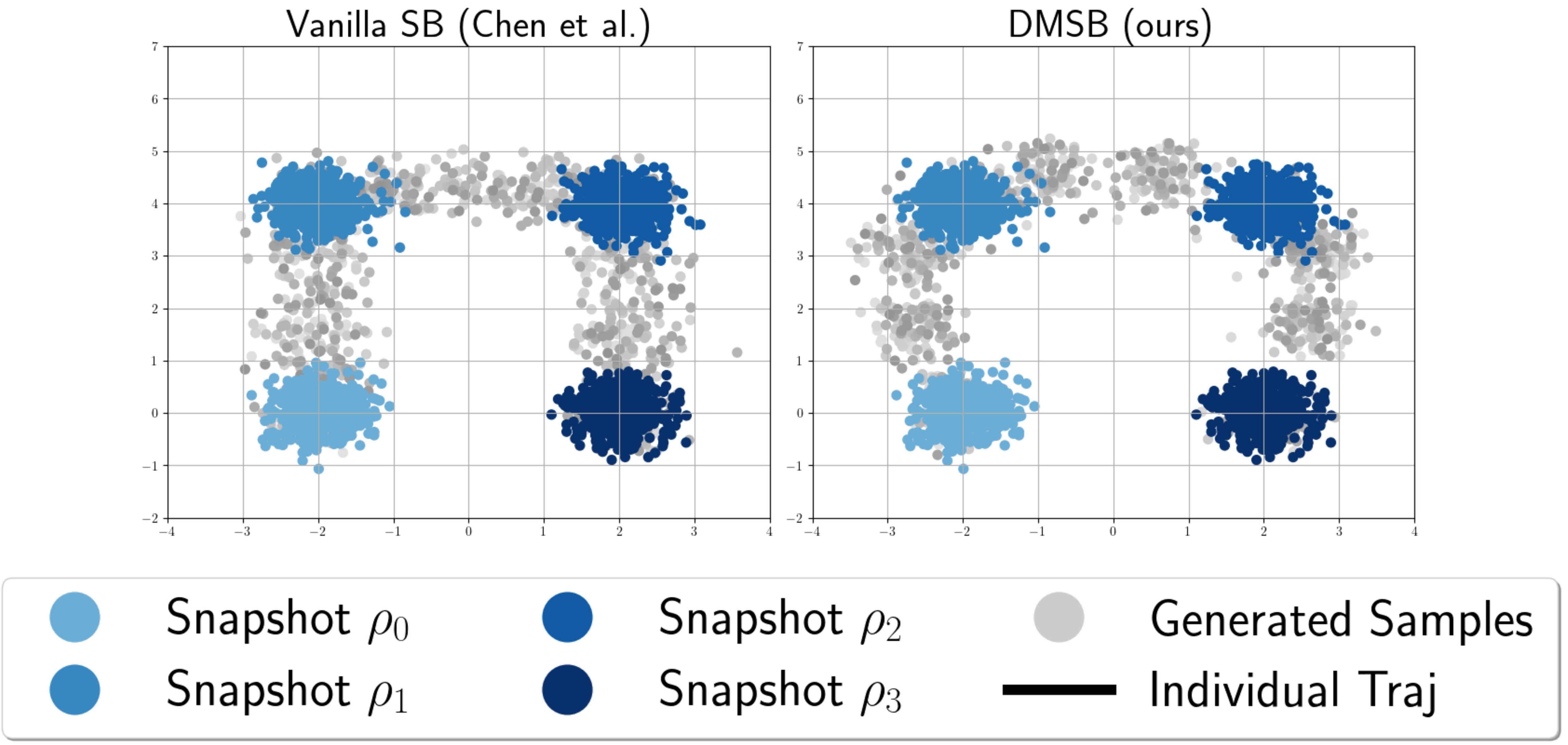
Problem Formulation

Requirement:

1. Preserve the boundaries marginals. — Maximizing likelihood.
2. Optimality Structure — Schrödinger Bridge
3. Smoothest Interpolants in density space — momentum Schrödinger Bridge (by product: pairing)

$$\min_{\pi} KL(\pi || \xi) \quad s.t \quad x_i \sim p_i$$



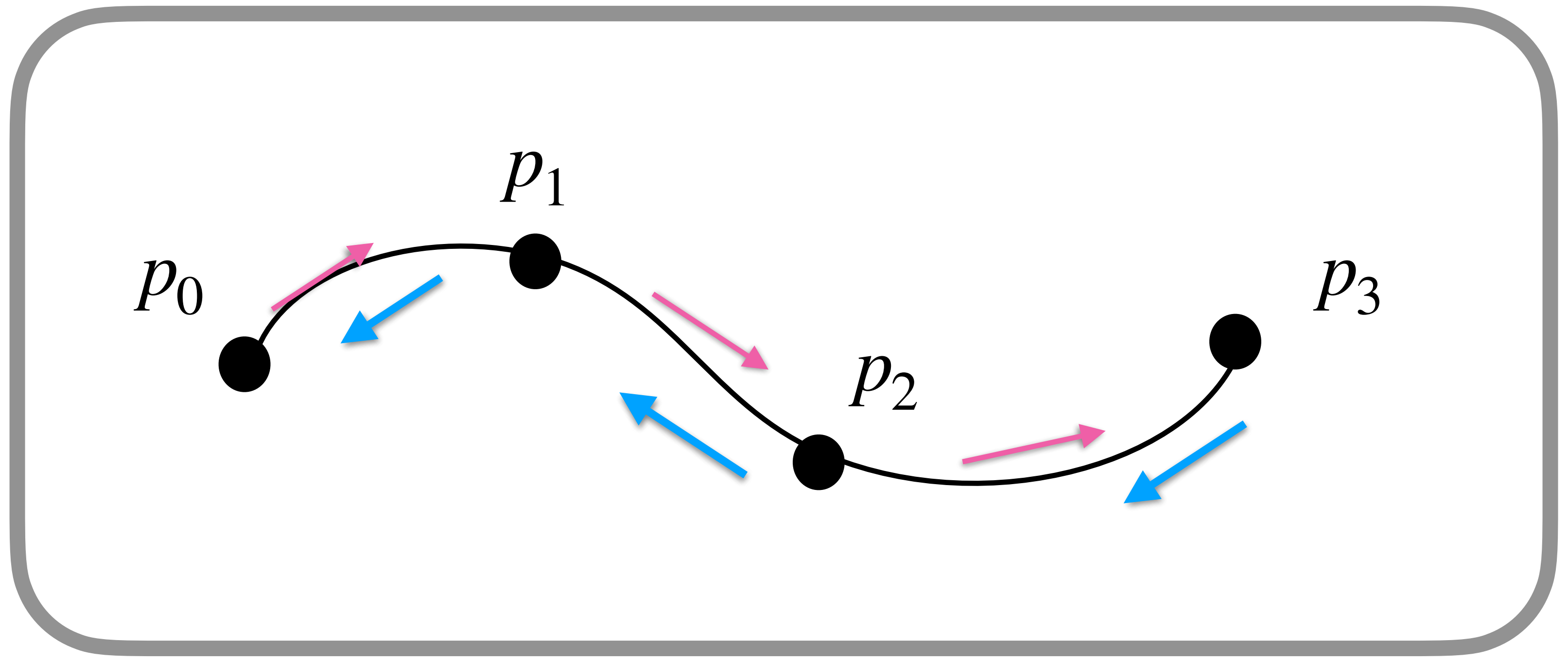


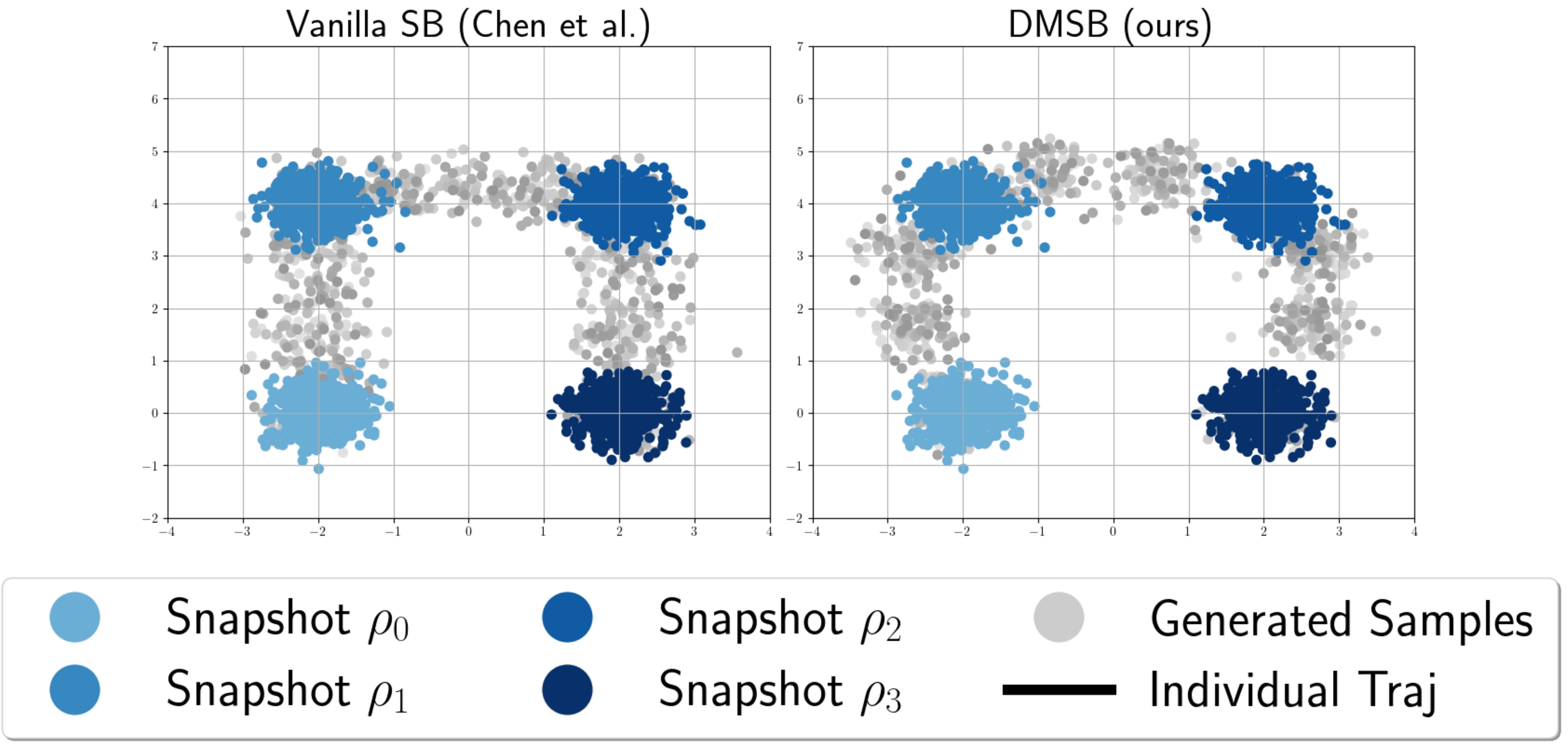
Problem Formulation

Requirement:

1. Preserve the boundaries marginals. — Maximizing likelihood.
2. Optimality Structure — Schrödinger Bridge
3. Smoothest Interpolants in density space — momentum Schrödinger Bridge (by product: pairing)

$$\min_{\pi} KL(\pi || \xi) \quad \cancel{s.t \quad x_i \sim p_i}$$



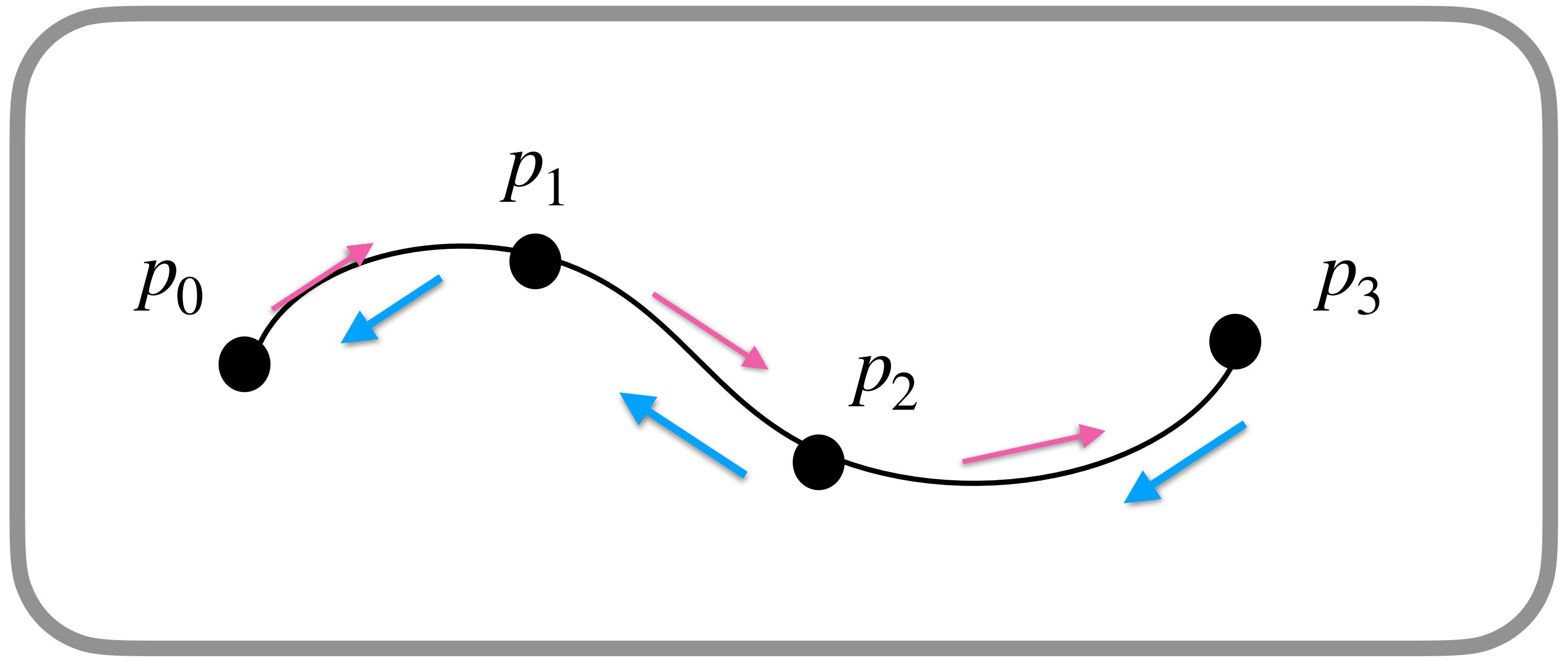


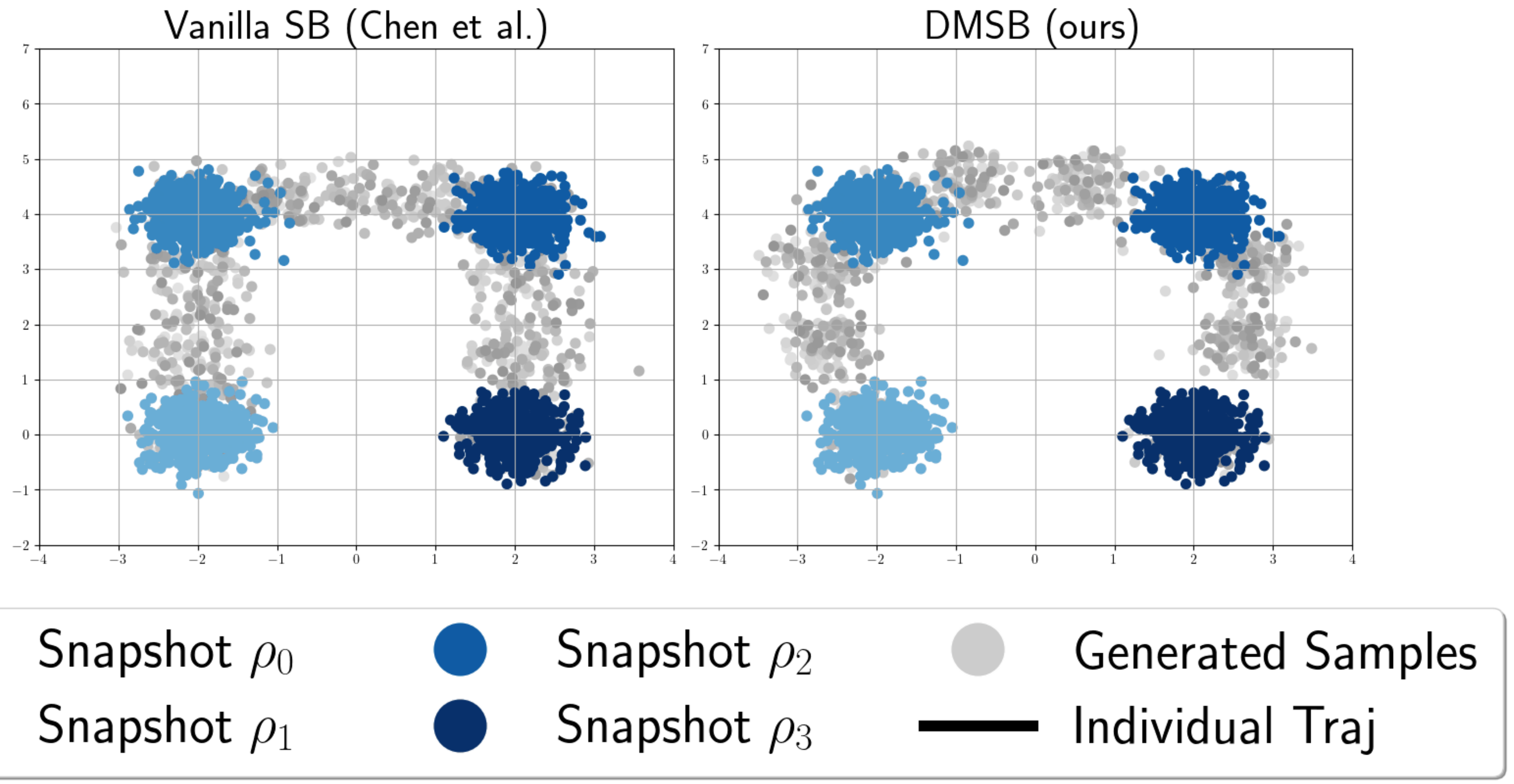
Problem Formulation

Requirement:

1. Preserve the boundaries marginals. — Maximizing likelihood.
2. Optimality Structure — Schrödinger Bridge
3. Smoothest Interpolants in density space — momentum Schrödinger Bridge (by product: pairing)

$$\min_{\pi \in \cap K_i} KL(\pi || \xi)$$

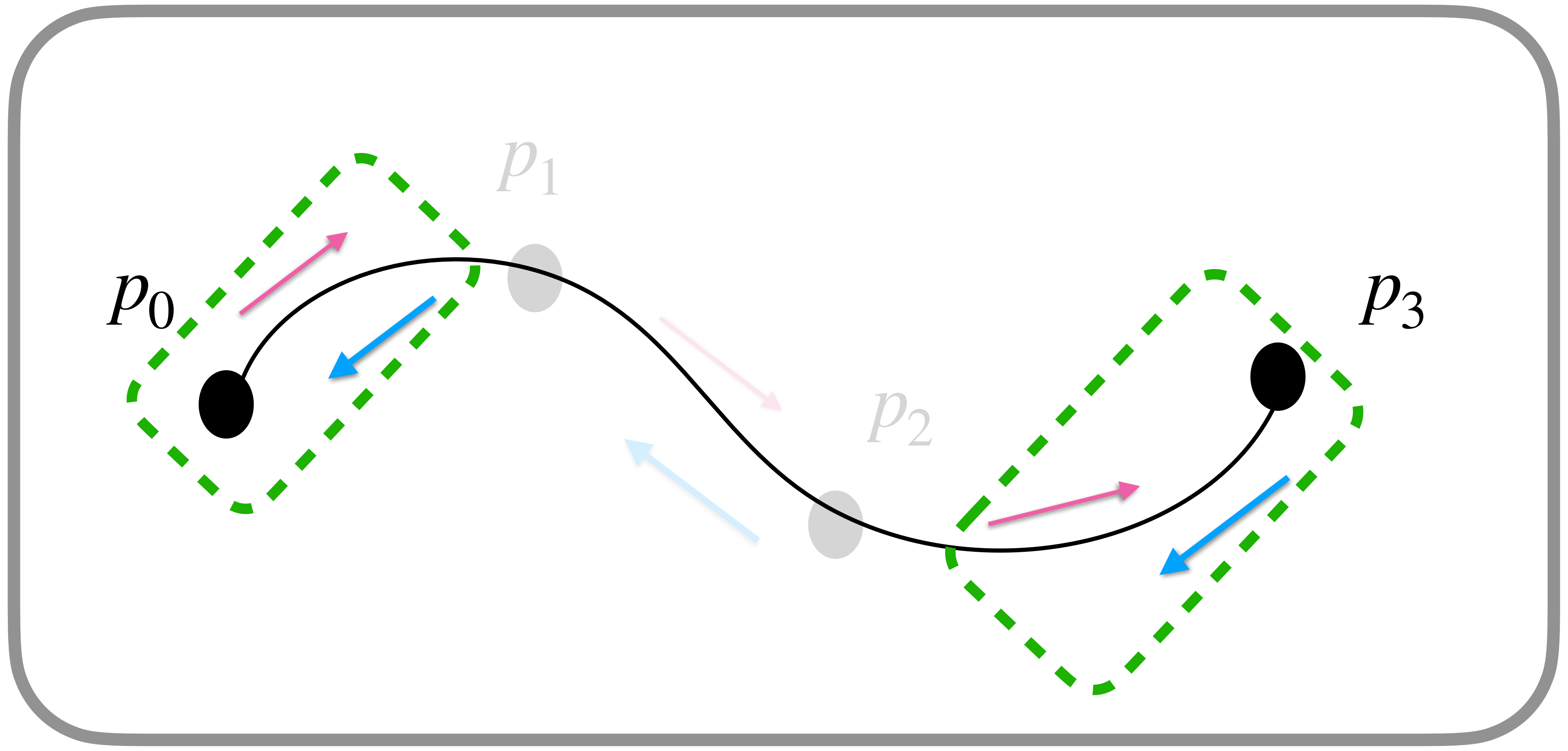




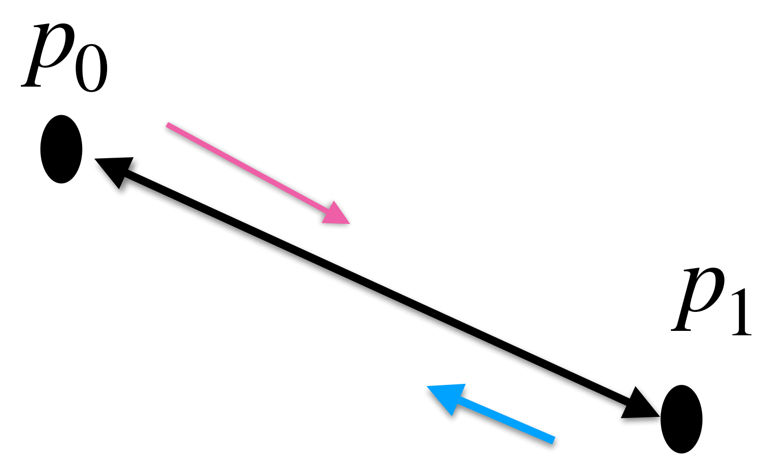
Solutions

- p_0 and p_N is similar to the training of SB, since there is only one side.

momentum Schrödinger Bridge



Schrödinger Bridge



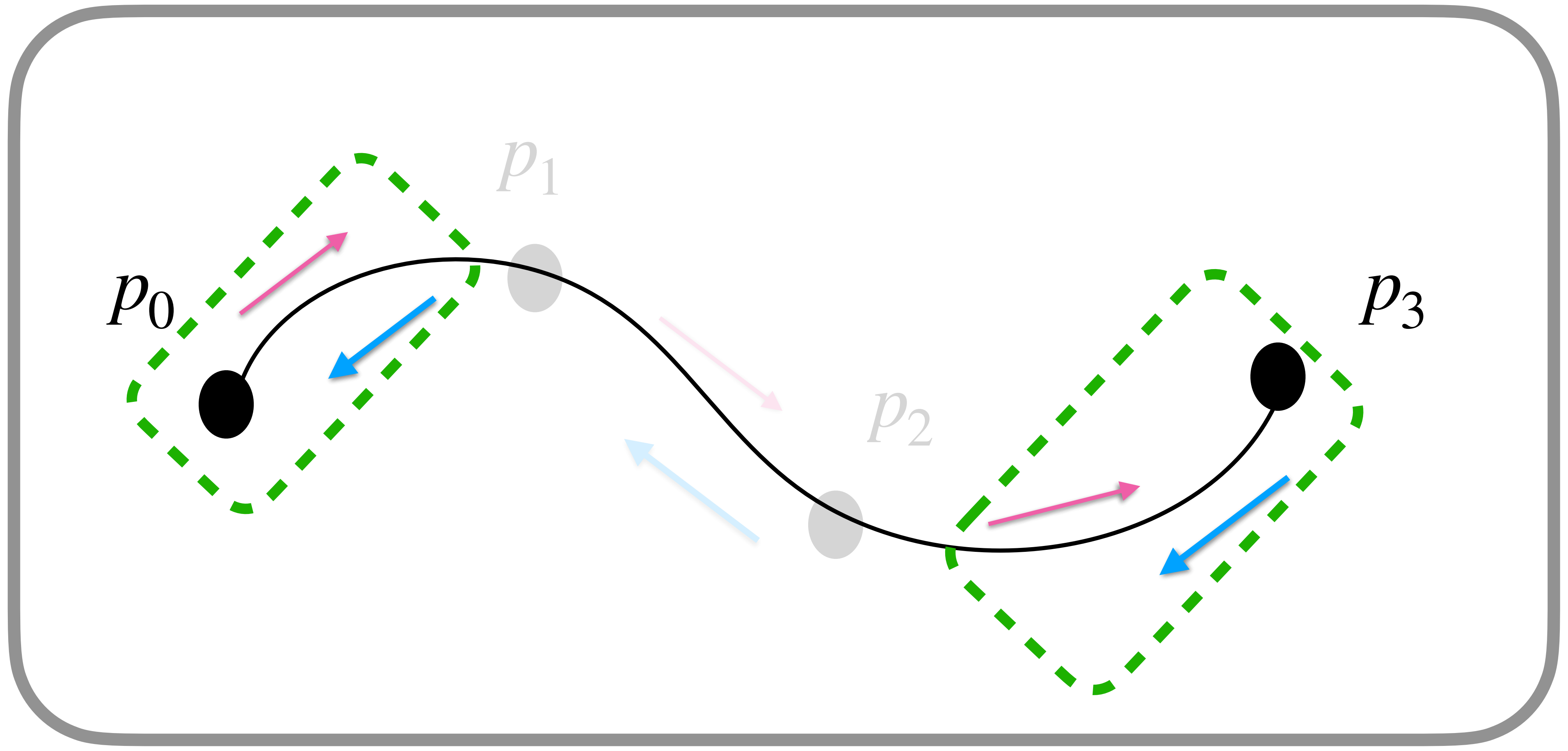
$$\min_{\theta} KL(\mu^{\phi} || \nu^{\theta}) \quad \nu \in \left\{ \int \pi_{0,1} dx_0 = p_3 \right\}$$

$$\min_{\phi} KL(\nu^{\theta} || \mu^{\phi}) \quad \mu \in \left\{ \int \pi_{0,1} dx_1 = p_0 \right\}$$

Solutions

- p_0 and p_N is similar to the training of SB, since there is only one side.

momentum Schrödinger Bridge



Boundaries/constrains:

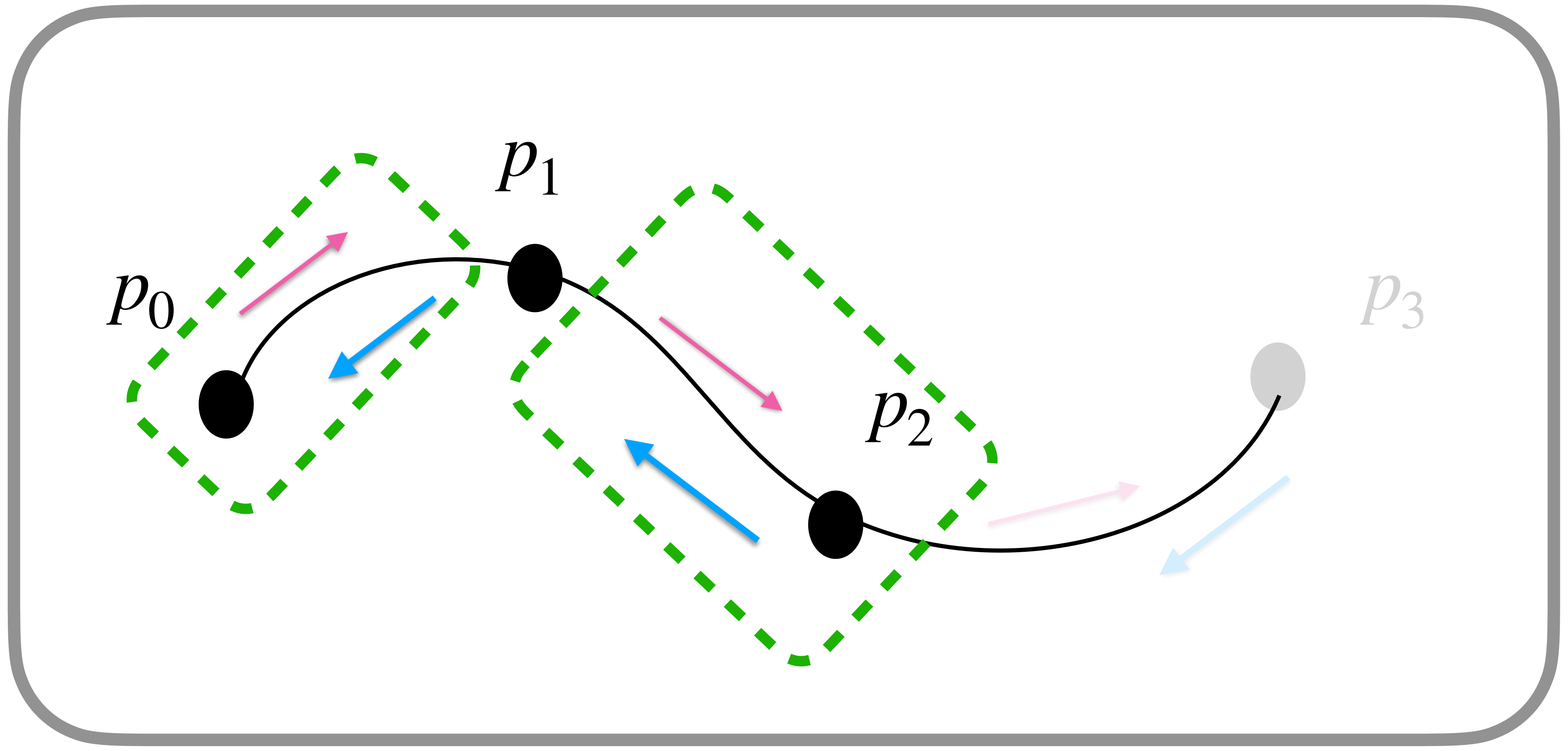
1. $K_0 = \left\{ \int\int \pi_{t_1,t_0} dx_1 dv_1 = p(x, v, 0) \right\}$
2. $K_3 = \left\{ \int\int \pi_{t_2,t_3} dx_2 dv_2 = p(x, v, 3) \right\}$

Preserve boundary

Solutions

- Intermediate marginal needs to consider boundary from two directions.

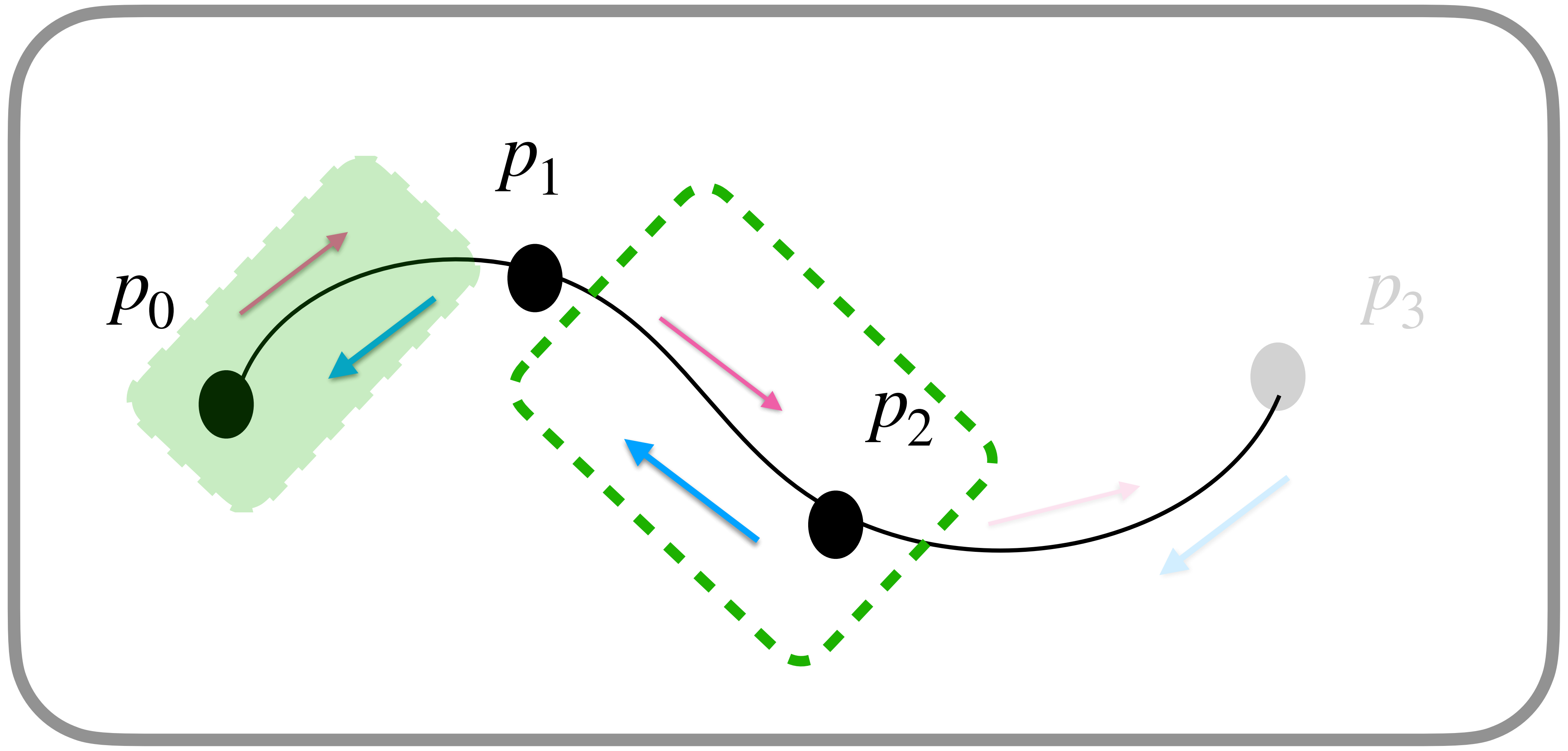
momentum Schrödinger Bridge



Solutions

- Intermediate marginal needs to consider boundary from two directions.

momentum Schrödinger Bridge



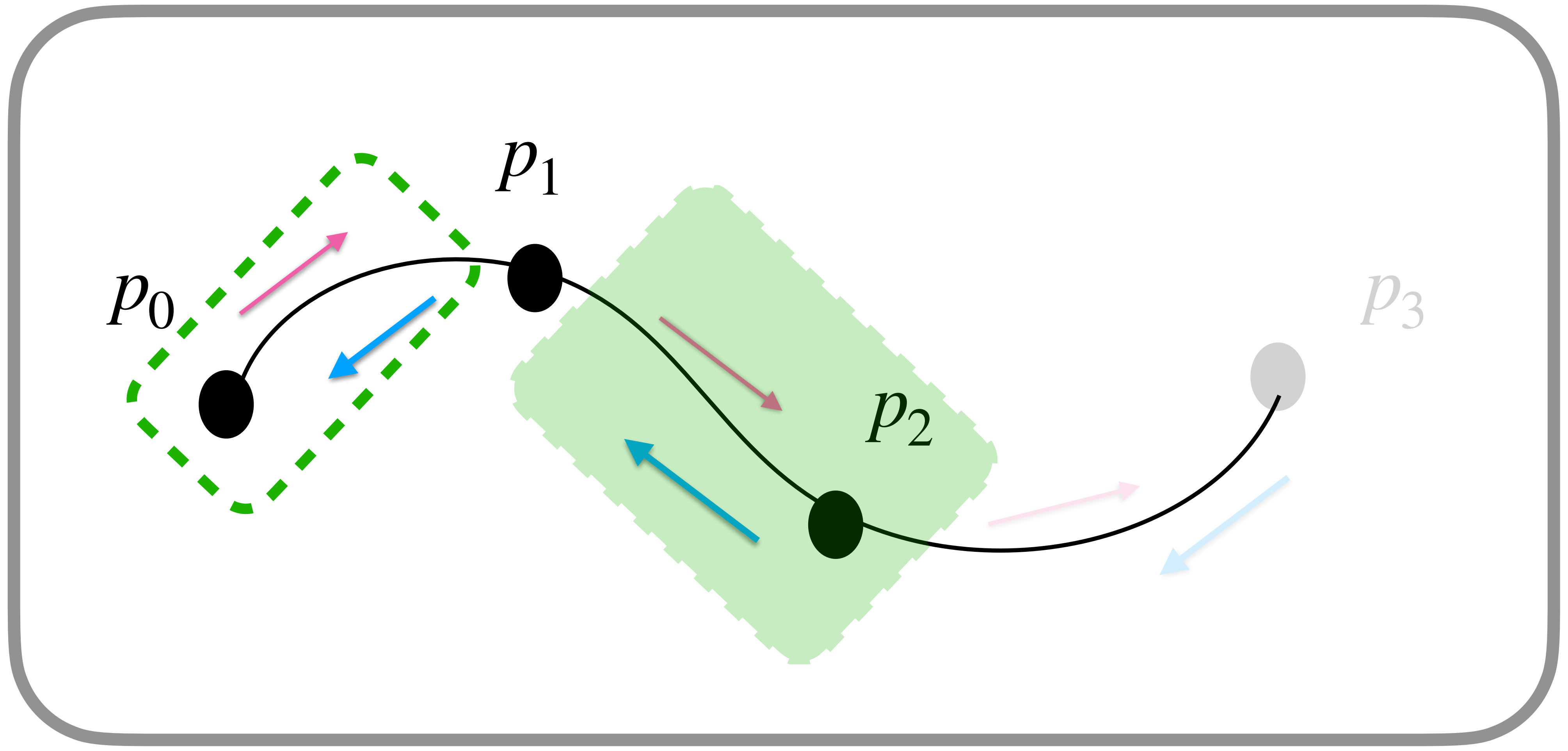
Boundaries/constrains:

1. $K_1 = \left\{ \int\int \pi_{t_0,t_1} dx_0 dv_0 = p(x, v, 1) \right\}$

Solutions

- Intermediate marginal needs to consider boundary from two directions.

momentum Schrödinger Bridge



Boundaries/constrains:

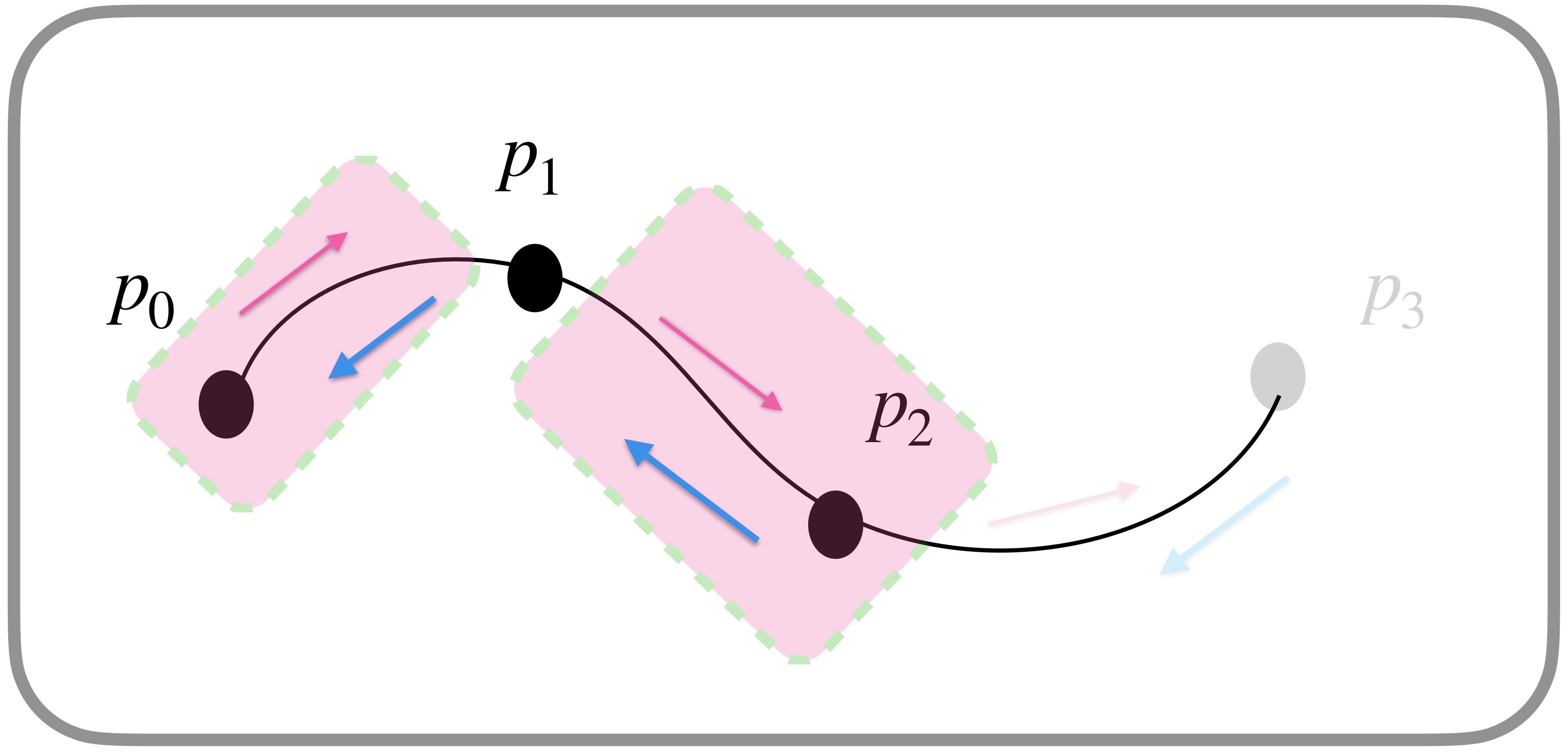
1. $K_1 = \left\{ \int\int \pi_{t_0,t_1} dx_0 dv_0 = p(x, v, 1) \right\}$

2. $K_2 = \left\{ \int\int \pi_{t_1,t_2} dx_2 dv_2 = p(x, v, 1) \right\}$

Solutions

- Intermediate marginal needs to consider boundary from two directions.

momentum Schrödinger Bridge



Boundaries/constrains:

1. $K_1 = \left\{ \int\int \pi_{t_0,t_1} dx_0 dv_0 = p(x, v, 1) \right\}$
2. $K_1 = \left\{ \int\int \pi_{t_1,t_2} dx_2 dv_2 = p(x, v, 1) \right\}$
3. $K_1^b = \left\{ \int\int \pi_{t_1,t_2} dx_2 dv_2 = \int\int \pi_{t_0,t_1} dx_0 dv_0 \right\}$

Preserve boundary

Bridge

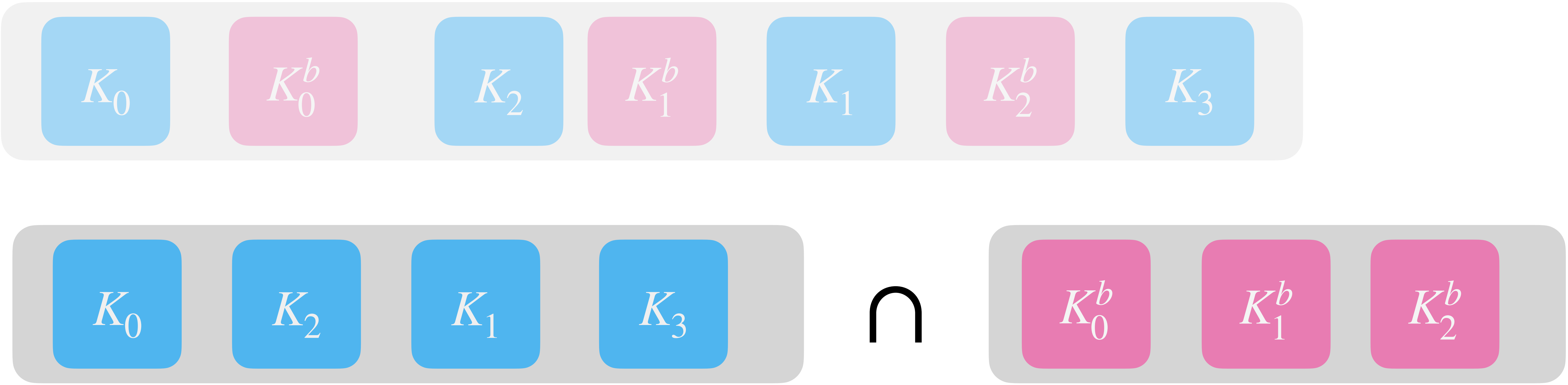
Solutions

$$\min_{\pi \in \cap K_i} KL(\pi || \xi)$$

K_0 K_0^b K_2 K_1^b K_1 K_2^b K_3

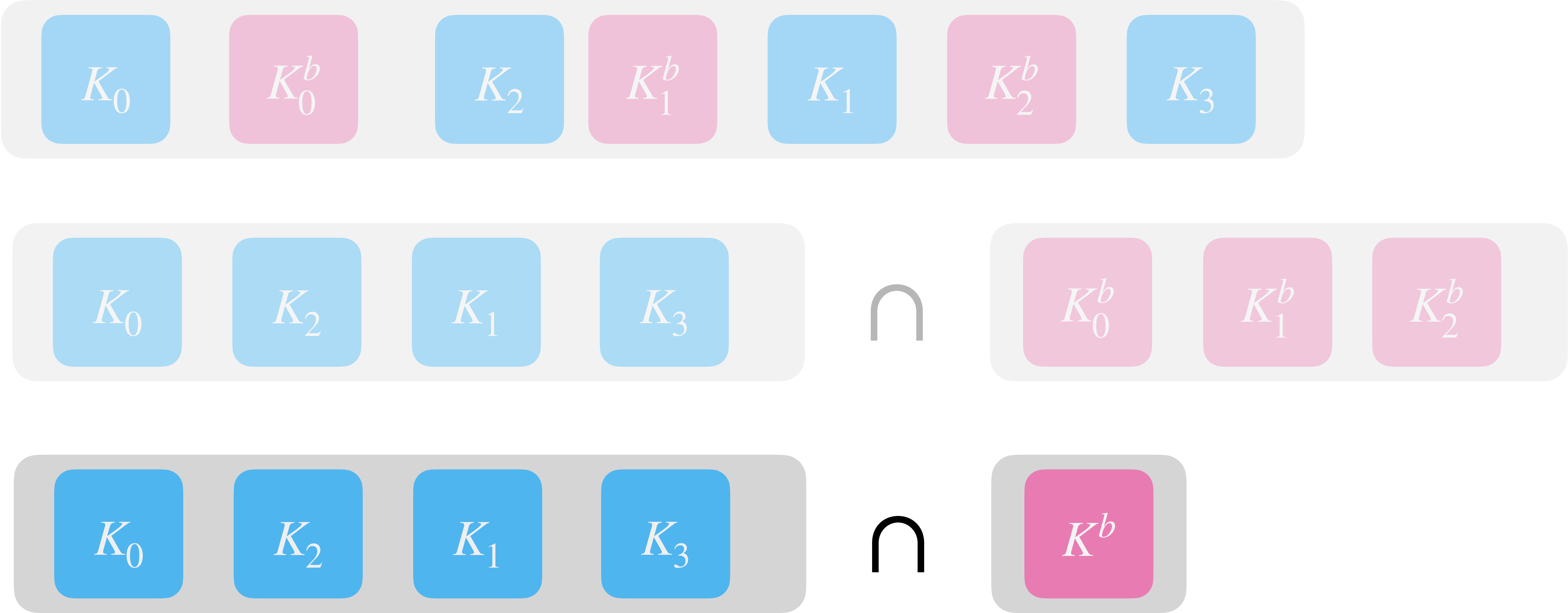
Solutions

$$\min_{\pi \in \cap K_i} KL(\pi || \xi)$$

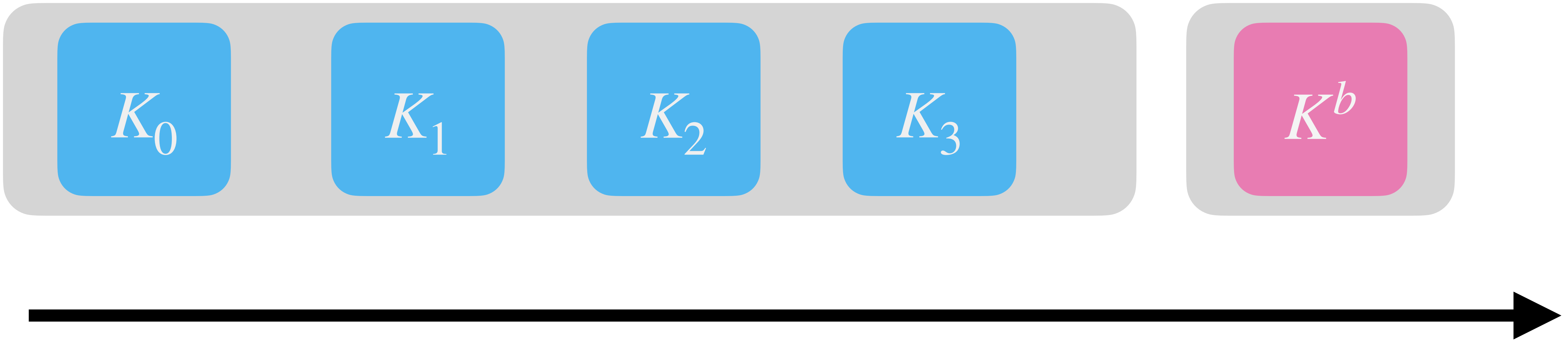


Solutions

$$\min_{\pi \in \cap K_i} KL(\pi || \xi)$$

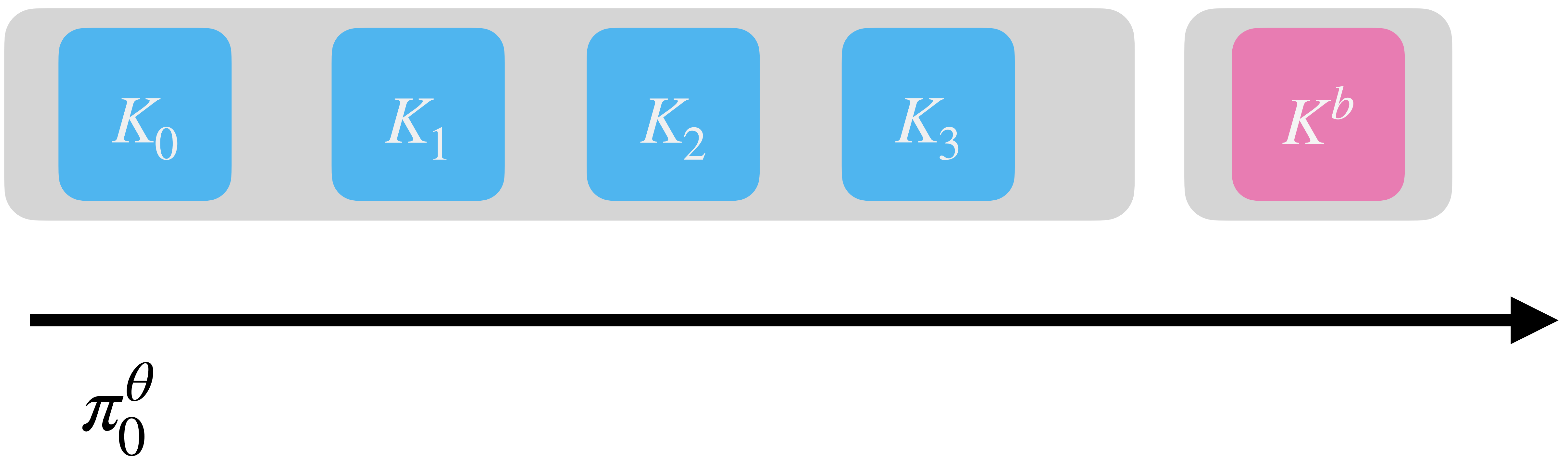


Solutions

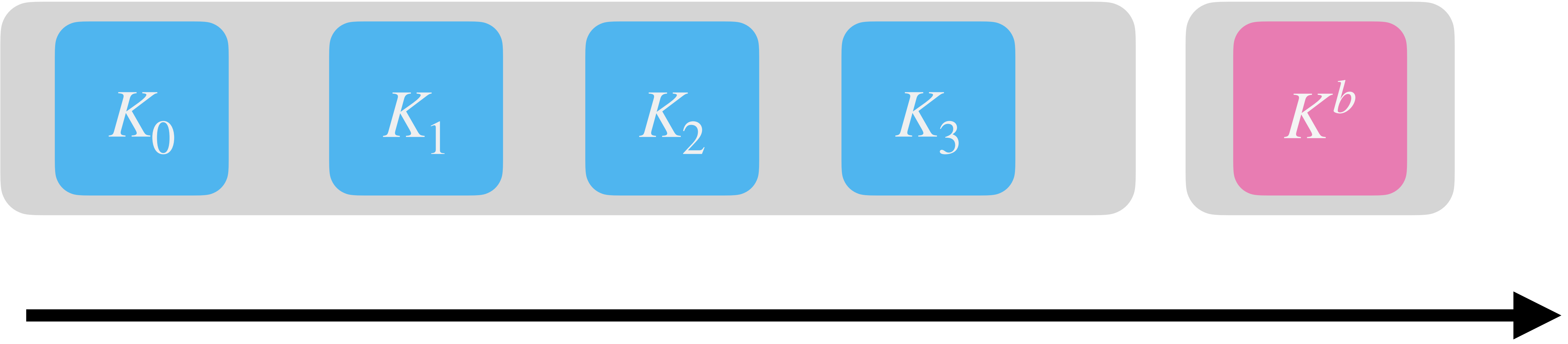


$$\min_{\pi \in K_0} KL(\pi || \xi)$$

Solutions

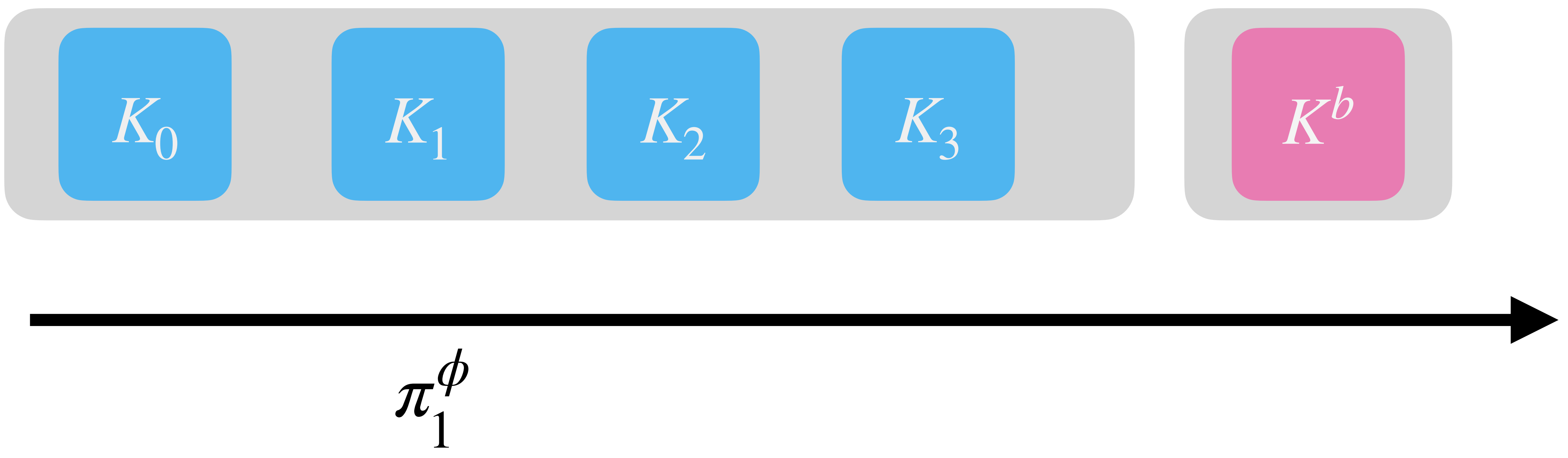


Solutions

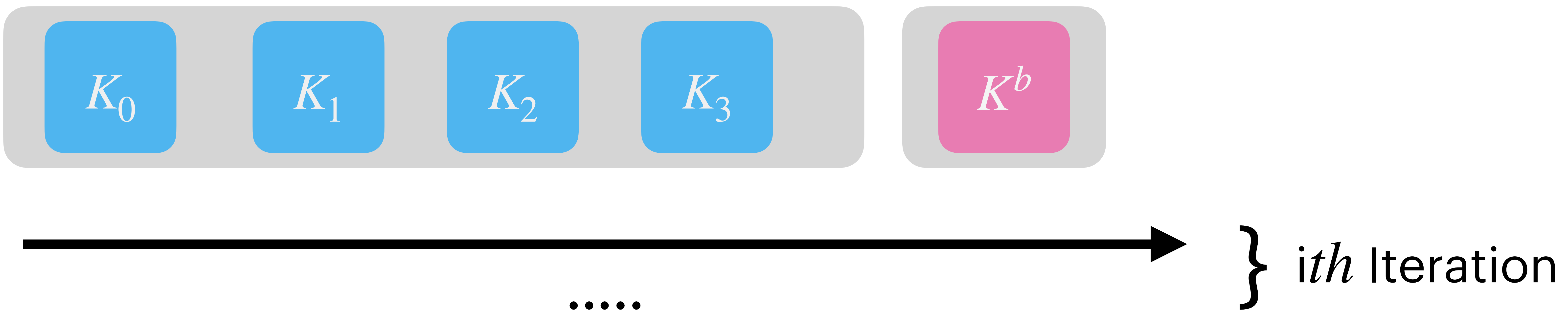


$$\min_{\pi \in K_0} KL(\pi \,||\, \pi_0^\theta)$$

Solutions

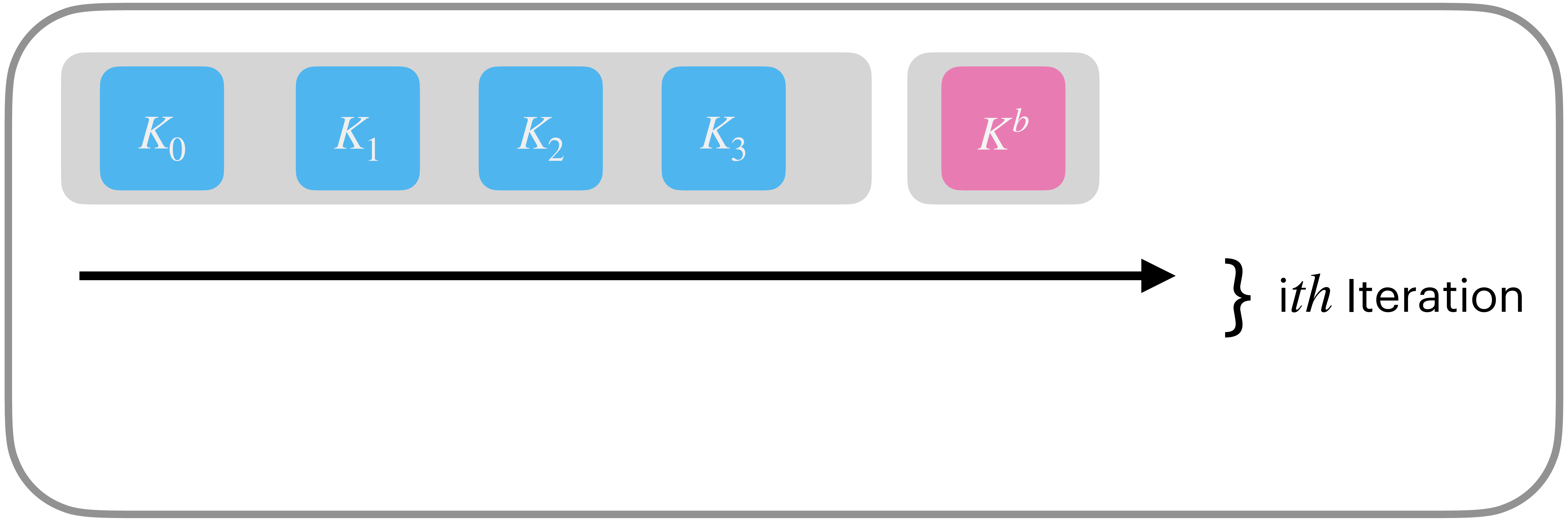


Solutions



Solutions

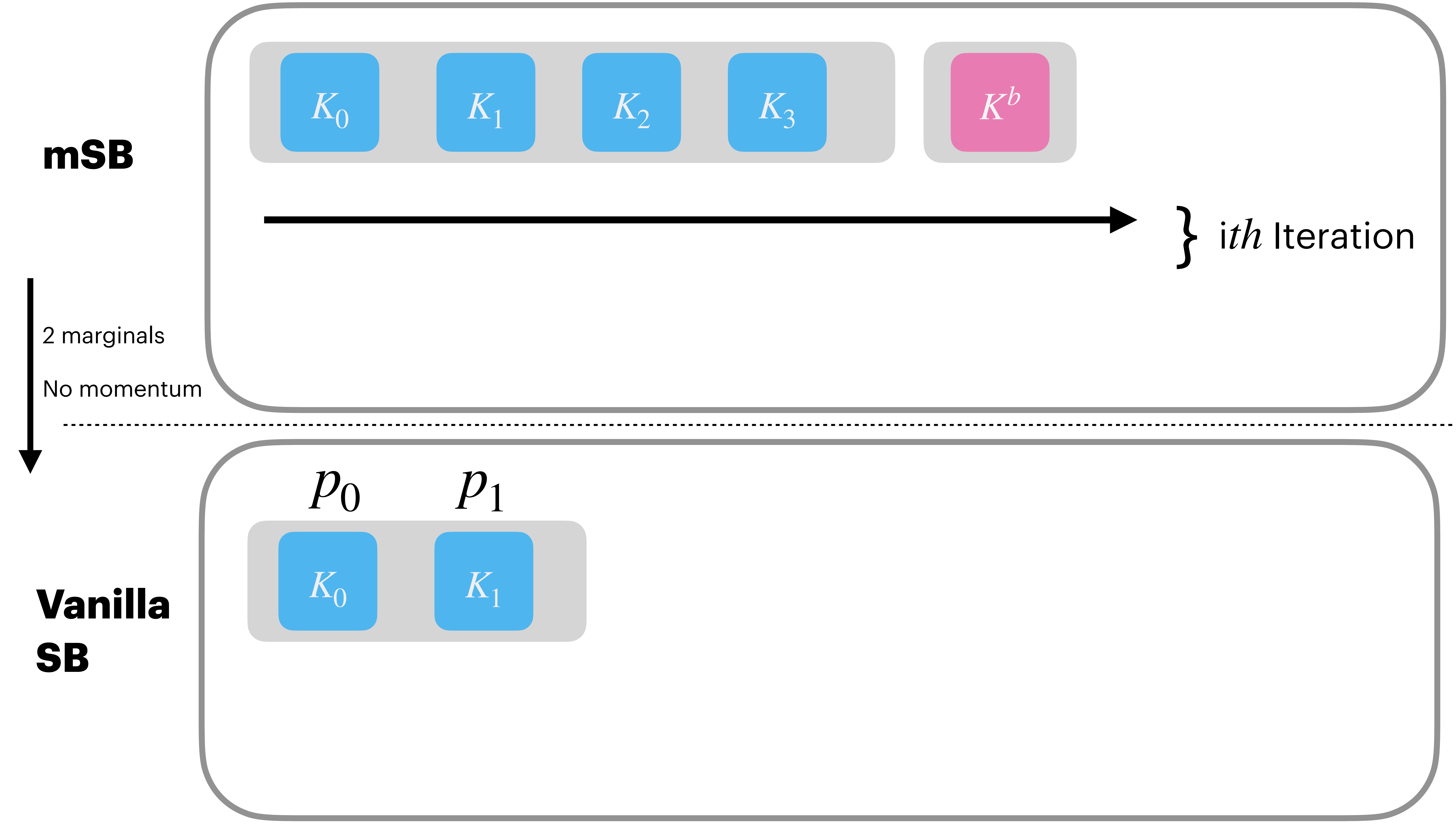
mSB



Bregman Iteration

$$\min_{\pi \in \cap K_i} KL(\pi || \xi)$$

Solutions


mSB
K_0
K_1
K_2
K_3
K^b
$i th$ Iteration
2 marginals
No momentum
p_0
p_1
K_0
K_1
Vanilla SB

Solutions

mSB

K_0 K_1 K_2 K_3 K^b

$\}$ ith Iteration

2 marginals

No momentum

Vanilla SB

p_0 p_1

K_0 K_1

$\min_{\theta} KL(\mu^{\phi} || \nu^{\theta})$

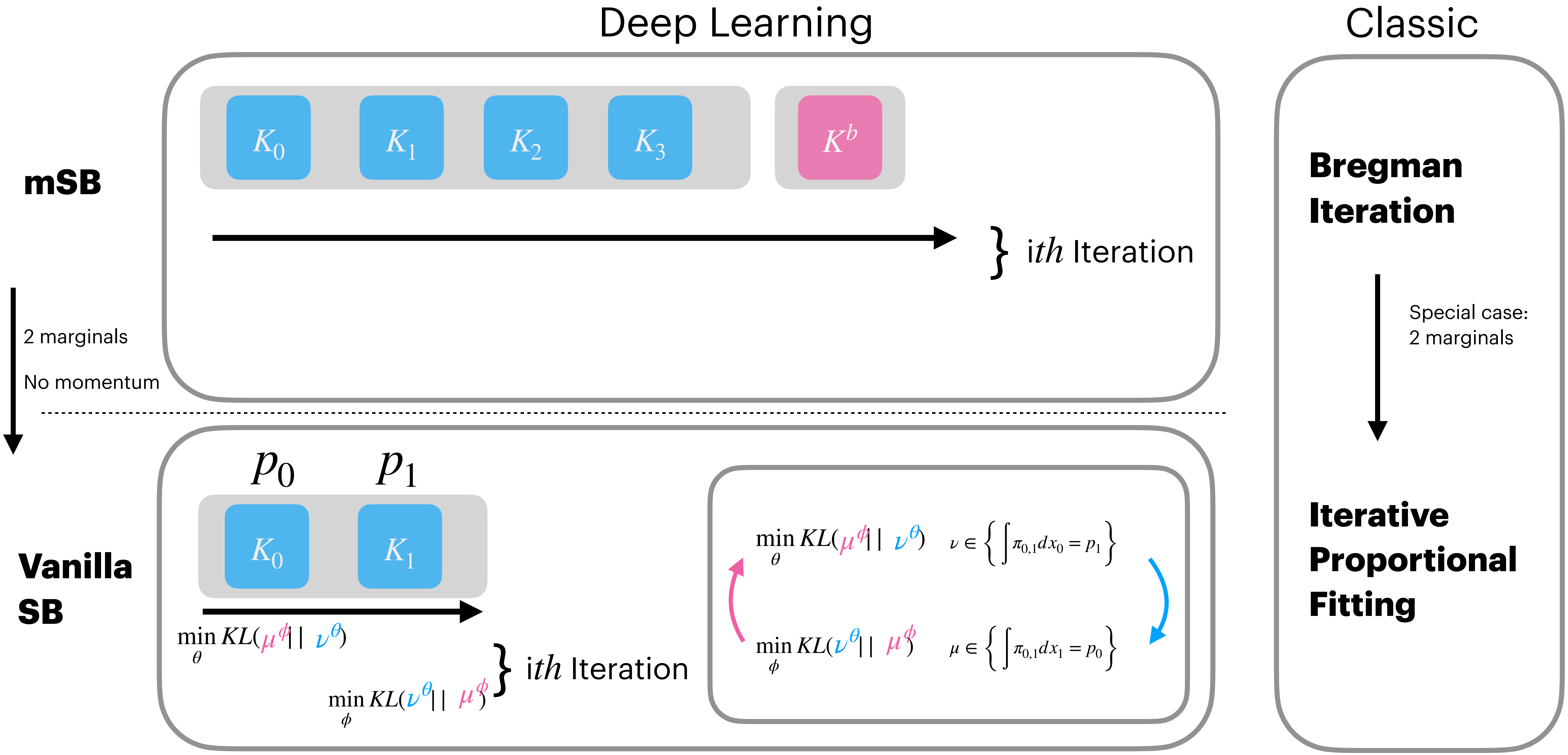
$\min_{\phi} KL(\nu^{\theta} || \mu^{\phi})$

$\}$ ith Iteration

$\min_{\theta} KL(\mu^{\phi} || \nu^{\theta}) \quad \nu \in \left\{ \int \pi_{0,1} dx_0 = p_1 \right\}$

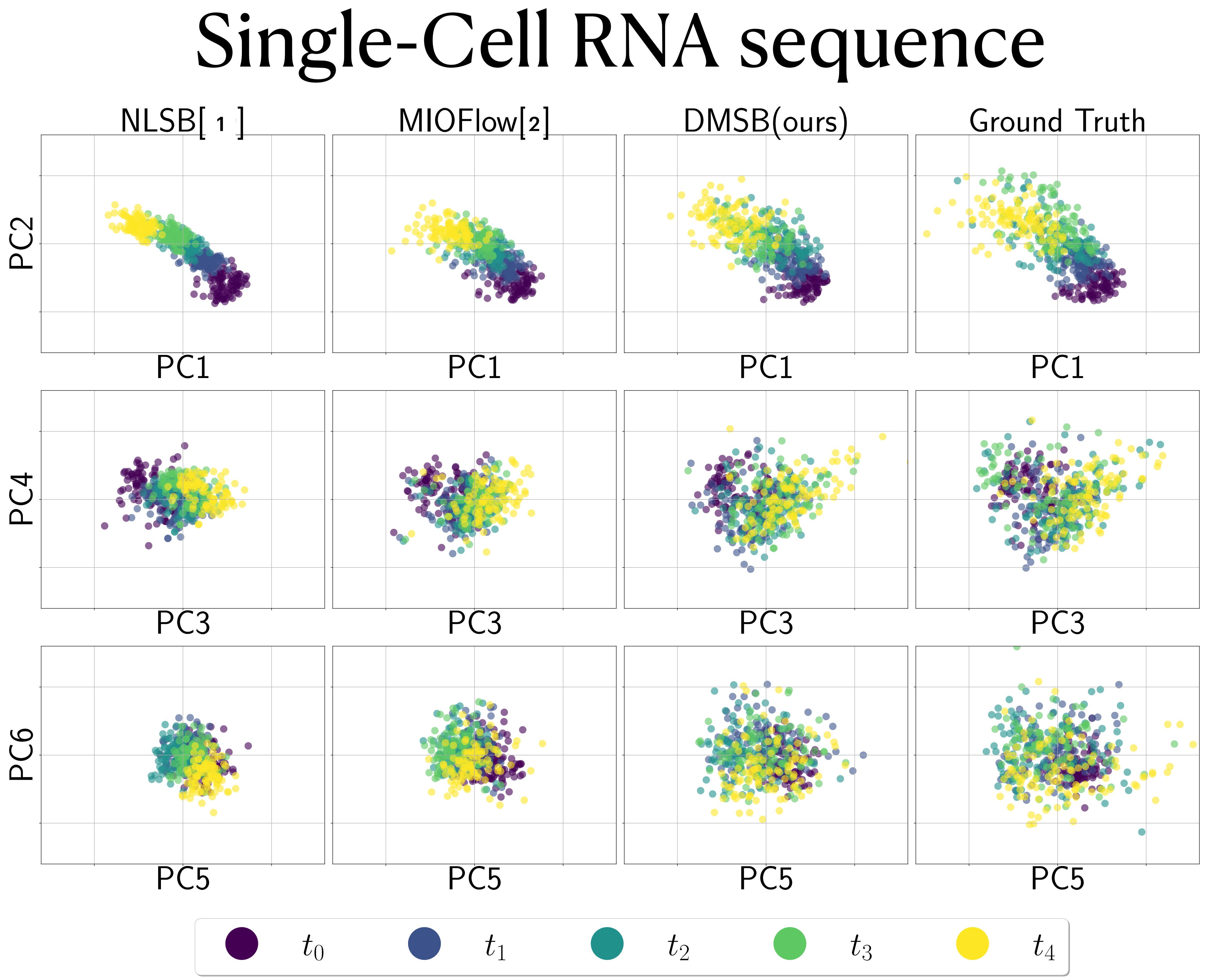
$\min_{\phi} KL(\nu^{\theta} || \mu^{\phi}) \quad \mu \in \left\{ \int \pi_{0,1} dx_1 = p_0 \right\}$

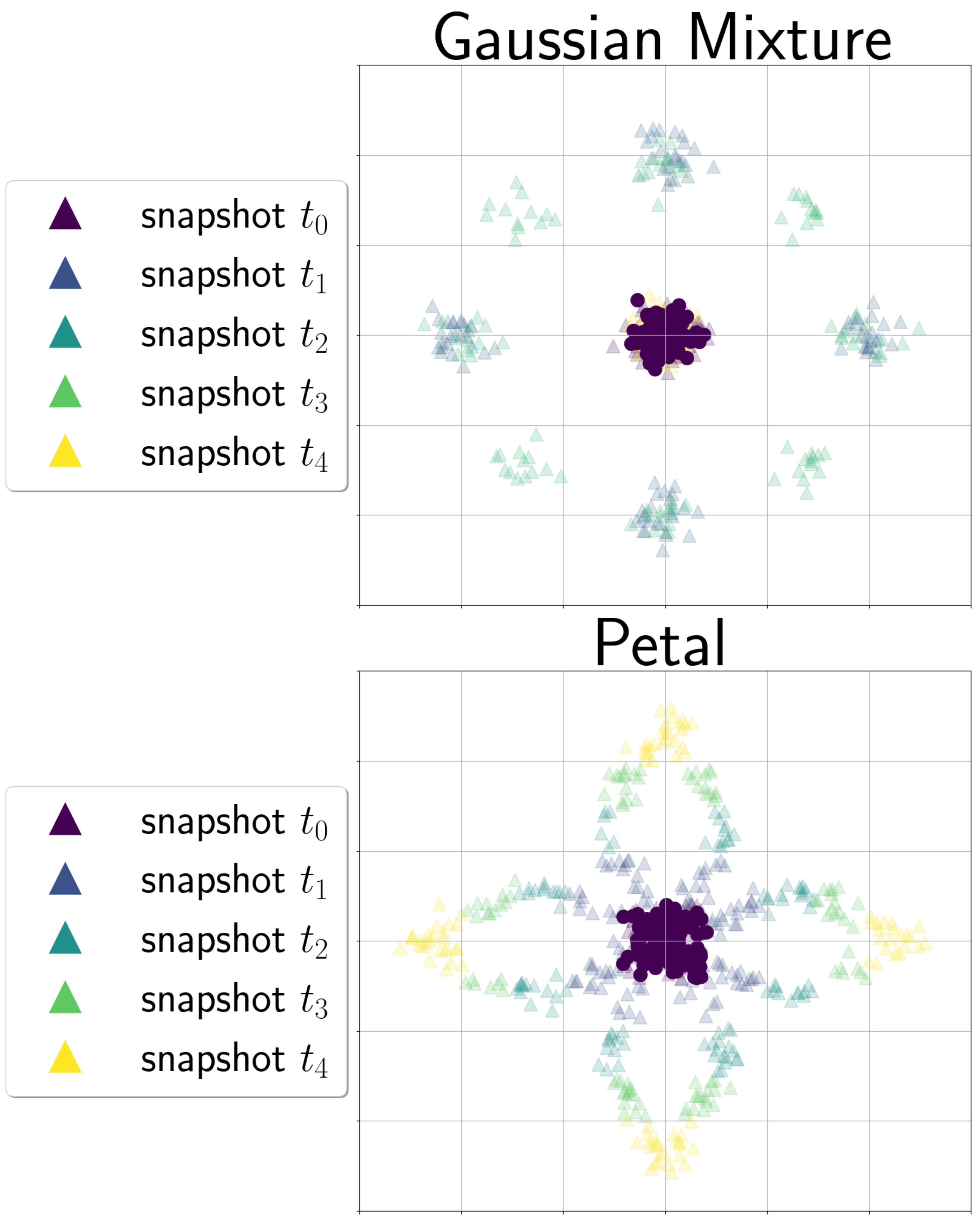
Solutions



Deep Learning
Classic
mSB
K_0
K_1
K_2
K_3
K^b
ith Iteration
2 marginals
No momentum
Vanilla SB
p_0
p_1
K_0
K_1
$\min_\theta KL(\mu^\phi || \nu^\theta)$
$\min_\phi KL(\nu^\theta || \mu^\phi)$
ith Iteration
$\min_\theta KL(\mu^\phi || \nu^\theta)$ $\nu \in \left\{ \int \pi_{0,1} dx_0 = p_1 \right\}$
$\min_\phi KL(\nu^\theta || \mu^\phi)$ $\mu \in \left\{ \int \pi_{0,1} dx_1 = p_0 \right\}$
Bregman Iteration
Special case:
2 marginals
Iterative Proportional Fitting

Results





	MMD ↓				SWD ↓			
Algorithm	w/o LO	LO-t_1	LO-t_2	LO-t_3	w/o LO	LO-t_1	LO-t_2	LO-t_3
NLSB[1]	0.66	0.38	0.37	0.37	0.54	0.55	0.54	0.55
MIOFlow[2]	0.23	0.23	0.90	0.23	0.35	0.49	0.72	0.50
DMSB(ours)	**0.03**	**0.04**	**0.04**	**0.04**	**0.20**	**0.20**	**0.19**	**0.18**

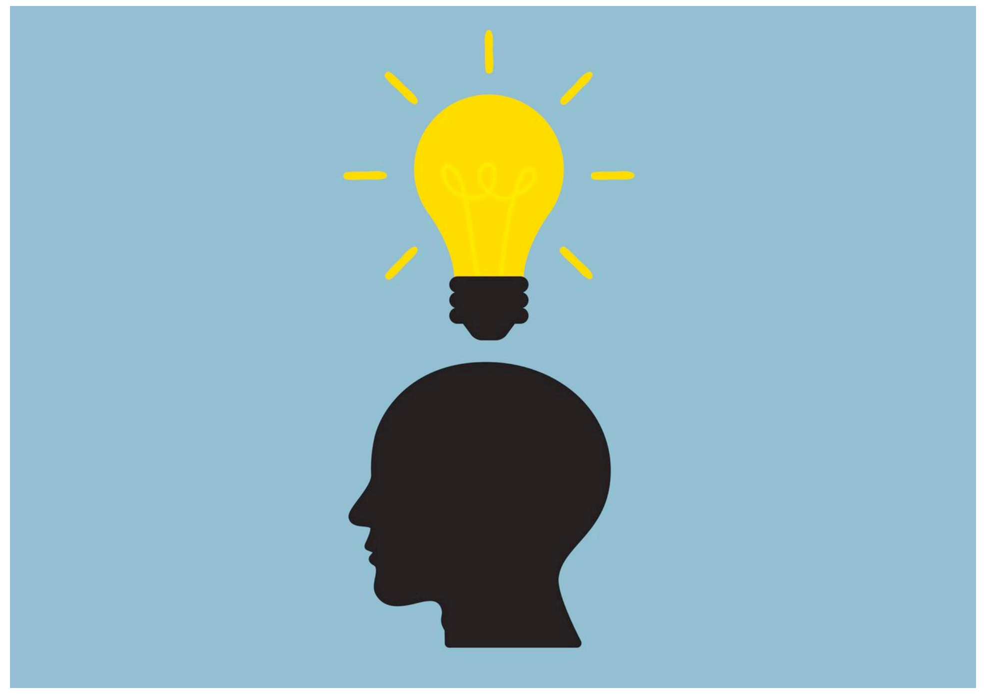
[1] T Koshizuka et al. "Neural Langrange Schrödinger Bridge"

[2] Guillaume Huguet et al. "Manifold Interpolating Optimal-Transport Flows for Trajectory Inference"

Possible Directions

Exploring the Structure in the Deep Learning

Human Prior



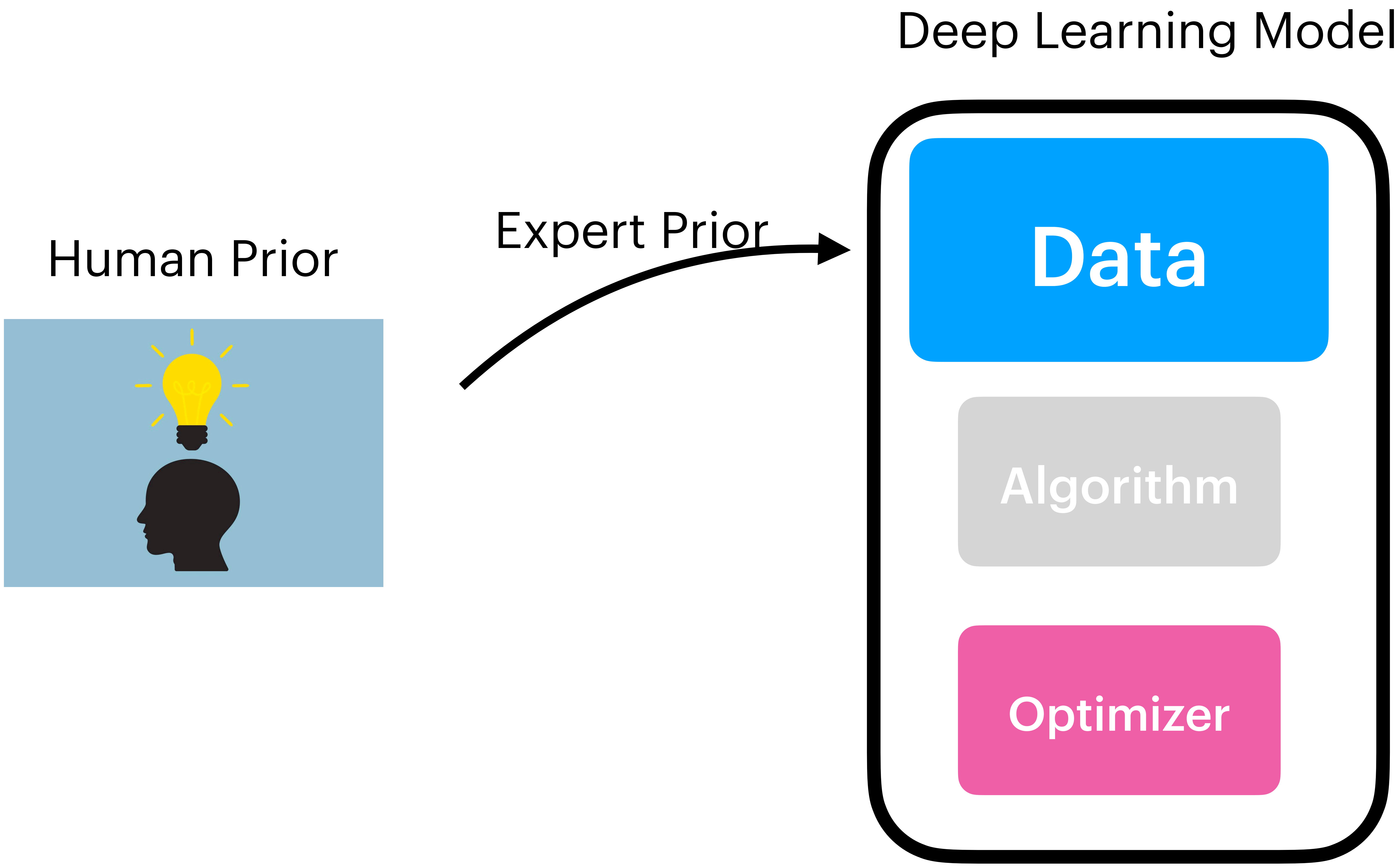
Deep Learning Model

Data

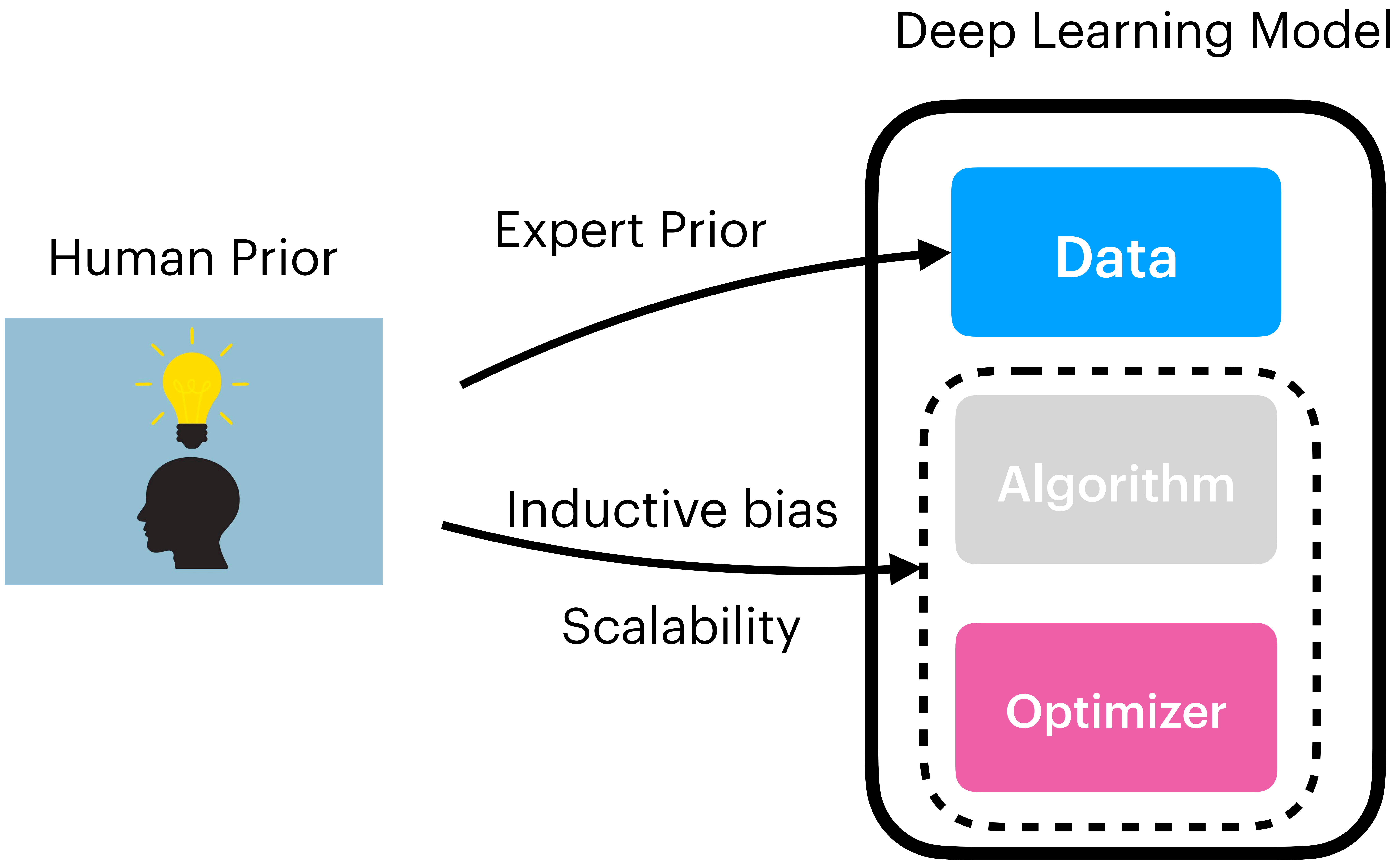
Algorithm

Optimizer

Exploring the Structure in the Deep Learning



Exploring the Structure in the Deep Learning



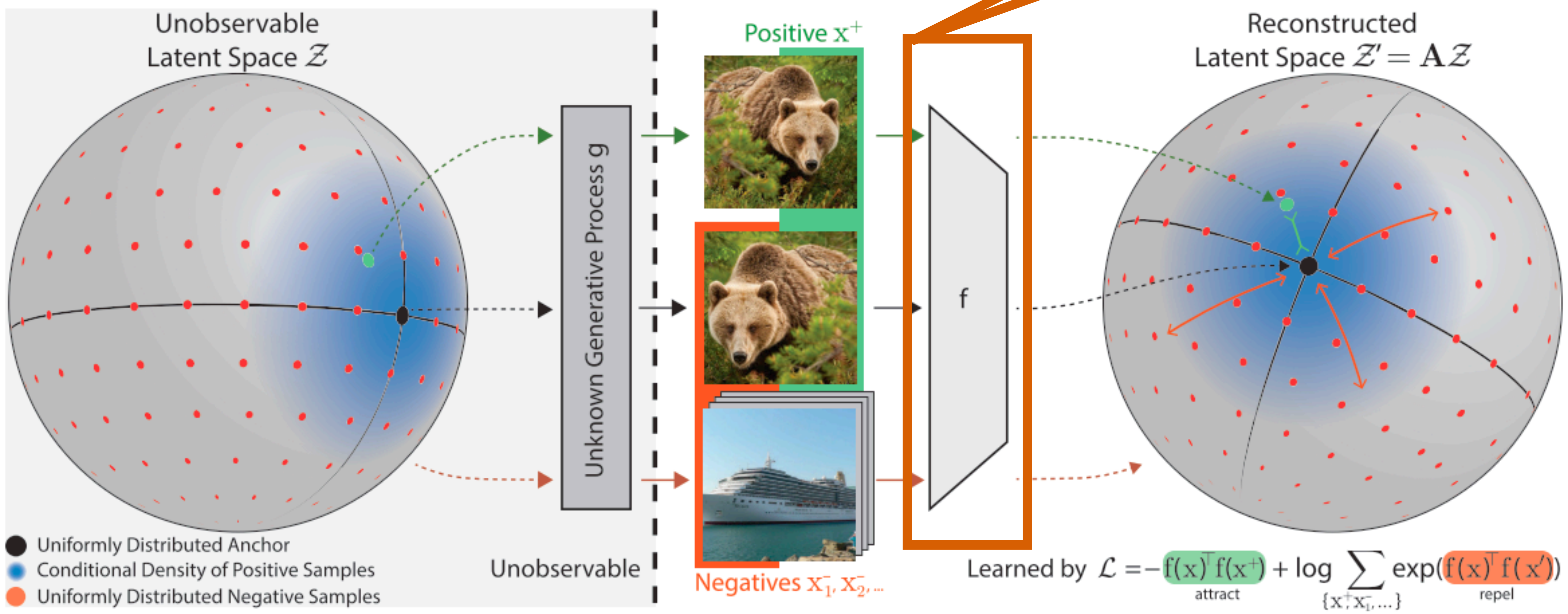
Exploring the Structure in the Deep Learning

1. **Data**
    - Contrastive Learning **<—> Manifold Theory**
2. **Algorithm**
    - Diffusion Model Video Generation **<—> McKean Vlasov Dynamics**
    - Investigating the Potential of Pairing for various problems**<—> OT/SB**

…

Self-Supervised Learning

Training: InfoNCE

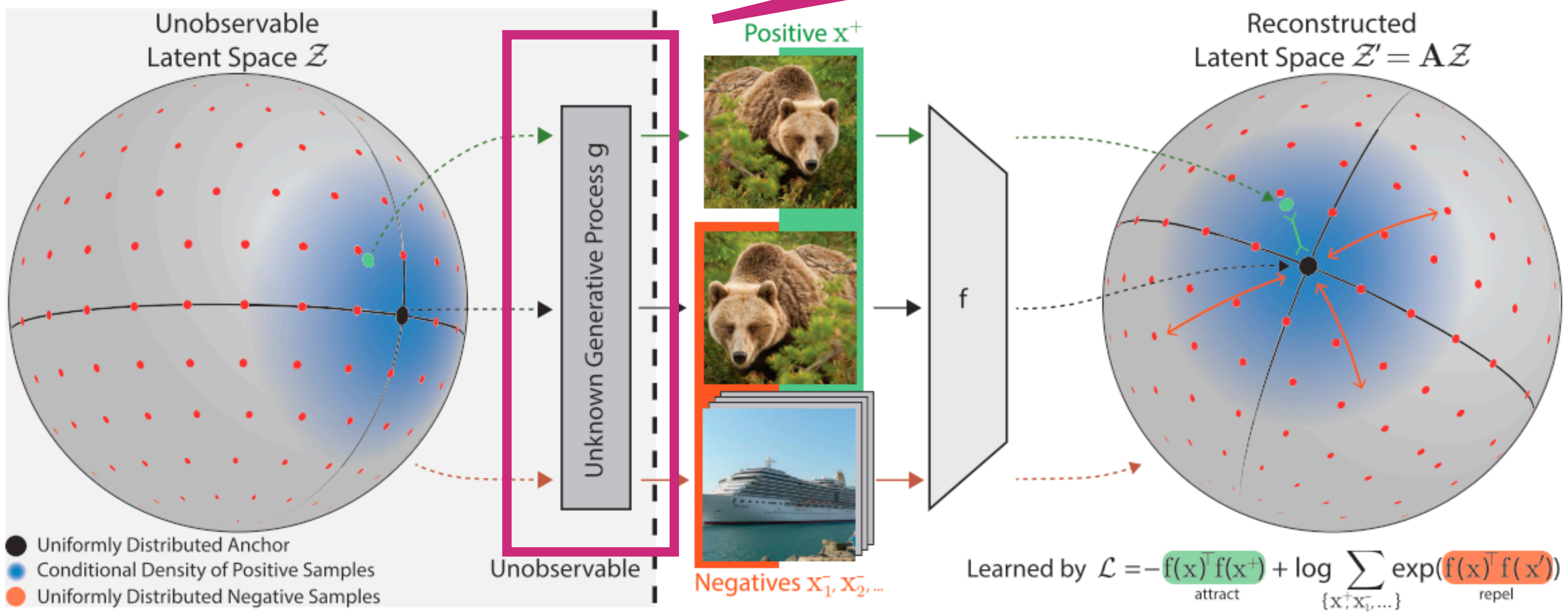


Statement: Contrastive Learning Inverts the Data Generating Process

Roland S. Zimmermann et al. “Contrastive Learning Inverts the Data Generating Process”

Self-Supervised Learning

Diffusion, GAN, Normalizing Flow...

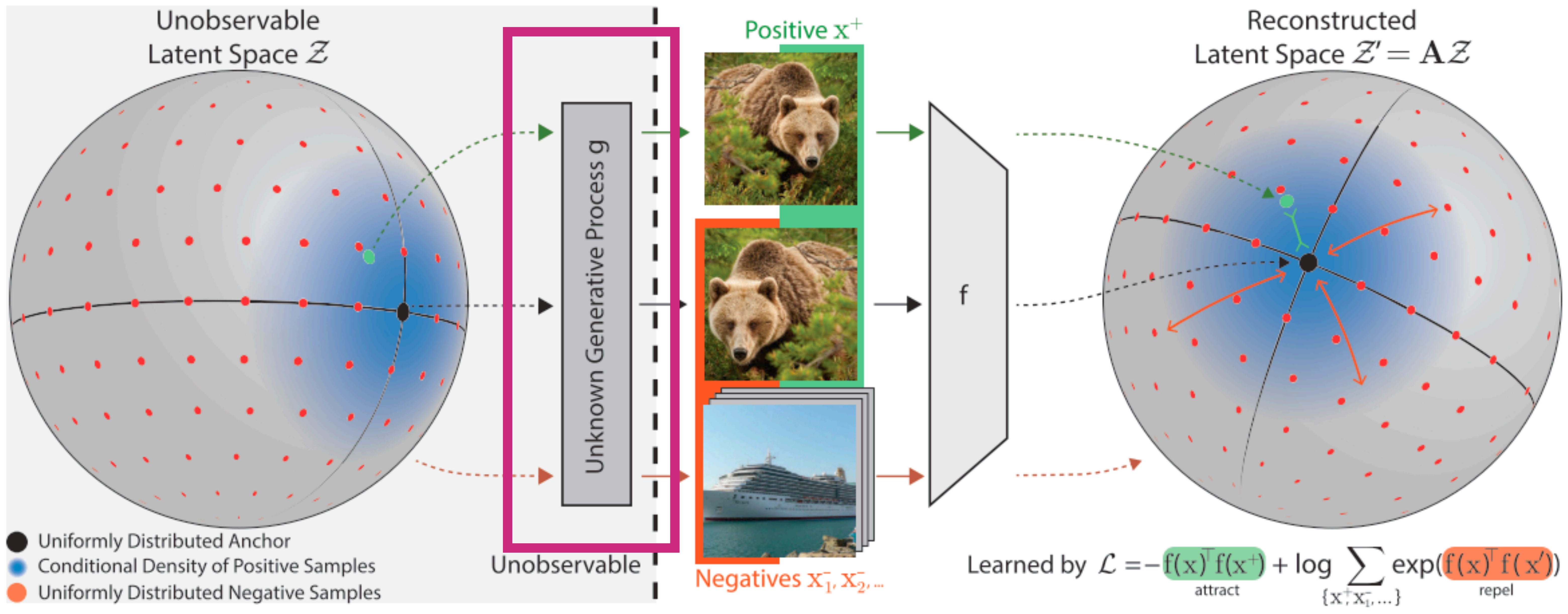


Statement: Contrastive Learning Inverts the Data Generating Process

Prior: We can do very good generation tasks for images!

Roland S. Zimmermann et al. "Contrastive Learning Inverts the Data Generating Process"

Self-Supervised Learning



Statement: Contrastive Learning Inverts the Data Generating Process

Maybe? Why can't we just train a Invertible Generative Model?

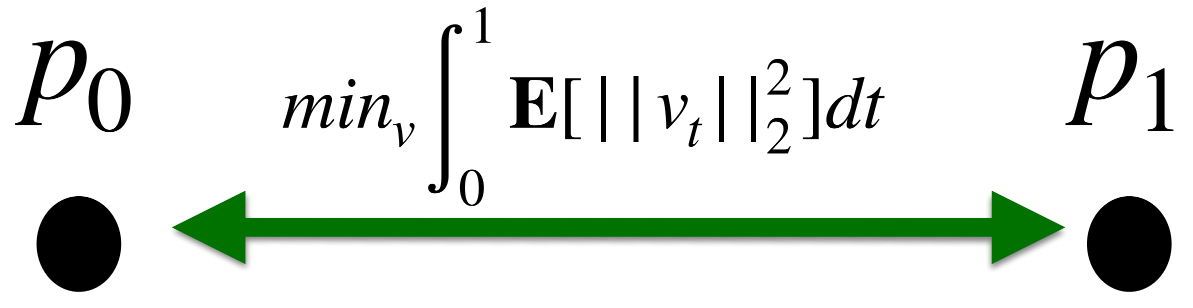
1. Dimension Reduction: VAE in LSDM.
2. Manifold assumption: specific dynamics for manifold prior.
3. Reverse Generation: Property of Dynamical Generative Modeling

Roland S. Zimmermann et al. "Contrastive Learning Inverts the Data Generating Process"

Pairing? Pairing!

Construct pairing: Optimal Transport/Schrödinger Bridge $\Pi^{OT}_{(p_0,p_1)}, \Pi^{SB}_{(p_0,p_1)}$:

1. Image/3D point cloud Registration
2. Transportation Operation
3. Earth Science:Seismic tomography and reflection seismology



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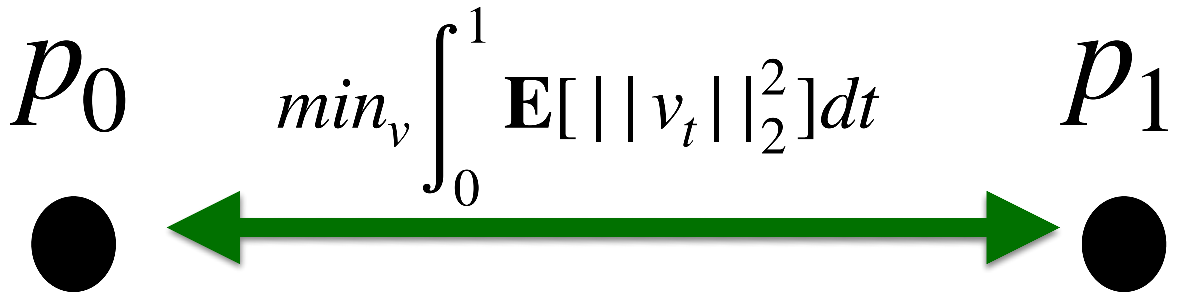
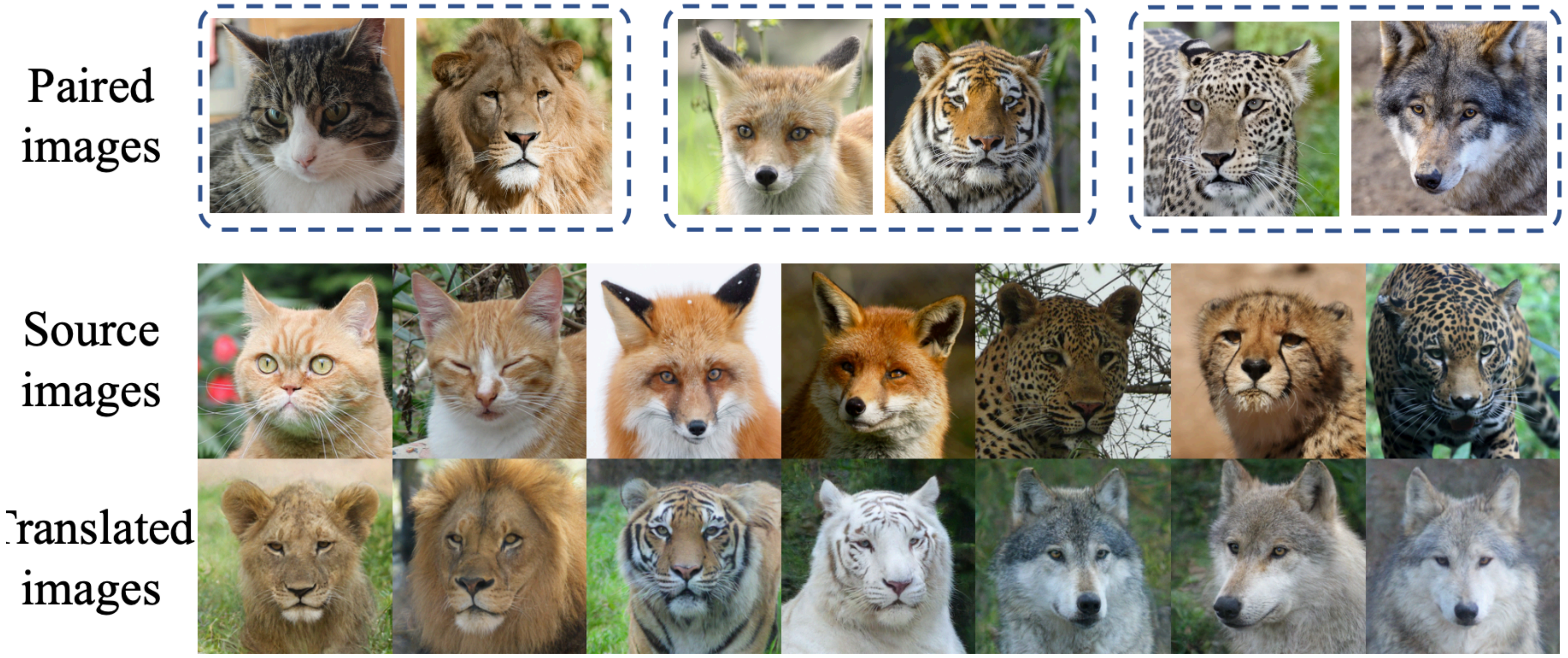
4. **Semi-supervised OT.**





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4. **Semi-supervised OT.**

$$p_0 \xleftrightarrow{min_v \int_0^1 \mathbf{E}[||v_t||_2^2]dt} p_1$$

Given Pairing $\Pi_{(p_0,p_1)}$:

1. Image to Image Transformation: I2SB [1].

$$p_0 \xleftrightarrow{y = Hx + \epsilon} p_1$$

[1] Guan-horng Liu et al. “I2SB”

Pairing? Pairing!

Construct pairing: Optimal Transport/Schrödinger Bridge $\Pi^{OT}_{(p_0,p_1)}, \Pi^{SB}_{(p_0,p_1)}$:

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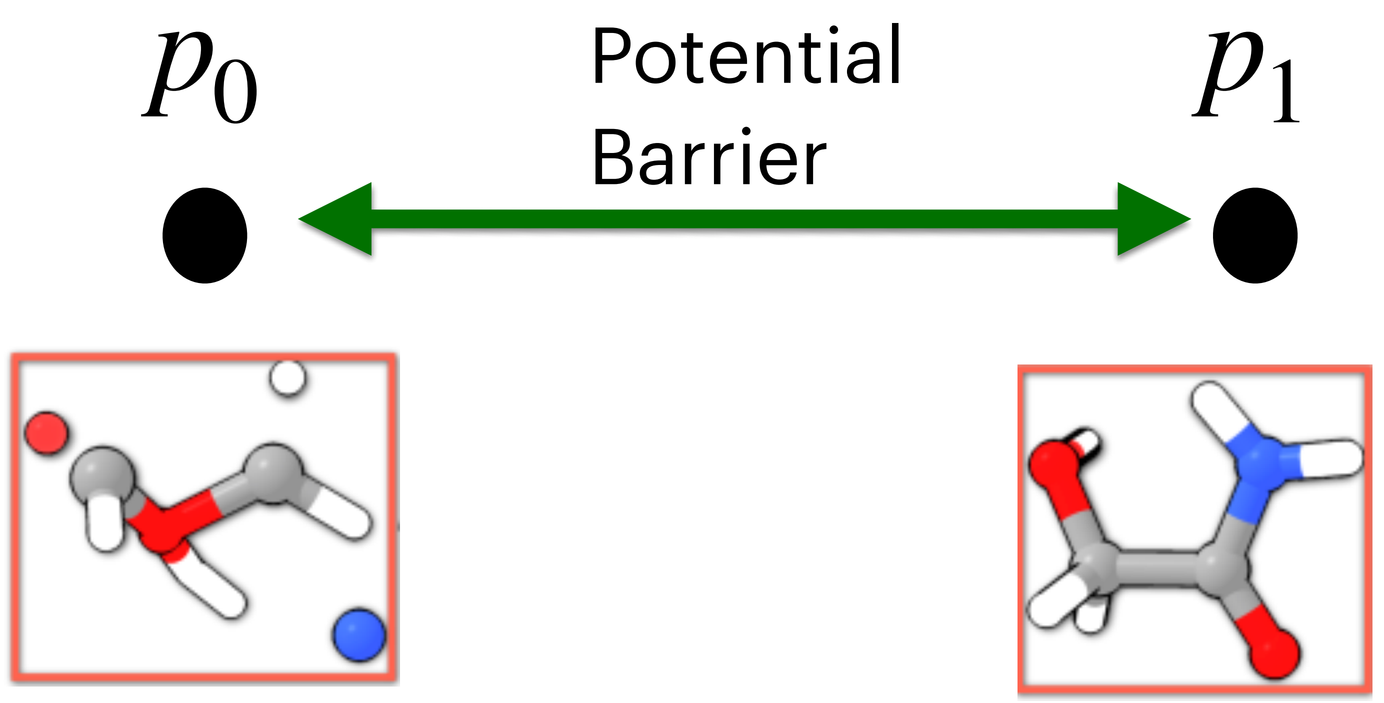


Given Pairing $\Pi_{(p_0,p_1)}$:

1. Image to Image Transformation: I2SB [1].
2. Drug Design, Reactor and Product prediction. (Ongoing)

[1] Guan-horng Liu et al. "I2SB"

[2] Chenru Duan et al. "Accurate transition state generation with an object-aware equivariant elementary reaction diffusion model"

Pairing? Pairing!

Construct pairing: Optimal Transport/Schrödinger Bridge $\Pi^{OT}_{(p_0,p_1)}, \Pi^{SB}_{(p_0,p_1)}$:

1. Image/3D point cloud Registration
2. Transportation Operation
3. Earth Science:Seismic tomography and reflection seismology
4. **Semi-supervised OT.**

$p_0 \quad \min_v \int_0^1 \mathbf{E}[||v_t||_2^2]dt \quad p_1$

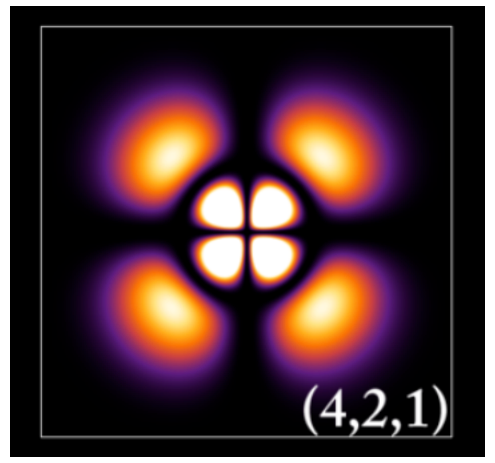
Given Pairing $\Pi_{(p_0,p_1)}$:

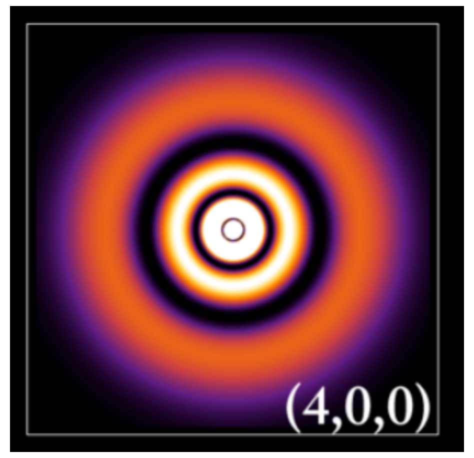
1. Image to Image Transformation: I2SB [1].
2. Drug Design, Reactor and Product prediction. [2]
3. Quantum State generation/Transformation. (Ongoing)

…

$tr(A) = 1, A = A^\dagger$

$p_0 \quad p_1$



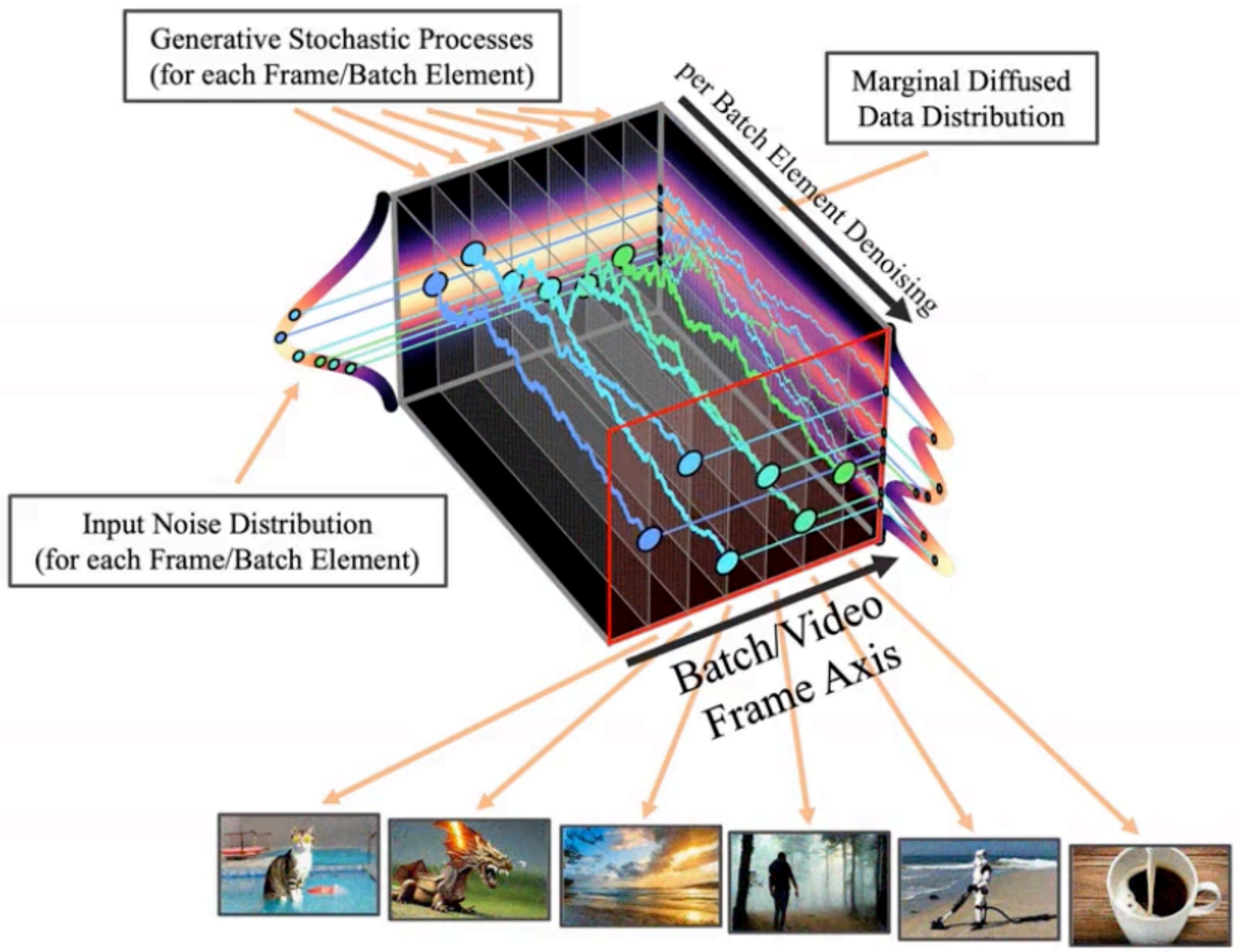


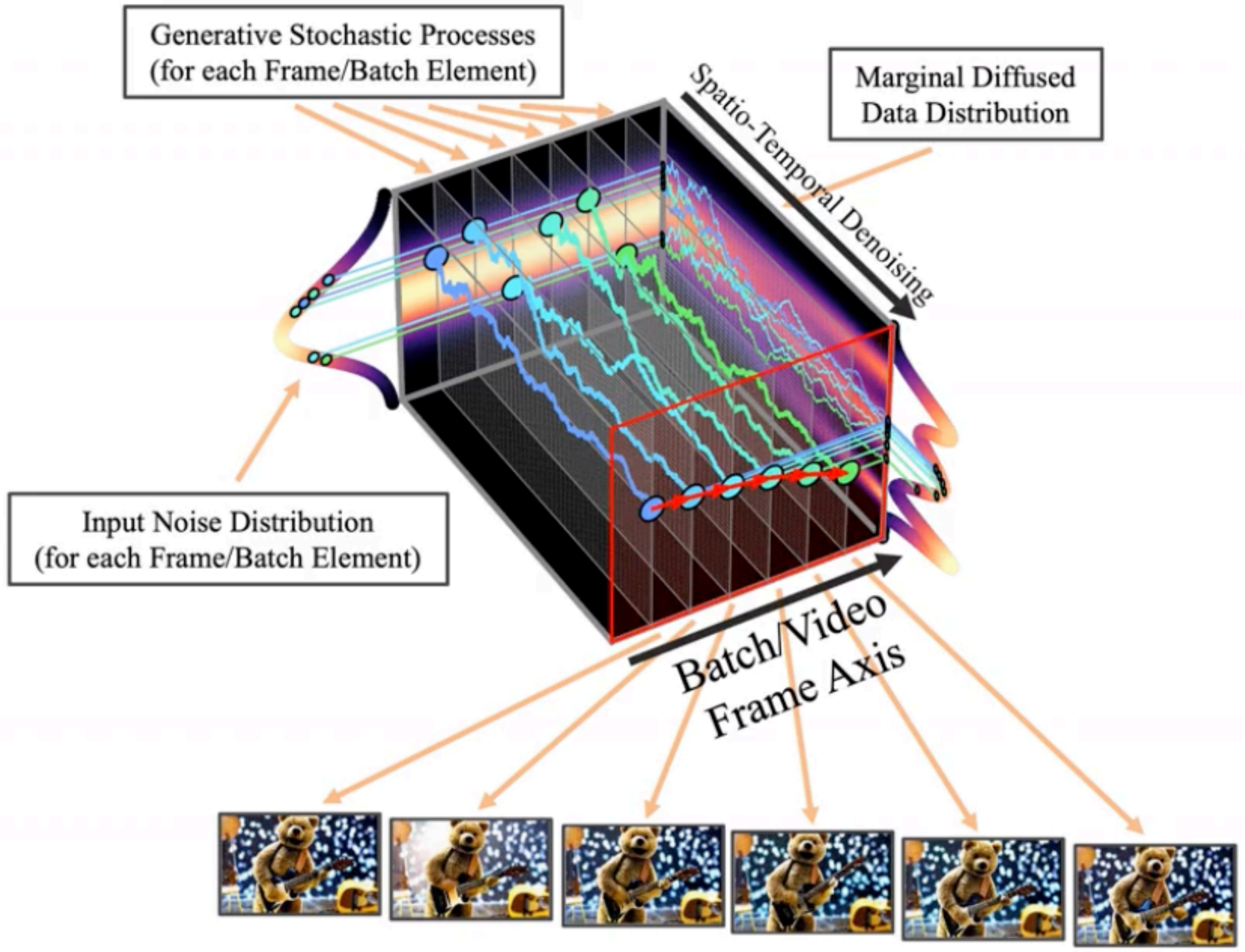
PC to https://www.wikiwand.com/en/Quantum_state#google_vignette

[1] Guan-horng Liu et al. “I2SB”

[2] Chenru Duan et al. “Accurate transition state generation with an object-aware equivariant elementary reaction diffusion model”

Video Generation



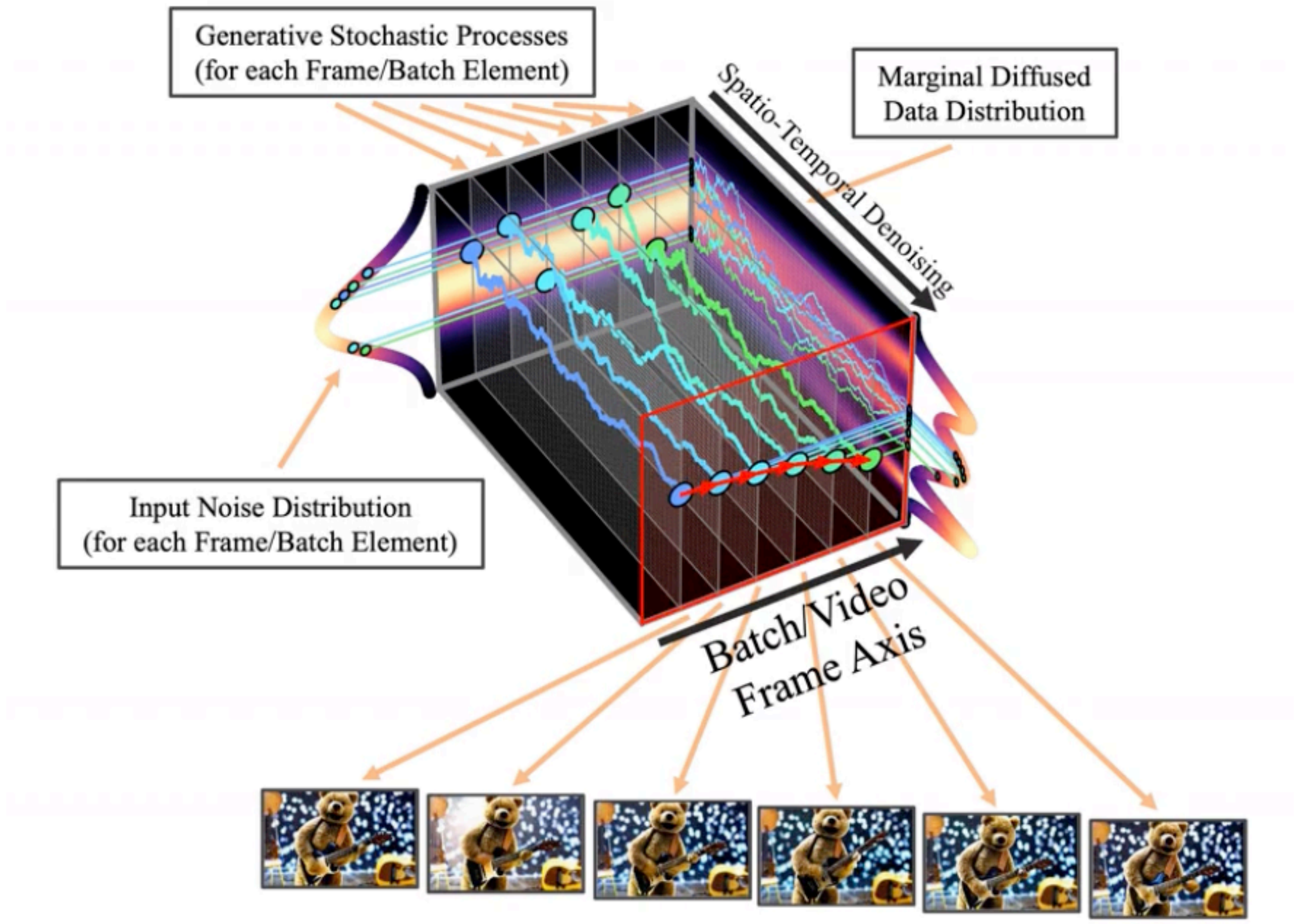


How in inject temporal information?

1. Latent Diffusion Model with fine-tuned Decoder $\mathscr{D}$.
2. Add temporal layer into the network.

Pc to Blattmann, Andreas, et al. "Align your latents: High-resolution video synthesis with latent diffusion models."

"Controlled" Video Generation



How in inject temporal information?

1. Latent Diffusion Model with fine-tuned Decoder $\mathscr{D}$.
2. Add temporal layer into the network.

$F_t(x,t)$:Base Drift

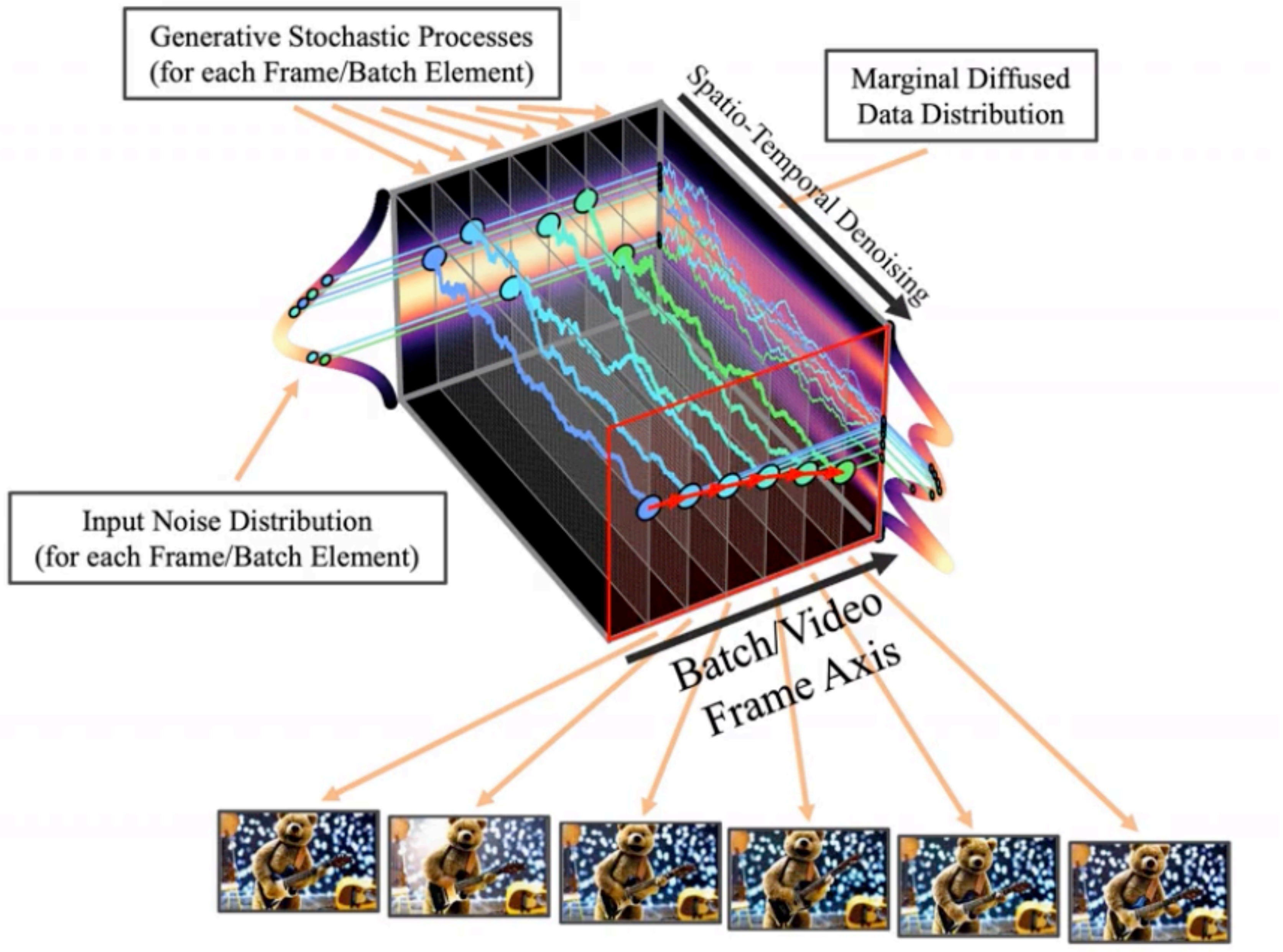
$$dx = \boxed{(f - g^2 \nabla_x \log p)} dt + g_t dw_t$$

$$x_0 \sim p_0 \qquad x_1 \sim p_1$$

Multi-agent control?

Pc to Blattmann, Andreas, et al. "Align your latents: High-resolution video synthesis with latent diffusion models."

"Controlled" Video Generation



How in inject temporal information?

1. Latent Diffusion Model with fine-tuned Decoder $\mathscr{D}$.
2. Add temporal layer into the network.

McKean Vlasov SDE/ODE

$$dx_t = F_t(x_t, t, \boxed{\mu_{x_t}})dt + g_t dw_t$$

$$x_0 \sim p_0^{video} \qquad x_1 \sim p_1$$

μ_{x_t} guidance module.

1. special case t=1: mixed noise model [1]
2. Explicit temporal Layer for all t.

How to construct F_t?

Pc to Blattmann, Andreas, et al. "Align your latents: High-resolution video synthesis with latent diffusion models."

[1] Songwei Ge et al. "Preserve Your Own Correlation: A Noise Prior for Video Diffusion Models"

Q&A