

# Sampling and friends with dynamic measure transport



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**informatics**

Mila

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A meme featuring two astronauts in white space suits floating in space. The astronaut on the right is pointing a silver handgun at the astronaut on the left. In the background, the Earth is visible, showing the Americas. The text is overlaid in a bold, white, sans-serif font.

**WAIT, IT WAS  
ENTROPY-REGULARISED OFF-POLICY RL  
ALL ALONG?**

**ALWAYS  
HAS BEEN**

# Summary

- ▶ Diffusion models review
- ▶ Survey of sampling with learned diffusions
  - ▶ Continuous-time case: Time reversal for SDEs
- ▶ Two views on stochastic measure transport in discrete time
  - ▶ Hierarchical variational inference
  - ▶ Deep entropy-regularised reinforcement learning
  - ▶ Limiting properties
- ▶ Some large-scale applications
  - ▶ Posteriors under diffusion and other generative model priors
- ▶ Schrödinger bridge generalisation
- ▶ Conclusion and outlook

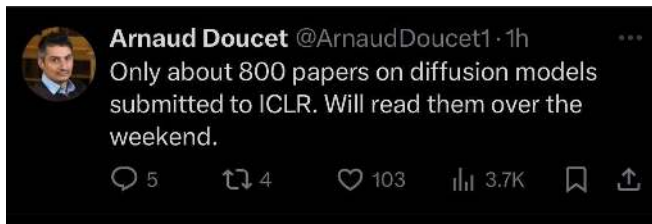
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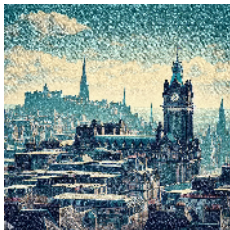
Thank you to all [inspirers] and [collaborators].  
In particular: J. Berner, L. Richter, M. Sendera  
K. Tamogashev, S. Venkatraman.

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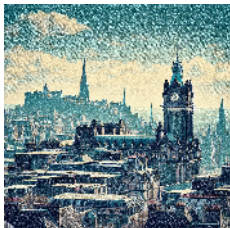


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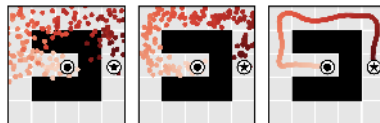


'Edinburgh from Calton Hill, pointillist style'

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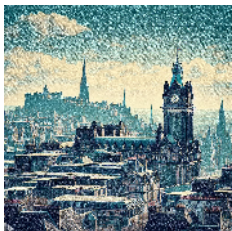
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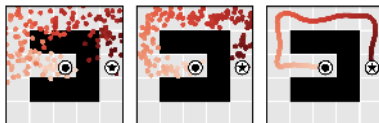
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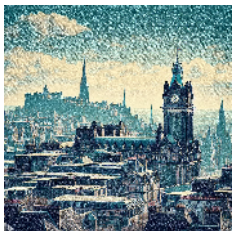
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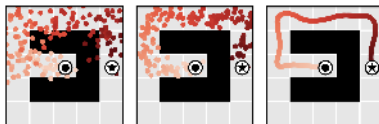
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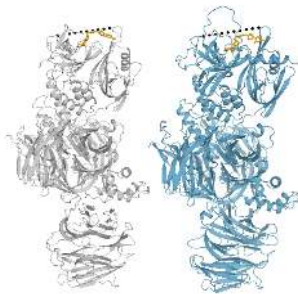
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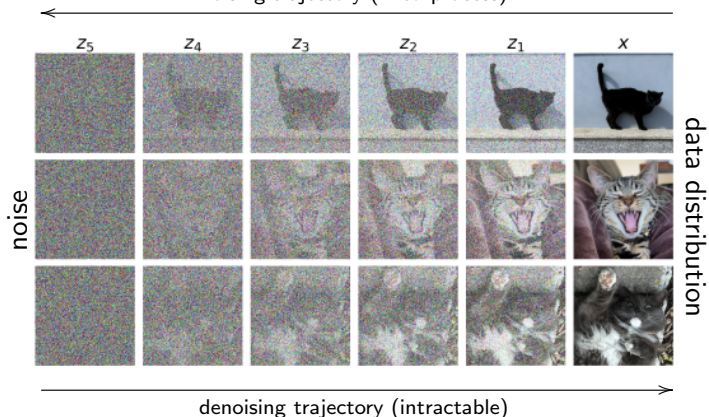


AlphaFold 3

# Diffusion models and time discretisation

$$\begin{array}{ccccccc}
 z_N & \xrightarrow{p(z_{N-1}|z_N;\theta)} & z_{N-1} & \xrightarrow{p(z_{N-2}|z_{N-1};\theta)} & \dots & \xrightarrow{\quad} & z_1 & \xrightarrow{p(x|z_1;\theta)} & z_0 = x \\
 & \nwarrow q(z_N|z_{N-1}) & & \nwarrow q(z_{N-1}|z_{N-2}) & & & \nwarrow q(z_1|x) & & 
 \end{array}$$

noising trajectory (fixed process)



# Hierarchical generative model training

The noising / destruction process  $q$  is a discretised SDE:

$$x_{t-\Delta t} = x_t - \Delta t C_t x_t + D_t \sqrt{\Delta t} \varepsilon_t, \varepsilon_t \sim \mathcal{N}(0, I)$$

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$$x_{t+\Delta t} = x_t + \Delta t \mu_\theta(x_t, t) + \sqrt{\Delta t} \sigma_\theta(x_t, t) \varepsilon_t, \quad \varepsilon_t \sim \mathcal{N}(0, I)$$



# Hierarchical generative model training

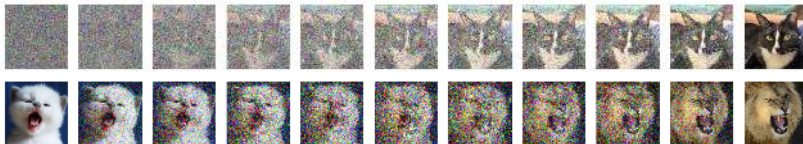
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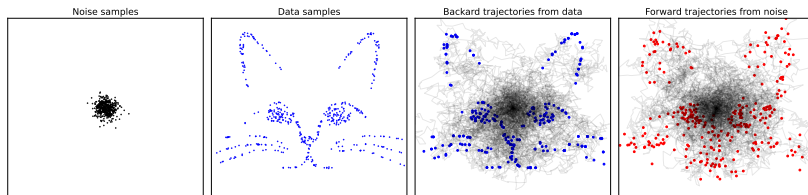


# Variational interpretation of diffusion model training

- ▶ Diffusion model training matches two distributions over trajectories (sequences of latents):
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  - ▶ Forward (denoising) from noise

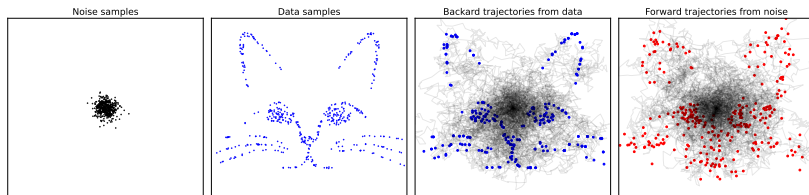
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In continuous time, denoising  $\leftrightarrow$  score matching  $\leftrightarrow$  minimising KL divergence between two path space measures

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# Diffusion models without data?

- Diffusion models are trained from data. . .

$$\text{KL}(\text{target distribution} \cdot \text{noising process} \parallel \text{denoising process}_{\theta})$$



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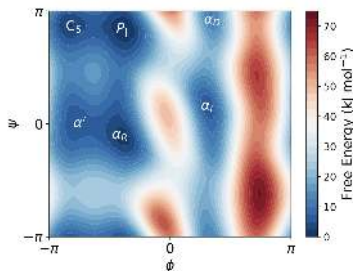
- ▶ Bayesian inference / sampling setting: we have only a target density / energy  $R(\mathbf{x}) = \exp(-\mathcal{E}(\mathbf{x}))$ 
  - ▶ Thought of as unnormalised 'reward' (e.g., a Bayesian posterior  $p(\mathbf{x} \mid \mathbf{y}) \propto p(\mathbf{x})p(\mathbf{y} \mid \mathbf{x})$ )
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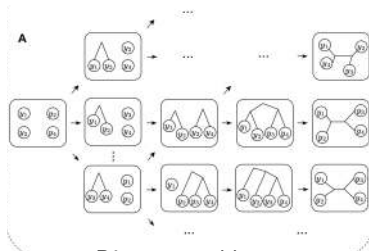
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[Phillips et al.,  $\chi$ :2408.15905]



Discrete problems:

[Zhou et al., ICLR'24,  $\chi$ :2310.08774]

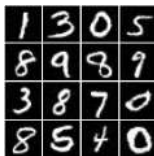
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diffusion model



+ classifier  
 $p(7 \mid x)$

→

conditional samples



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Approaches to training a diffusion model without data:

- ▶ Optimise the reverse KL ( $\leftrightarrow$  stochastic control methods)

$\text{KL}(\text{denoising process}_\theta \parallel \text{target distribution} \cdot \text{noising process})$

- ▶ KL: Memory issues from deep reparametrisation trick
- ▶ Mode-seeking behaviour

- ▶ PDE approaches

[Nüsken & Richter, PDEA,  $\chi$ :2005.05409], [Máté & Fleuret, TMLR,  $\chi$ :2301.07388], [Sun et al.,  $\chi$ :2407.07873] and others

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- ▶ Monte Carlo methods to estimate  $\nabla \log(R * \mathcal{N}(0, V(t)))$

- ▶ Diffusion samplers are annealed importance samplers

[Doucet et al., NeurIPS'22,  $\chi$ :2208.07698]

- ▶ SMC to sample posterior under diffusion priors

[Cardoso et al., ICLR'24,  $\chi$ :2308.07983] and others

- ▶ High variance (but sometimes amortisable)

[Akhound-Sadegh et al., ICML'24,  $\chi$ :2402.06121] and others

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Examples of estimates amenable to importance sampling:

- ▶ DEM [Akhound-Sadegh et al., ICML'24, [χ:2402.06121](#)]:

$$\nabla \log(R * \mathcal{N}(0, V_t))(x_t) = \frac{\mathbb{E}_{x_0 \sim \mathcal{N}(x_t, V_t)}[\nabla R(x_0)]}{\mathbb{E}_{x_0 \sim \mathcal{N}(x_t, V_t)}[R(x_0)]}$$

(estimated using diagonal joint proposal)

- ▶ RDMC [Huang et al., ICLR'24, [χ:2307.02037](#)]:

$$\nabla \log(R * \mathcal{N}(0, V_t))(x_t) = \frac{\mathbb{E}_{x_0 \sim \mathcal{N}(x_t, V_t)}[R(x_0) \nabla \log \mathcal{N}(x_0; x_t, V_t)]}{\mathbb{E}_{x_0 \sim \mathcal{N}(x_t, V_t)}[R(x_0)]}$$

- ▶ Others proposed for diffusion posterior sampling

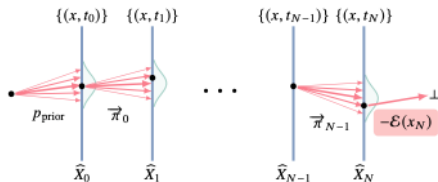
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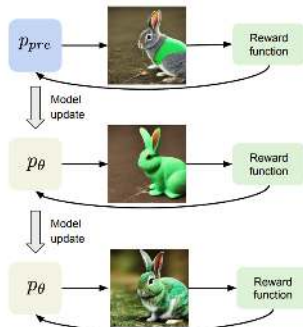
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- ▶ PDE approaches
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- ▶ Off-policy RL: diffusion samplers are diversity-seeking agents



[Berner et al.,  $\chi$ :2501.06148]  $\uparrow$

[Fan et al., 'DPOK...']  $\rightarrow$



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Example of a **consistency objective**: For a denoising trajectory  $\tau = \mathbf{x}_0 \rightarrow \mathbf{x}_{\Delta t} \rightarrow \dots \rightarrow \mathbf{x}_1$ , minimise a divergence such as

$$\mathcal{L}_{\text{TB}}(\tau) = \left( \log \frac{Z_\theta \cdot \text{denoising process}_\theta(\tau)}{R(\mathbf{x}_1) \cdot \text{noising process}(\tau \mid \mathbf{x}_1)} \right)^2$$

- ▶ Multi-objective problem; need to select  $\tau$
- ▶ ‘Off-policy’ = preconditioning
- ▶ But, on-policy, we recover the reverse KL gradient (this later)

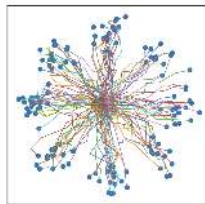
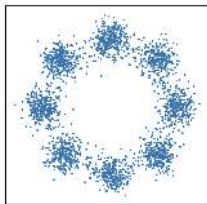


# Time reversal for SDEs

We have two SDEs  $\rightsquigarrow$  path space measures:

$$\overrightarrow{\mathbb{P}} : dX_t = \overrightarrow{\mu}(X_t, t) dt + \sigma(t) dW_t, \quad X_0 \sim p_{\text{prior}},$$

$$\overleftarrow{\mathbb{P}} : dY_t = \overleftarrow{\mu}(Y_t, t) dt + \sigma(t) d\overleftarrow{W}_t, \quad X_1 \sim p_{\text{target}}$$



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Radon-Nikodym derivative via Girsanov theorem:

$$\begin{aligned} \log \frac{d\overrightarrow{\mathbb{P}}}{d\overleftarrow{\mathbb{P}}} = \log \frac{p_{\text{prior}}(X_0)}{p_{\text{target}}(X_1)} &+ \int_0^1 \frac{\|\overleftarrow{\mu}(X_t, t)\|^2 - \|\overrightarrow{\mu}(X_t, t)\|^2}{2\sigma(t)^2} dt \\ &+ \int_0^1 \frac{\overrightarrow{\mu}(X_t, t)}{\sigma(t)^2} \cdot dX_t - \int_0^1 \frac{\overleftarrow{\mu}(X_t, t)}{\sigma(t)^2} \cdot d\overleftarrow{X}_t \end{aligned}$$

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and the KL, giving a stochastic control cost with control  $\overrightarrow{\mu}$ :

$$\begin{aligned} \text{KL}(\overrightarrow{\mathbb{P}} \parallel \overleftarrow{\mathbb{P}}) = \log Z + \mathbb{E}_{X \sim \overrightarrow{\mathbb{P}}} &\left[ \log p_{\text{prior}}(X_0) + \mathcal{E}(X_T) \right. \\ &\left. + \int_0^1 \left( \frac{\|\overrightarrow{\mu}(X_t, t) - \overleftarrow{\mu}(X_t, t)\|^2}{2\sigma(t)^2} - \nabla \cdot \overleftarrow{\mu}(X_t, t) \right) dt \right] \end{aligned}$$

The two SDEs define the same process with marginal densities  $p_t$  if and only if the following three are satisfied:

- ▶ Boundary conditions:  $p_0 = p_{\text{prior}}$  or  $p_1 = p_{\text{target}}$
- ▶ Nelson's (1965) / Anderson's (1982) identity:

$$\overleftarrow{\mu}(x, t) = \overrightarrow{\mu}(x, t) - \sigma(t)^2 \nabla \log p_t(x)$$

- ▶ Fokker-Planck equation for either process:

$$\partial_t p_t = -\nabla \cdot (p_t \overrightarrow{\mu}) + \frac{\sigma^2}{2} \Delta p_t$$

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This leads to objectives that enforce the above conditions through appropriate parametrisations or losses (see [\[Máté & Fleuret, TMLR,  \$\chi\$ :2301.07388\]](#), [\[Sun et al.,  \$\chi\$ :2407.07873\]](#), others)

# Key references on the various approaches

- ▶ KL minimisation: [Zhang & Chen, ICLR'22,  $\chi$ :2111.15141], [Vargas et al., ICLR'23,  $\chi$ :2302.13834]
- ▶ Off-policy losses: [Nüsken & Richter, PDEA,  $\chi$ :2005.05409], [Richter & Berner, ICLR'24,  $\chi$ :2307.01198]
  
- ▶ Connections with SMC, control, etc.: [Vargas et al., ICLR'24,  $\chi$ :2307.01050], [Chen et al., ICLR'25,  $\chi$ :2412.07081], [Albergo & Vanden-Eijnden, ICML'25,  $\chi$ :2410.02711], [Choi et al.,  $\chi$ :2510.11711]

# Key references on the various approaches

- ▶ KL minimisation: [Zhang & Chen, ICLR'22,  $\chi$ :2111.15141], [Vargas et al., ICLR'23,  $\chi$ :2302.13834]
- ▶ Off-policy losses: [Nüsken & Richter, PDEA,  $\chi$ :2005.05409], [Richter & Berner, ICLR'24,  $\chi$ :2307.01198]

My work on this (shameless plug):

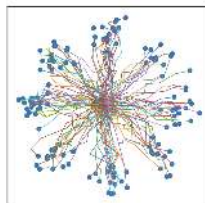
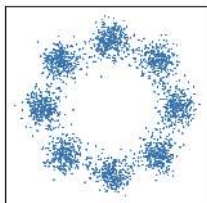
- ▶ RL techniques: [Sendera et al., NeurIPS'24,  $\chi$ :2402.05098], [Kim et al., ICLR'25,  $\chi$ :2410.01432], [Gritsaev et al.,  $\chi$ :2506.01541], ...
- ▶ Unifying theory and continuous-time limit: [Lahlou et al., ICML'23,  $\chi$ :2301.12594], [Berner et al.,  $\chi$ :2501.06148]
- ▶ Inverse problems and scaling: [Venkatraman et al., NeurIPS'24,  $\chi$ :2405.20971], [Venkatraman et al., ICML'25,  $\chi$ :2502.06999]
- ▶ Connections with SMC, control, etc.: [Vargas et al., ICLR'24,  $\chi$ :2307.01050], [Chen et al., ICLR'25,  $\chi$ :2412.07081], [Albergo & Vanden-Eijnden, ICML'25,  $\chi$ :2410.02711], [Choi et al.,  $\chi$ :2510.11711]

- ▶ Diffusion models review
- ▶ Survey of sampling with learned diffusions
  - ▶ Continuous-time case: Time reversal for SDEs
- ▶ Two views on stochastic measure transport in discrete time
  - ▶ Hierarchical variational inference
  - ▶ Deep entropy-regularised reinforcement learning
  - ▶ Limiting properties
- ▶ Some large-scale applications
  - ▶ Posteriors under diffusion and other generative model priors
- ▶ Schrödinger bridge generalisation
- ▶ Conclusion and outlook



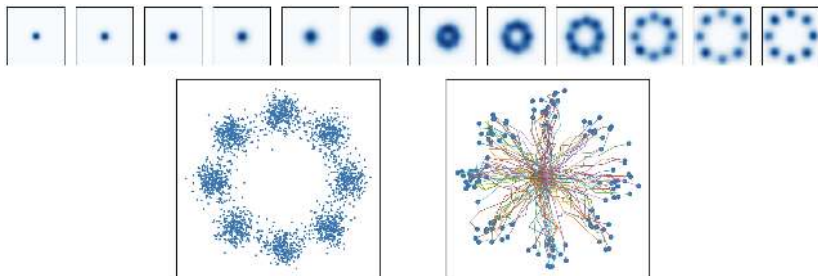
# Again: Sampling with learned diffusions

Recall the problem: sampling a distribution  $p_{\text{target}}$  on  $\mathbb{R}^d$  given its unnormalised density  $\rho = \exp(-\mathcal{E}(\cdot))$



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- Assume a pair of SDEs  $\rightsquigarrow$  path space measures:

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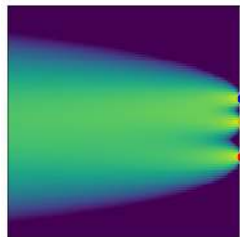
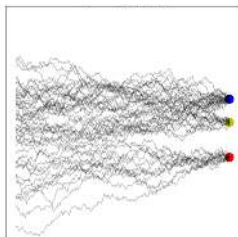
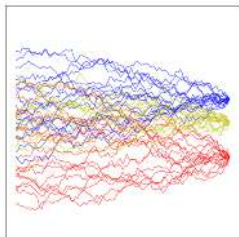
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- Match the two processes (PINN/PDEs, KL, off-policy divergences)
- If they are equal, then  $(\text{ev}_1)_\# \overrightarrow{\mathbb{P}} = (\text{ev}_1)_\# \overleftarrow{\mathbb{P}}$ , so  $X_1 \sim p_{\text{target}}$ .



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The discrete-time version of this: hierarchical variational inference

# Hierarchical variational inference

- ▶ Assume a Markov chain with states valued in  $\mathbb{R}^d$ :

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- ▶ For  $\vec{p}$  to satisfy  $X_T \sim p_{\text{target}}$ , need

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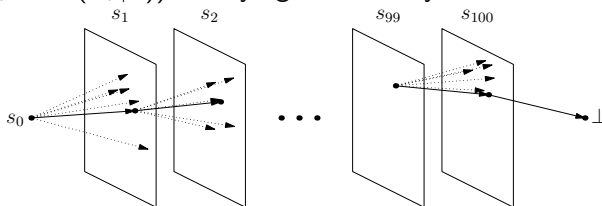
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- ▶ HVI: Match  $p_{\text{prior}} \otimes \vec{p} \otimes \dots \otimes \vec{p}$  and  $p_{\text{target}} \otimes \overleftarrow{p} \otimes \dots \otimes \overleftarrow{p}$  by minimising the KL divergence
- ▶ Data processing inequality:  $0 \leq \text{KL}(X_T \parallel Y_T) \leq \text{KL}(p_{\text{prior}} \otimes \vec{p} \otimes \dots \otimes \vec{p} \parallel p_{\text{target}} \otimes \overleftarrow{p} \otimes \dots \otimes \overleftarrow{p})$

# Reinforcement learning setup

- ▶ Consider a **deterministic graded Markov decision process**  $\approx$  directed graph with set of states  $\mathcal{S} = \mathcal{S}_0 \sqcup \mathcal{S}_1 \sqcup \dots \sqcup \mathcal{S}_T$ , reward  $r(s_t, s_{t+1})$  associated with transition from  $s_t$  to  $s_{t+1}$
- ▶ A **policy**  $\pi$  is a collection of functions  $\pi_{\text{prior}} \in \mathcal{P}(\mathcal{S}_0)$ ,  $\pi_t : \mathcal{S}_t \rightarrow \mathcal{P}(\mathcal{S}_{t+1})$  satisfying reachability constraints





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- ▶ Goal: find a policy that maximises the expected reward

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(Solution not always unique; deterministic maximiser exists.)

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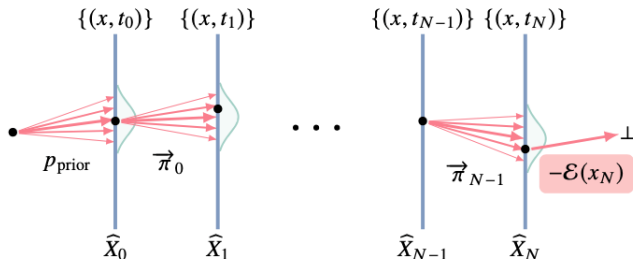
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- ▶ Entropy-regularised objective:  $R(\pi) + \alpha \mathcal{H}[\pi]$
- ▶ Solution to maximum-entropy RL problem:

$$\pi^*(x_0, x_1, \dots, x_T) \propto \exp \left( \frac{1}{\alpha} \sum_{t=0}^{T-1} r(x_t, x_{t+1}) \right)$$

# MDPs and policies associated with diffusion



The policies are given by neural networks predicting the parameters of transition kernels (e.g., Gaussian mean and variance) from  $(x_t, t)$

- Note that the reverse of a process with Gaussian transitions is not generally Gaussian (but it is in the continuous-time limit)

# HVI as entropy-regularised RL

Setting up HVI as a maximum-entropy RL problem:

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- Set  $p_{\text{init}} = p_{\text{prior}}, \alpha = 1$ , reward

$$r(\overbrace{x_t}^{\in \mathcal{S}_t}, \overbrace{x_{t+1}}^{\in \mathcal{S}_{t+1}}) = \begin{cases} \log \overleftarrow{p}(x_t | x_{t+1}), & t < T - 1, \\ \log \overleftarrow{p}(x_t | x_{t+1}) - \mathcal{E}(x_T), & t = T - 1 \end{cases}$$

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- ▶ Optimal policy  $\pi^* \rightsquigarrow$  kernel  $\vec{p}$  such that

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Note: no assumption that spaces  $\mathcal{S}_t$  are all identical (more later)

# Local and global objectives for entropic RL

How to learn the optimal policy  $\pi^*$ ? [M. et al., ICLR'23,  $\chi$ :2210.00580],  
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- ▶ Local objective (soft Q-learning):
  - ▶ Learn **value functions**  $V_t : \mathcal{S}_t \rightarrow \mathbb{R}$  to enforce **soft Bellman equation**:

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- ▶ Algebraic manipulation recovers the nested VI [Zimmermann et al., NeurIPS'21,  $\chi$ :2106.11302] / detailed balance constraint for the transition kernels:

$$\tilde{V}_t(x_t) + \log \vec{p}(x_{t+1} | x_t) = \tilde{V}_{t+1}(x_{t+1}) + \log \overleftarrow{p}(x_t | x_{t+1})$$

where  $\tilde{V}_t(x_t) = V_t(x_t)$  for  $t < T$  and  $\tilde{V}_T(x_T) = -\mathcal{E}(x_T)$

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- ▶ Iterating the soft Bellman equation gives a **path consistency** condition [Nachum et al., NIPS'17, [χ:1702.08892](#)]

- ▶ In our setting, this recovers the following HVI constraint:

$$V_0(x_0) + \log \prod_{t=0}^{T-1} \vec{p}(x_{t+1} | x_t) = -\mathcal{E}(x_T) + \log \prod_{t=0}^{T-1} \overleftarrow{p}(x_t | x_{t+1})$$

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- ▶ Does not involve intermediate value functions!

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- ▶ Both constraints can be turned into optimisation objectives
  - ▶ Minimising some divergence between the two sides over trajectories/transitions sampled from some behaviour policy

# Off-policy hierarchical VI

- Recall the trajectory balance constraint:

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- Optimising the squared difference over a training distribution  $p_{\text{beh}}$  recovers VarGrad [Richter et al., NeurIPS'20, [χ:2010.10436](#)]:

$$\mathcal{L}_{\text{LV}}^{p_{\text{beh}}}(\vec{p}, \overleftarrow{p}) = \text{Var}_{p_{\text{beh}}} \left( \log \frac{p_{\text{prior}}(x_0) \prod_{t=0}^{T-1} \vec{p}(x_{t+1} | x_t)}{\exp(-\mathcal{E}(x_T)) \prod_{t=0}^{T-1} \overleftarrow{p}(x_t | x_{t+1})} \right)$$



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- Optimising the squared difference over a training distribution  $p_{\text{beh}}$  recovers VarGrad [Richter et al., NeurIPS'20, [χ:2010.10436](#)]:

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- But we can do better than reverse KL...

# Exploratory policies for training diffusion samplers

Rather than sampling trajectories from the current distribution  $\vec{p}$ , we can sample from a more exploratory policy  $\pi_{\text{beh}}$ :

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- ▶ Or even **learn** the exploratory policy to favour high-loss trajectories [Kim et al., ICLR'25,  $\chi$ :2410.01432]



Goal distr.



Student (1/5)



Teacher (1/5)



Goal distr.



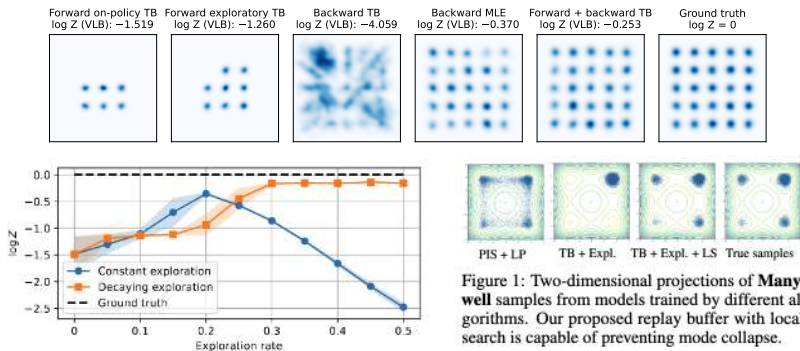
Student (2/5)



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# Exploratory policies for training diffusion samplers

## Exploration methods work



- ▶ The error in the detailed balance constraint

$$\tilde{V}_i(x_{t_i}) + \log \vec{p}(x_{t_{i+1}} | x_{t_i}) - \tilde{V}_{t+1}(x_{t_{i+1}}) - \log \overleftarrow{p}(x_{t_i} | x_{t_{i+1}})$$

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# Connections with SMC

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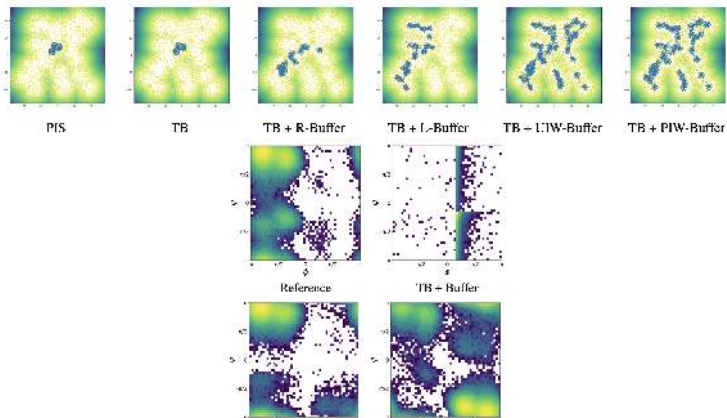
- ▶ NVI/DB (resp. HVI/VarGrad) training minimise **variance of log-IWs** over steps (resp. over trajectories)
- ▶ Deep entropic RL is a twisted SMC algorithm (cf. [\[Chen et al.,  \$\chi\$ :2412.07081\]](#))

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[Choi et al.,  $\chi$ :2510.11711]:

particle filters (SMC) + group importance sampling in replay buffers



# Why drop the continuous-time assumption?

- ▶ In the continuous-time setting, we are matching two processes:

$$\overrightarrow{\mathbb{P}} : \quad dX_t = \overrightarrow{\mu}(X_t, t) dt + \sigma(t) dW_t, \quad X_0 \sim p_{\text{prior}},$$

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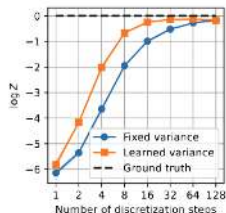
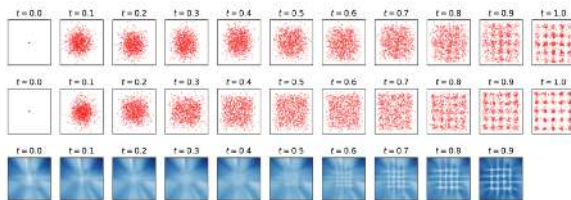
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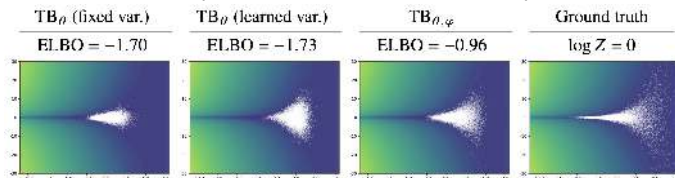
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[Gritsaev et al.,  $\chi$ :2506.01541]

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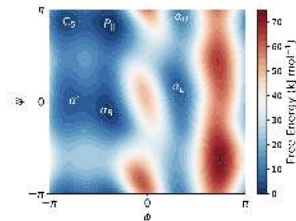
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Easy generalisation to non-Gaussian kernels, kernels on manifolds, etc.

- ▶ [Phillips et al., [χ:2408.15905](https://arxiv.org/abs/2408.15905)], mixture-of-von-Mises kernel on torus



- ▶ Diffusion models review
- ▶ Survey of sampling with learned diffusions
  - ▶ Continuous-time case: Time reversal for SDEs
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# VI with Euler-Maruyama kernels and consistency

If we **do** assume underlying SDEs, how are HVI/RL approaches related to the continuous-time setting? [Berner et al., [χ:2501.06148](#)]

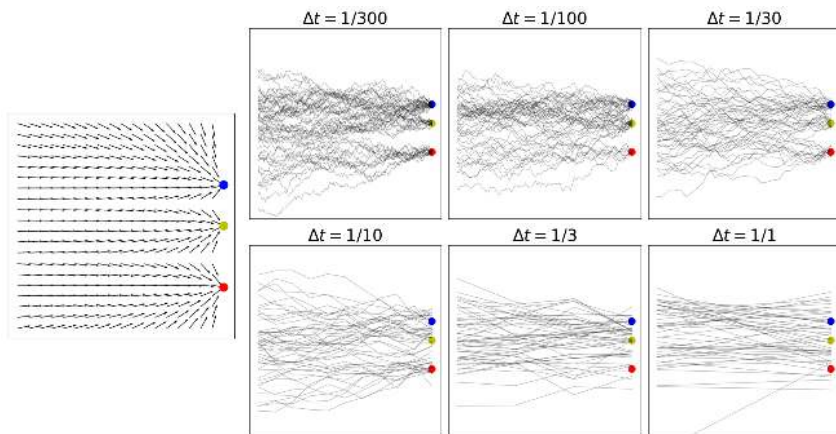
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SDE  $\rightsquigarrow$  Euler-Maruyama discretisation as a policy:

- ▶ Given a time discretisation  $0 < t_0 < t_1 < \dots < t_T = 1$  with  $\Delta t_i := t_{i+1} - t_i$ , we get a Gaussian Markov kernel by

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What happens as  $\max_i \Delta t_i \rightarrow 0$ ? Under mild assumptions:

- **Theorem 1:** Global objectives (VarGrad) are consistent:

$$\lim_{\max_i \Delta t_i \rightarrow 0} \mathcal{L}_{\text{LV}}^{p_{\text{beh}}}(\vec{p}, \overleftarrow{p}) = \mathcal{L}_{\text{LV}}^{\mathbb{P}_{\text{beh}}}(\vec{\mathbb{P}}, \overleftarrow{\mathbb{P}}) \text{ almost surely}$$

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- ▶ **Theorem 2:** Local constraints (soft Q-learning) approach PDEs. Considering the detailed balance discrepancy

$$\tilde{V}_i(x_{t_i}) + \log \vec{p}(x_{t_{i+1}} | x_{t_i}) - \tilde{V}_{t+1}(x_{t_{i+1}}) - \log \overleftarrow{p}(x_{t_i} | x_{t_{i+1}}),$$

- ▶ Vanishing of the  $O(\sqrt{\Delta t_i}) \rightarrow$  Nelson's identity:

$$\vec{\mu}(x_{t_i}, t_i) = \overleftarrow{\mu}(x_{t_i}, t_i) + \sigma(t_i)^2 \nabla V_i(x_{t_i})$$

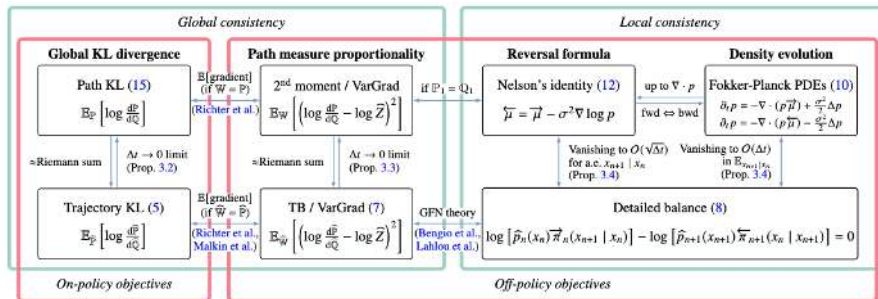
- ▶ Vanishing of the expected  $O(\Delta t_i) \rightarrow$  Fokker-Planck:

$$\partial_t p_t = -\nabla \cdot (\vec{\mu}(x_t, t) p_t) + \frac{\sigma(t)^2}{2} \nabla \cdot \nabla p_t$$

where  $p_{t_i}(x) = \exp(V_i(x))$ .

- ▶ The two jointly imply the forward and reverse SDEs define the same process and have marginal densities  $p_t$

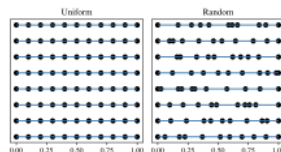
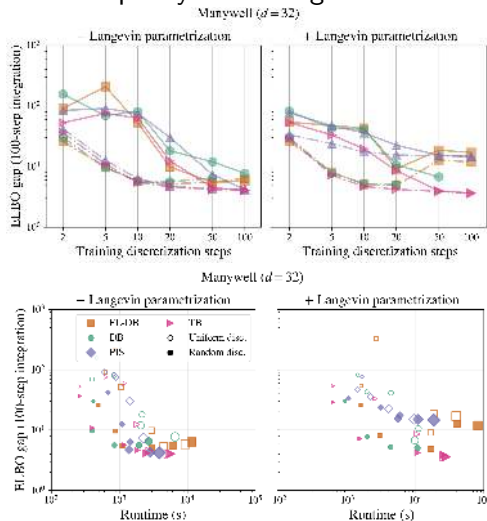
# VI with Euler-Maruyama kernels and consistency



[Berner et al.,  $\chi$ :2501.06148]

# Implications for training with variable time steps

We can train models using HVI/RL losses with very few time steps, then sample by simulating SDEs with much finer discretisation:



Interestingly, the coarse discretisation needs to be nonuniform.

- ▶ Diffusion models review
- ▶ Survey of sampling with learned diffusions
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# Amortising intractable posteriors under diffusion priors

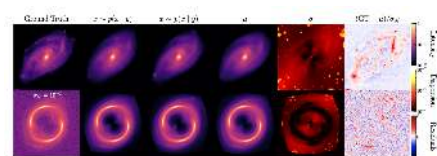
What about sampling  $x_T$  from  $p(x_T | y) \propto p(x_T)p(y | x_T)$ , where  $p(x_T)$  is a pretrained **diffusion prior** and  $p(y | x_T)$  is a likelihood?

- ▶ Intractable in general; MC and SMC-based methods exist
- ▶ Extracting information from pretrained foundation models for images, text, proteins, etc. is important in generative AI

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a lion reading the newspaper\*



a steam engine train, high resolution\*

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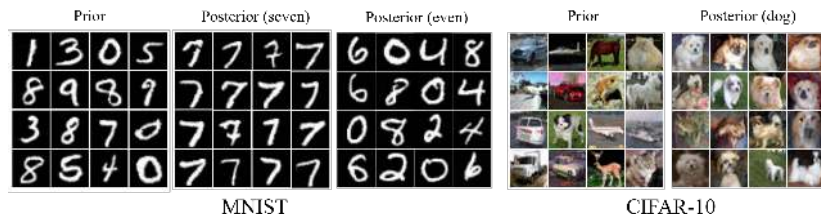
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By renormalising the base measure from Lebesgue to one defined by the prior diffusion model, convert this into an entropic RL problem as above

- ▶ ‘Relative’ VarGrad and other objectives [Venkatraman et al., NeurIPS’24, [χ:2405.20971](#)]
- ▶ Apply the same methods to **fine-tune** the prior diffusion model into a posterior model

# Amortising intractable posteriors under diffusion priors

## Class-conditional image models from unconditional priors

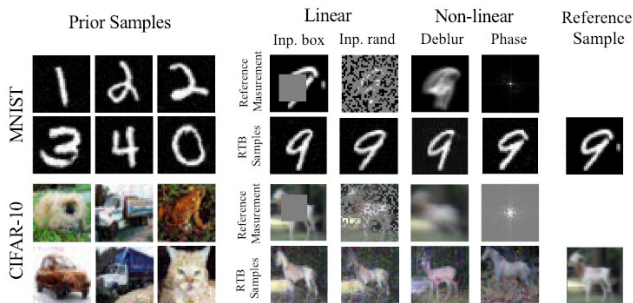


[Venkatraman et al., NeurIPS'24,  $\chi$ :2405.20971]

- ▶ Unconditional diffusion model + classifier  $\rightsquigarrow$  class-conditional model
- ▶ Classifier guidance approximations and RL baselines are biased

# Amortising intractable posteriors under diffusion priors

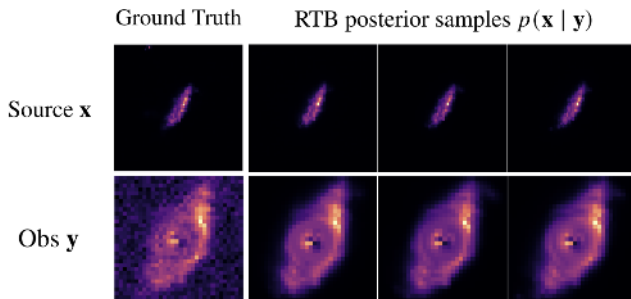
(Non-!)linear inverse problems (with applications in inverse imaging)



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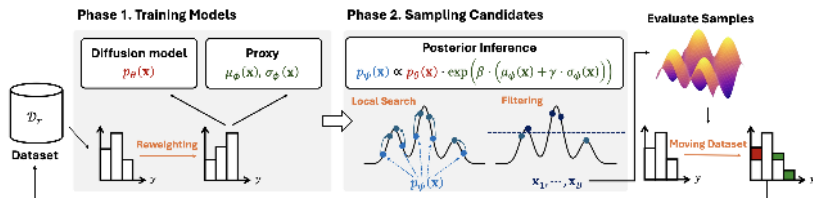
# Amortising intractable posteriors under diffusion priors

Table 1: Sources of diffusion priors and constraints.

Domain	Prior $p(\mathbf{x})$	Constraint $r(\mathbf{x})$	Posterior
Conditional image generation (§4.1)	Image diffusion model $p(\mathbf{x})$	Classifier likelihood $p(c   \mathbf{x})$	Class-conditional distribution $p(\mathbf{x}   c)$
Text-to-image generation (§4.2)	Text-to-image foundation model	RLHF reward model	Aligned text-to-image model
Language infilling (§4.3)	Discrete diffusion model	Autoregressive completion likelihood	Infilling distribution
Offline RL policy extraction (§4.4)	Diffusion model as behavior policy	Boltzmann dist. of $Q$ -function	Optimal KL-constrained policy

Other applications:

- ▶ Discrete-space diffusion (text)
- ▶ Offline RL policy extraction
- ▶ Black-box Bayesian optimisation [Yun et al.,  $\chi$ :2502.16824]



# Inference in latent spaces of generative models

‘Outsourced’ diffusion sampling: sample posteriors in latent spaces of GANs, VAEs, etc., given a constraint on the output space

Table 2. The priors and constraints studied in §5. Outsourced diffusion sampling works in noise spaces of a wide range of generative models and is agnostic to their specific form.

Task	Constraint	Prior	Prior type	$d_{\text{noise}}$	$d_{\text{latent}}$
CIFAR-10 classifier guidance	CIFAR-10 classifier	SN-GAN	GAN	128	$3 \times 32 \times 32$
		I-CFM	CNF	$3 \times 32 \times 32$	$3 \times 32 \times 32$
FFHQ text conditioning	ImageReward	StyleGAN3	GAN	512	$3 \times 256 \times 256$
		NVAE	Hierarchical VAE	$4 \times 20 \times 8 \times 8$	$3 \times 256 \times 256$
Text-to-Image model RLHF	ImageReward	Stable Diffusion 3	Latent-CNF	$16 \times 64 \times 64$	$3 \times 512 \times 512$
Protein structure	Structure Diversity	FoldFlow 2	Riemannian CNF	$7 \times 64$	$7 \times 64$



[Venkatraman et al., ICML'25,  $\chi$ :2502.06999]



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A cat and a dog.



Prior



Posterior

A cat riding a llama.



Prior



Posterior

[Venkatraman et al., ICML'25,  $\chi$ :2502.06999]

# Schrödinger bridge problem

- ▶ The SB problem (for processes on  $[0, 1]$  taking values in  $\mathbb{R}^d$ ):

$$\mathbb{P}_t^* = \arg \min_{\mathbb{P}_t} \{ \text{KL}(\mathbb{P}_t \parallel \mathbb{Q}_t) : (\pi_0)_\# \mathbb{P}_t = p_0, (\pi_1)_\# \mathbb{P}_t = p_1 \}$$

where  $\mathbb{Q}_t$  is a reference process and  $p_0, p_1$  are given

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then so (under regularity conditions) is the solution  $\mathbb{P}_t^*$

- ▶ For  $\mathbb{P}_t : dX_t = F(X_t, t) dt + \sigma_t dW_t, X_0 \sim p_0$ , KL is a control cost:

$$\text{KL}(\mathbb{P}_t \parallel \mathbb{Q}_t) = \text{KL}(p_0 \parallel q_0) + \mathbb{E}_{X_t \sim \mathbb{P}_t} \int_0^1 \frac{\|F_{\text{ref}}(X_t, t) - F(X_t, t)\|^2}{2\sigma_t^2} dt,$$

showing that  $\sigma_t \rightarrow 0$  gives dynamic optimal transport

- ▶ Marginally entropic OT between  $p_0, p_1$  with entropy coefficient  $2\sigma_t^2$ )

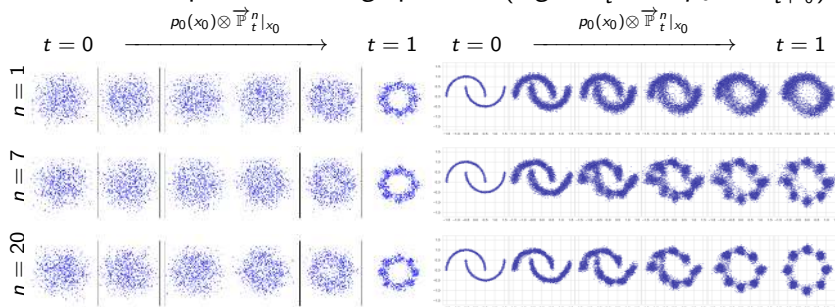
# Iterative proportional fitting

IPF [Sinkhorn, 1964] is a recursion initialised at  $\overrightarrow{\mathbb{P}}_t^0 = \mathbb{Q}_t$ :

$$\overleftarrow{\mathbb{P}}_t^{n+1} = \arg \min_{\mathbb{P}_t} \left\{ \text{KL}(\mathbb{P}_t \parallel \overrightarrow{\mathbb{P}}_t^n) \text{ s.t. } (\pi_0)_\# \mathbb{P}_t = \rho_0 \right\},$$

$$\overrightarrow{\mathbb{P}}_t^{n+1} = \arg \min_{\mathbb{P}_t} \left\{ \text{KL}(\mathbb{P}_t \parallel \overleftarrow{\mathbb{P}}_t^{n+1}) \text{ s.t. } (\pi_1)_\# \mathbb{P}_t = \rho_1 \right\}$$

where each step is a *half-bridge* problem (e.g.,  $\overleftarrow{\mathbb{P}}_t^{n+1} = \rho_0 \otimes \overrightarrow{\mathbb{P}}_t^n|_{x_0}$ )



The processes  $\overrightarrow{\mathbb{P}}_t$  and  $\overleftarrow{\mathbb{P}}_t$  converge in KL to the SB solution  $\mathbb{P}_t^*$

# Schrödinger bridge with diffusion sampling objectives

Existing IPF implementations assume samples from  $p_0, p_1$  are given

- ▶ If  $p_1$  is given by samples, training  $\overrightarrow{\mathbb{P}}_t$  is maximum-likelihood training (as in diffusion)
- ▶ If  $p_0$  is given by samples, training  $\overrightarrow{\mathbb{P}}_t$  is also maximum-likelihood training (trivial in diffusion)
  - ▶ Diffusion training (with noising process converging to  $p_0$ ) is a case of IPF that converges in one step

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  - ▶ Diffusion training (with noising process converging to  $p_0$ ) is a case of IPF that converges in one step
- ▶ If one of both of the distributions is given by an unnormalised density, we can use generalisations of the RL/VI objectives above (and appropriate off-policy training)

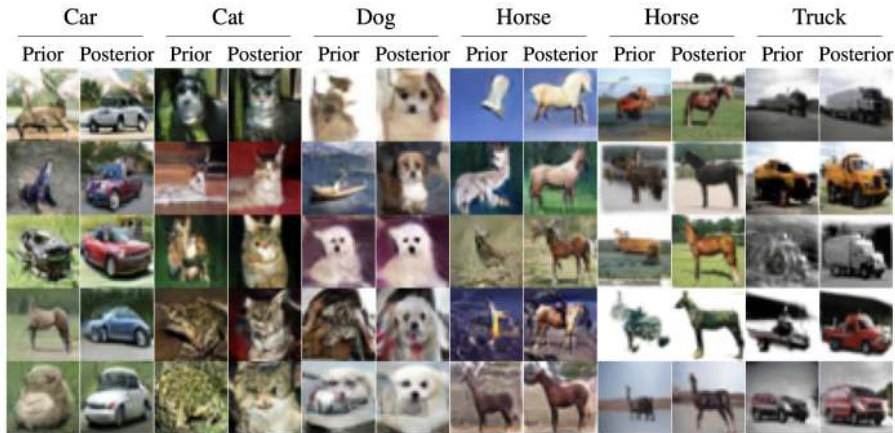
# Outsourced Schrödinger bridge

Translation  $p_{\text{prior}} \leftrightarrow p_{\text{prior}} \cdot p(\text{class} \mid \cdot)$  in the latent space of a generative model

Prior		Fives		Prior		Even		Prior		Odd	
9	16295	5	56565	8	70797	8	40448	2	69767	1	59797
0	89164	8	59565	9	02821	0	02022	8	75609	7	75339
3	55710	5	55555	3	09443	2	20460	9	00764	9	95759
5	53806	5	55555	6	58148	6	88748	4	17800	5	17733
0	15399	5	55555	1	51724	4	02026	6	16734	6	15754
5	48340	5	55555	4	98500	0	68066	9	90435	7	95937

# Outsourced Schrödinger bridge

Translation  $p_{\text{prior}} \leftrightarrow p_{\text{prior}} \cdot p(\text{class} \mid \cdot)$  in the latent space of a generative model

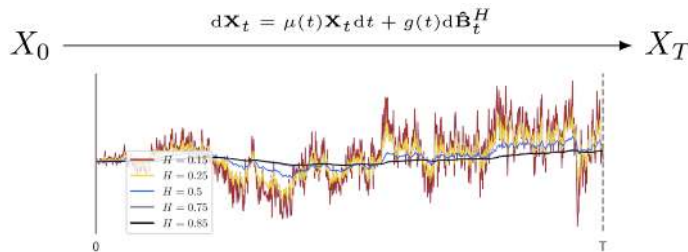




- ▶ Diffusion models review
- ▶ Survey of sampling with learned diffusions
  - ▶ Continuous-time case: Time reversal for SDEs
- ▶ Two views on stochastic measure transport in discrete time
  - ▶ Hierarchical variational inference
  - ▶ Deep entropy-regularised reinforcement learning
  - ▶ Limiting properties
- ▶ Some large-scale applications
  - ▶ Posteriors under diffusion and other generative model priors
- ▶ Schrödinger bridge generalisation
- ▶ Conclusion and outlook

# Open directions in modelling

- ▶ SMC as an RL exploration strategy; diffusion samplers as adaptive importance samplers [with S. Choi, V. Elvira, ...]
- ▶ Non-Markovian generation: Friction, momentum, persistent latent state [with R. Rajpal, B. Leimkuhler]
- ▶ Discrete-time optimal approximation with nondiagonal diffusion [with T. Gritsaev, D. Vetrov, ...]
- ▶ Samplers and bridges in discrete space [with A. Carter, K. Tamogashev, ...]



[Nobis et al., 'Generative fractional diffusion models', 2024]

# Conclusion

- ▶ SDE generative processes as distribution approximators in inference/sampling tasks using RL and control methods
  - ▶ Discrete-time formulation allows for flexible models and training schemes
  - ▶ Connections with SMC, optimal transport, Schrödinger bridges
- ▶ Many open directions in modelling, algorithms, and applications
  - ▶ And, of course, theory: sample complexity bounds, discretisation error, ...

# Conclusion

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Thank you for your attention.

More: [malkin1729.github.io](https://github.com/malkin1729)

[Always looking for new applications, collaborations, ...]

## **Temporary page!**

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