Probabilistic Modeling with Flows

Deep Probabilistic Modeling with Flows

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Sharif University of Technology
Department of Mathematical Sciences

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Density Estimation

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GAN, Diffusion, Autoregressive(e.g. LLMs), VAE, Flows ...

Density Estimation

What do they have in common?

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What is the difficulty of generative modeling?

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More importantly...

How to design a new generative model?

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by going through a fundamental and old problem

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That offers:

- Density estimation for continuous data
- A normalized distribution and exact likelihood computation
- Efficient and straightforward way to sample i.i.d data

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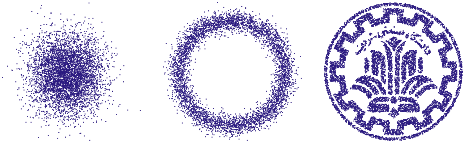

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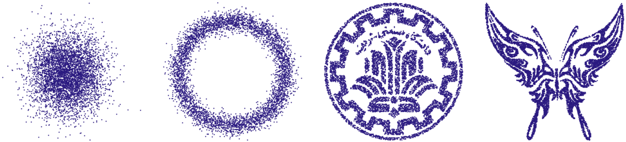

Normalizing Flow and Transport

Basic idea:

Transforming a simple density p to a complicated target p^*

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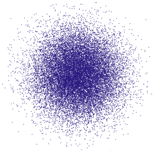

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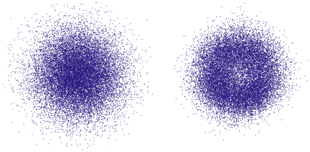

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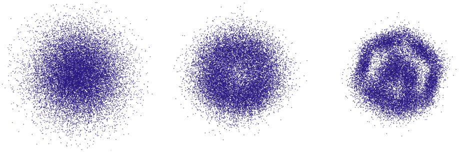

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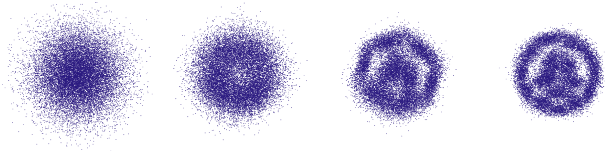

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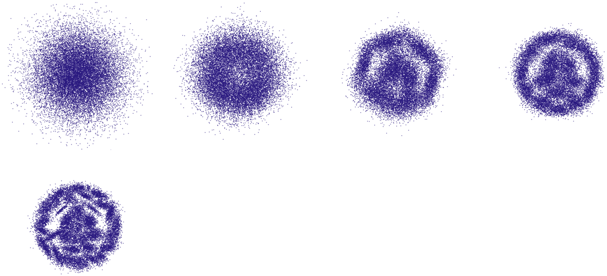

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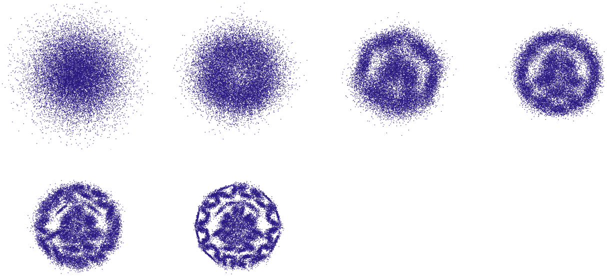

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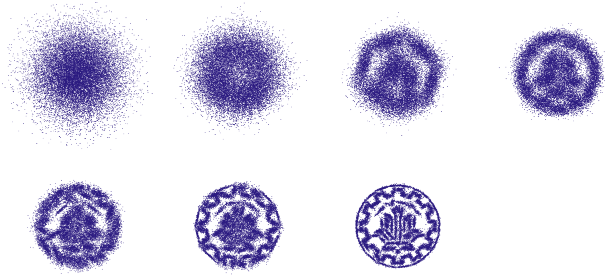

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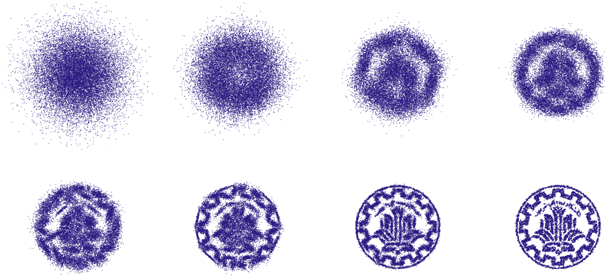

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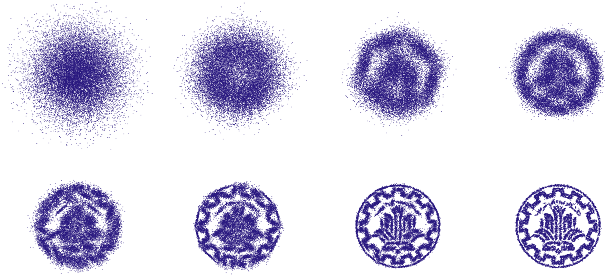

Is it possible!?

Example

$$T : X \to Y$$

$$X \sim \mathcal{N}(\mu, \Sigma)$$

$$(y_1, y_2) = T(x_1, x_2) = (0.75x_1 + 0.4, 0.5x_2 - 0.2)$$

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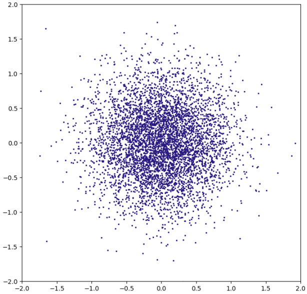

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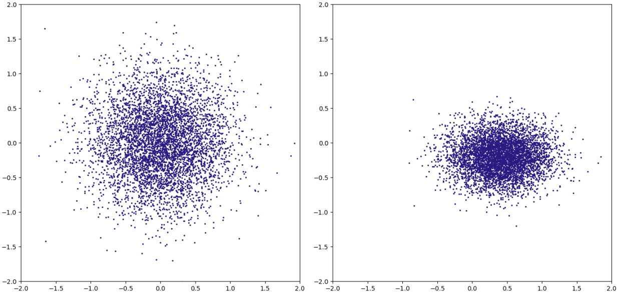

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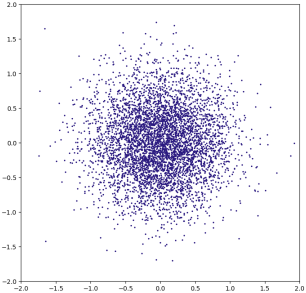

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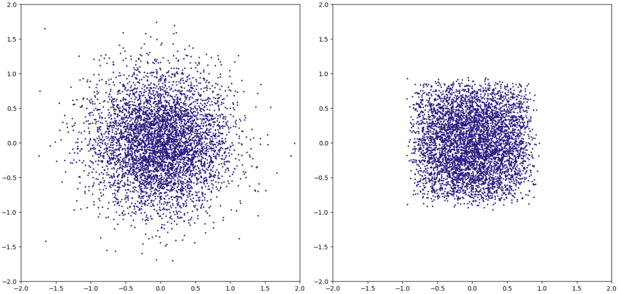

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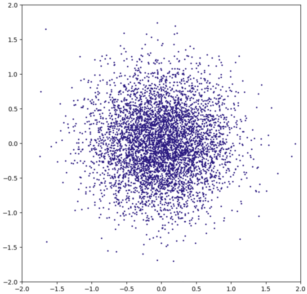

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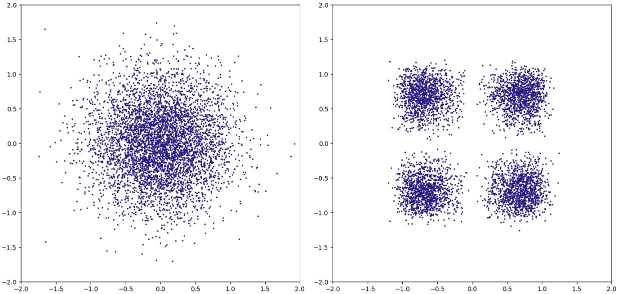

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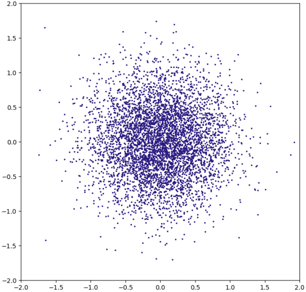

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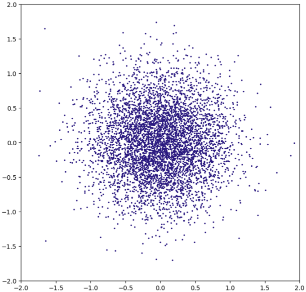

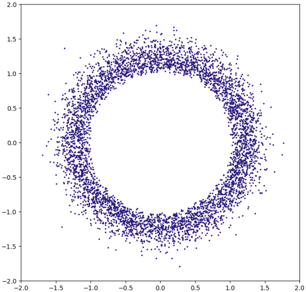

Transport

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Can we obtain any density by transforming a simple one?

Under reasonable assumptions, such a transformation always exists!

Change of Variable (Discrete Case)

Okay but how to find the transformed density?

$$p_y(y) = p_x(T^{-1}(y))|\det J_{T^{-1}}(y)|$$

Change of Variable

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Unfortunately NO!

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Only simple transformations satisfy the above conditions.

Example: Coupling Flow

Consider a simple invertible map like

$$h((x_1, x_2, ..., x_d)) = (a_1 x_1 + b_1, ..., a_d x_d + b_d)$$

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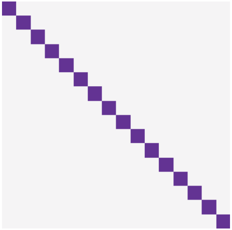

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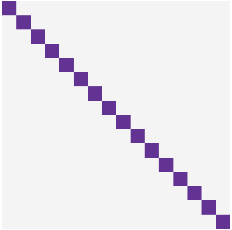

Why such a map is not so useful?

Example: Coupling Flow

Now define h as before:

$$h((x_1, x_2, ..., x_d); \theta) = (\theta_{11} x_1 + \theta_{12}, ..., \theta_{d1} x_d + \theta_{d2})$$

Take some partition of dimensions, like:

$$A : \{x_1, x_2, ..., x_m\}, B : \{x_{m+1}, ..., x_d\}$$

Define a map parametrized by θ in the following way:

$\theta = g(x_1, ..., x_m)$

$T(x_1, x_2, ..., x_m) = x_1, x_2, ..., x_m$

$T(x_{m+1}, ..., x_d) = h(x_{m+1}, ..., x_d; \theta)$

Is T invertible?

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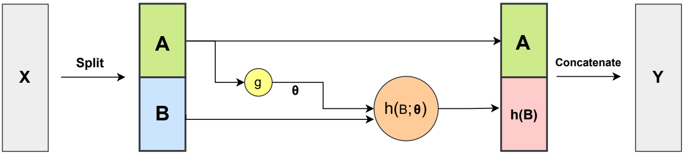

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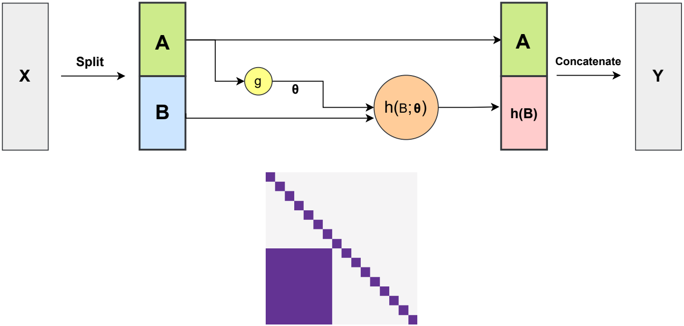

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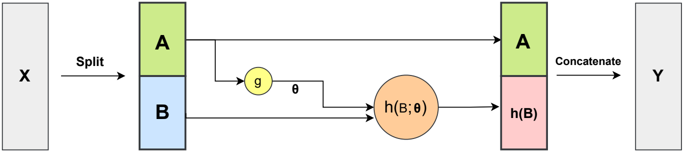

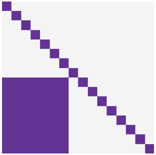

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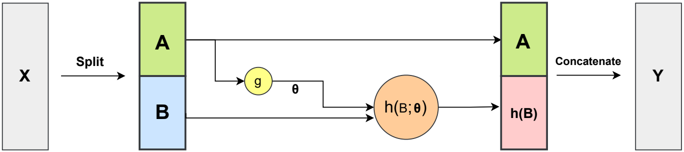

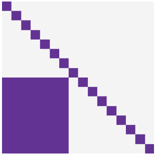

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Coupling provides an elegant framework to design invertible maps

Example: Coupling Flow

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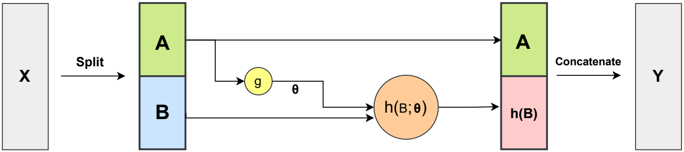

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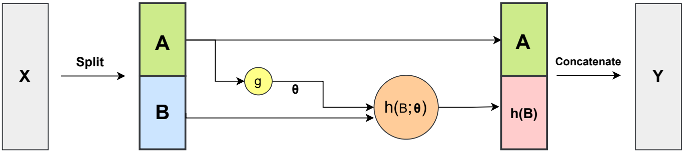

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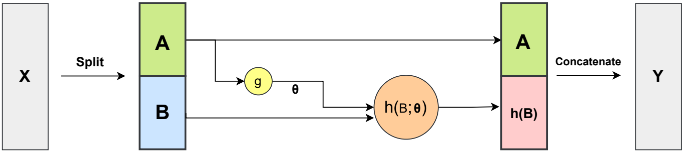

It doesn't touch half of the variables!!
So we can do it many times on different partitions!

$$T = T_1 \circ T_2 \circ ... \circ T_n$$

Summary

It's hard to find a expressive map T such that:

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Is there any other way?

Deterministic Continuous Transformations

Let's increase the number of transformations while making them simpler...

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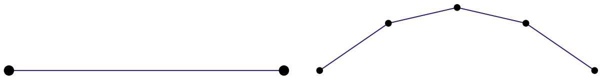

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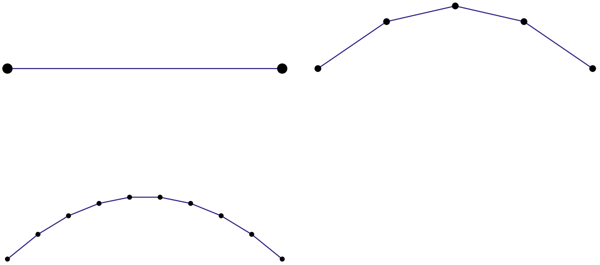

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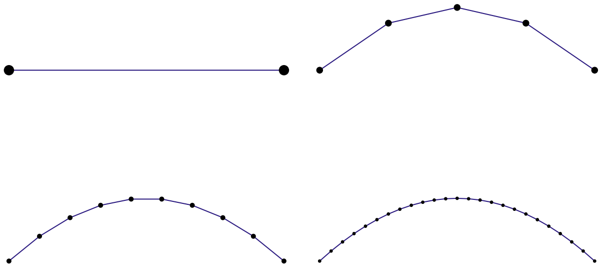

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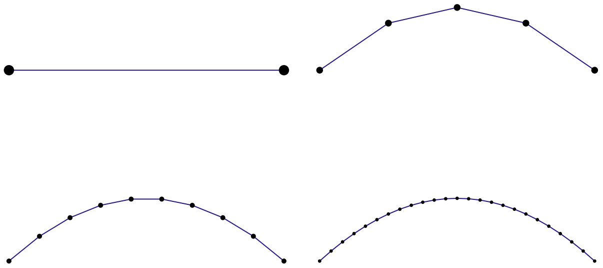


$$N \to \infty \ !??$$

Deterministic Continuous Transformations

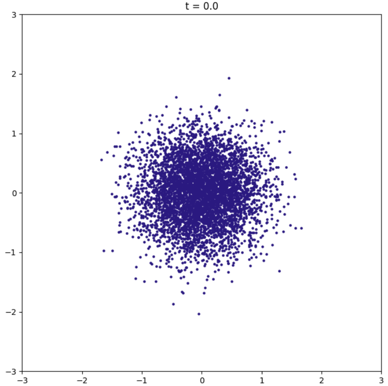
Now we define the transformed particles with a differential equation

$$dX_t = f(X_t, t)\, dt$$

Example

$$dX_t = -X_t \, dt$$

$$X_0 \sim \mathcal{N}(\mu, \Sigma)$$



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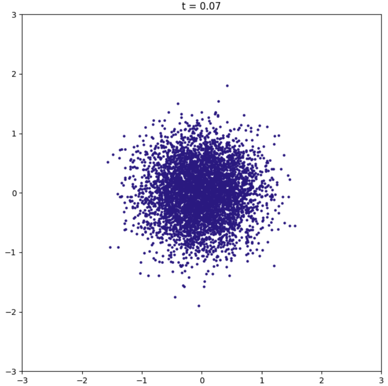

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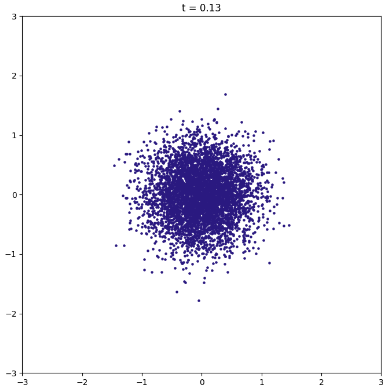

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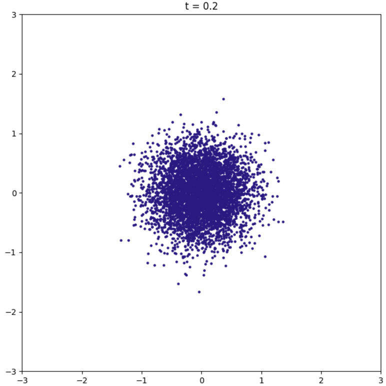

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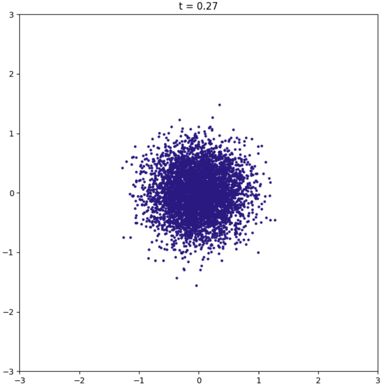

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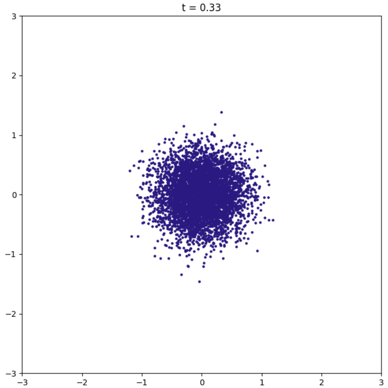

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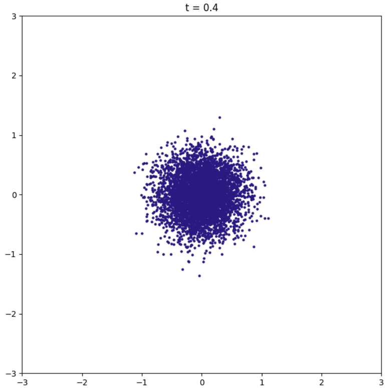

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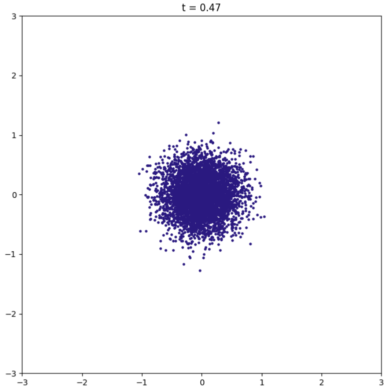

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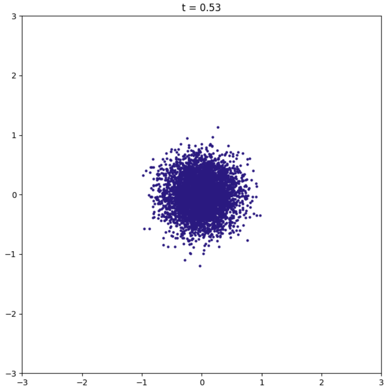

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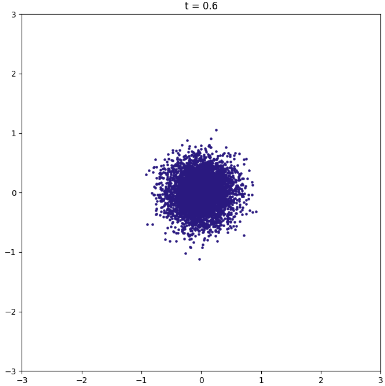

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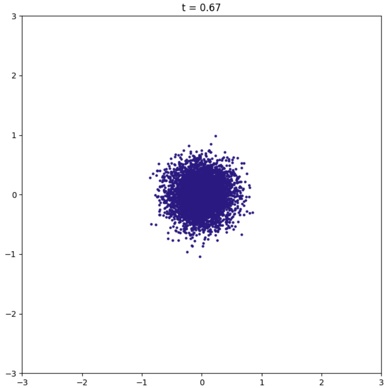

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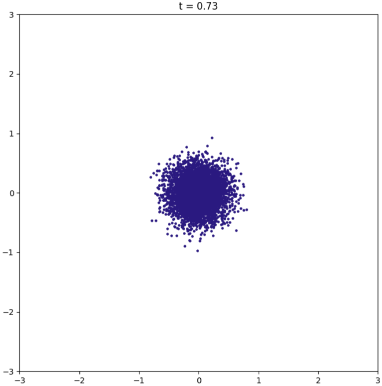

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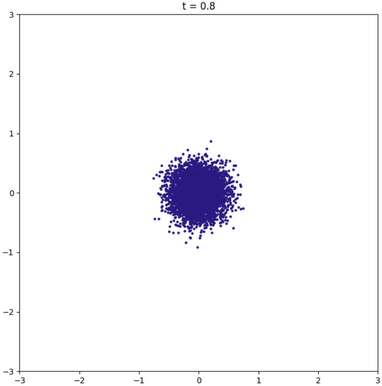

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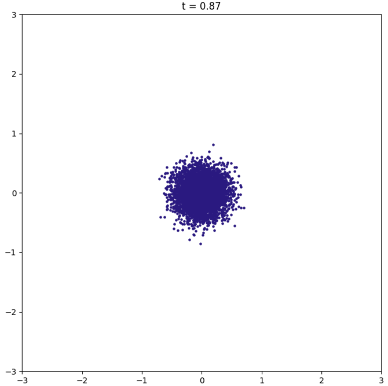

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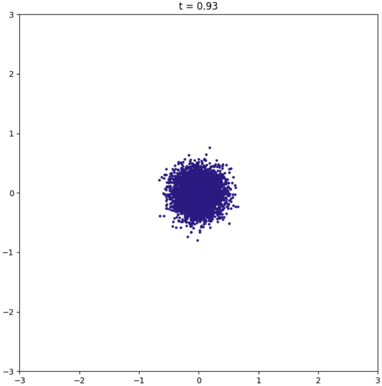

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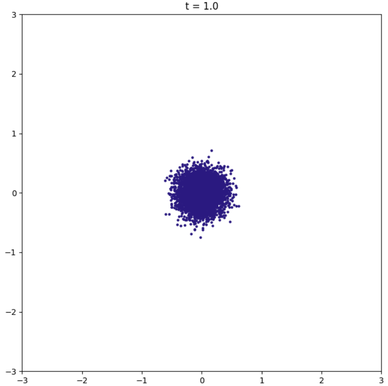

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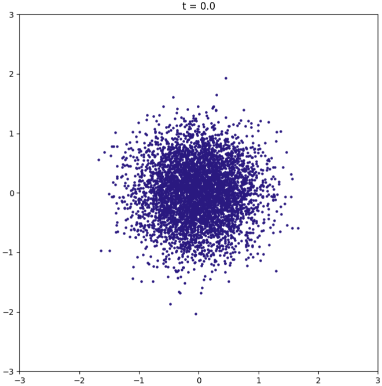

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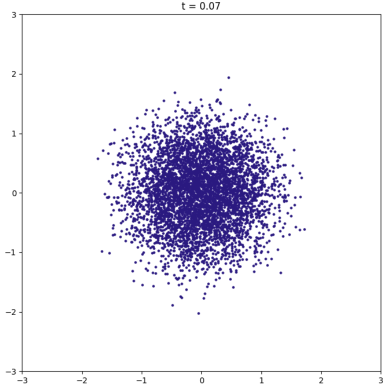

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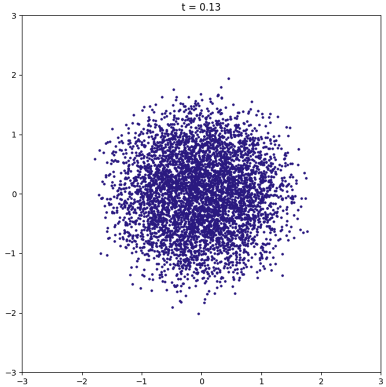

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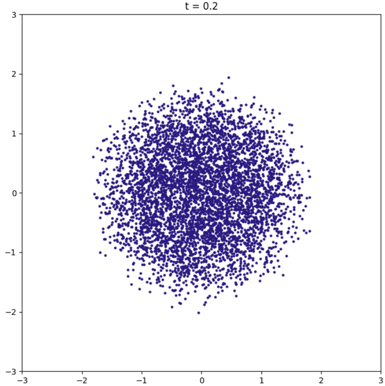

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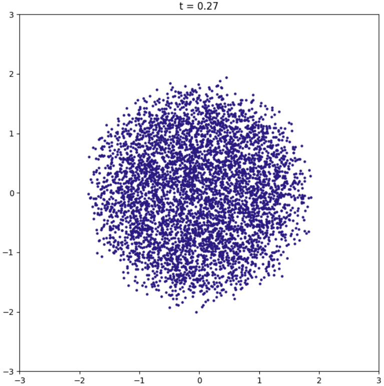

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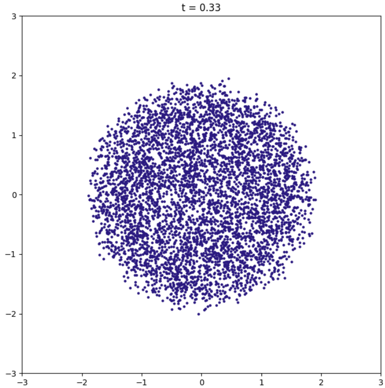

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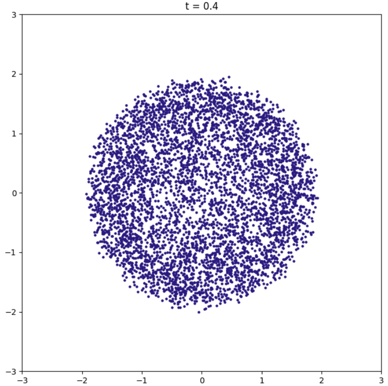

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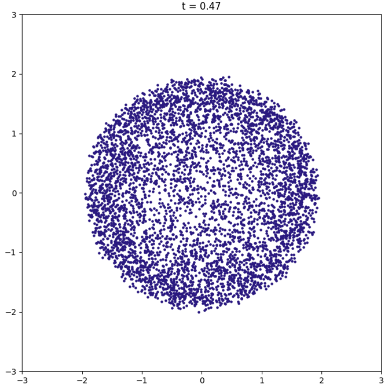

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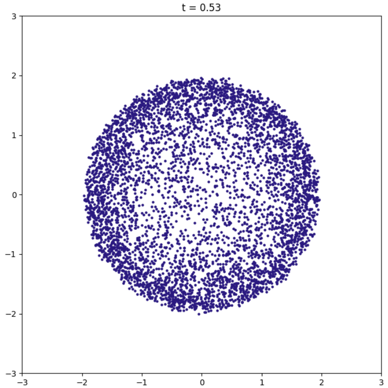

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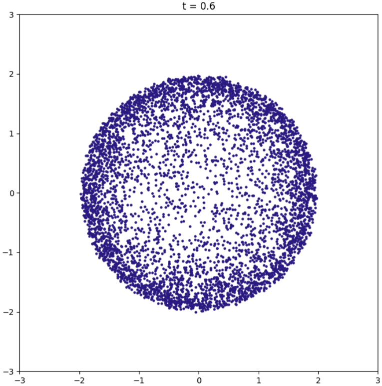

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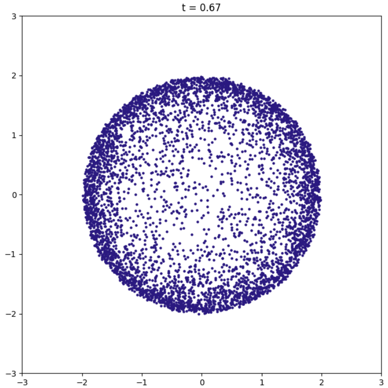

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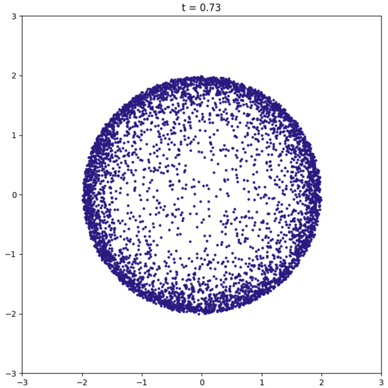

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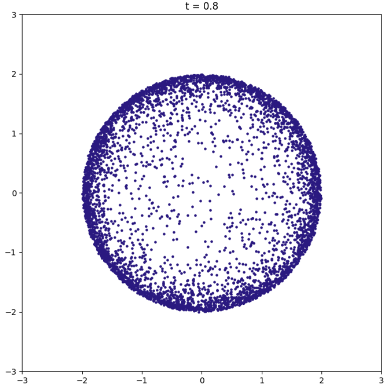

Example

Probabilistic Modeling with Flows

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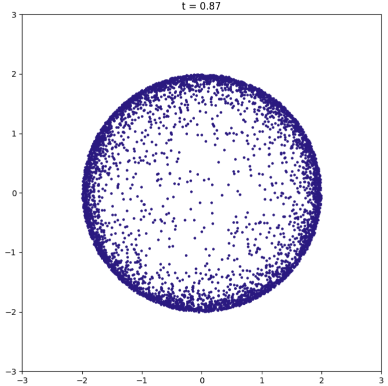

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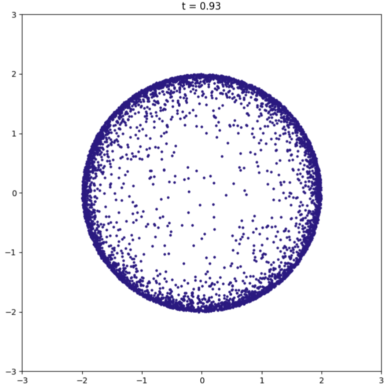

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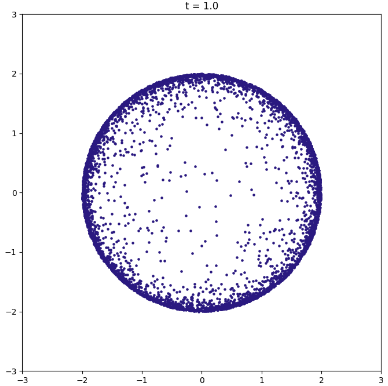

Instantaneous Change of Variables Theorem

$$dX_t = f(X_t, t)\,dt$$

Neural Ordinary Differential Equations, arXiv:1806.07366 [cs.LG]

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$$\frac{\partial \log p(x)}{\partial t} = \lim_{\epsilon \to 0^+} \frac{\log p(x) - \log \left|\det(\frac{\partial T_\epsilon}{\partial x})\right| - \log p(x)}{\epsilon}$$

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$$\frac{\partial \log p(x)}{\partial t} = -\mathrm{Tr}(\frac{df}{dx})$$

Neural Ordinary Differential Equations, arXiv:1806.07366 [cs.LG]

Continuity equation

$$dX_t = f(X_t, t)\, dt$$

Then the density of the transformed rvs is the solution of:

$$\frac{\partial p(x,t)}{\partial t} = -\frac{\partial}{\partial x}[f(x,t)p(x,t)]$$

Neural ODE

$$dX_t = f(X_t, t)\, dt$$

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A Neural Network with continuous depth!

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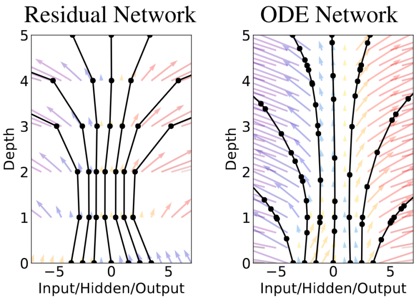
But How can we train such a model?

Neural ODE



Continuous Depth needs Continuous Backpropagation!

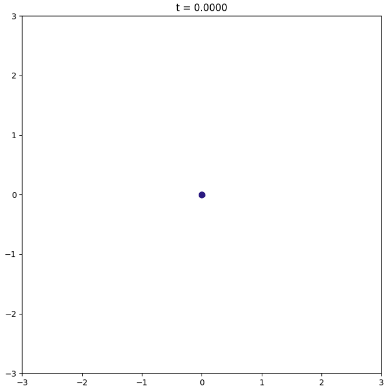
Neural Ordinary Differential Equations, arXiv:1806.07366 [cs.LG]

Deterministic Continuous Transformations

Let's see our last example of deterministic transports

Example: Gradient Flow

$$dX_t = \tau \nabla_x U(X_t)dt$$



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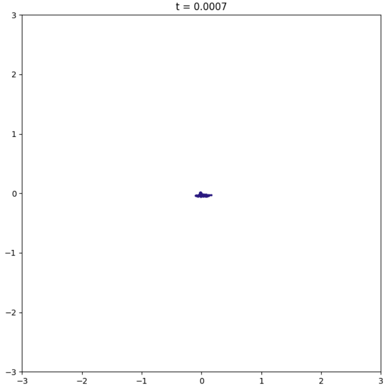

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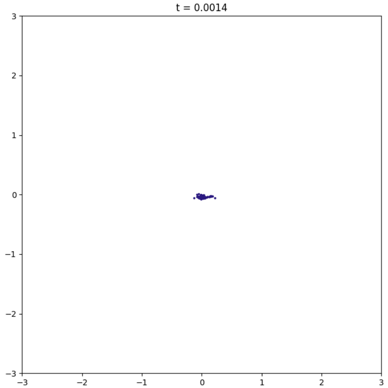

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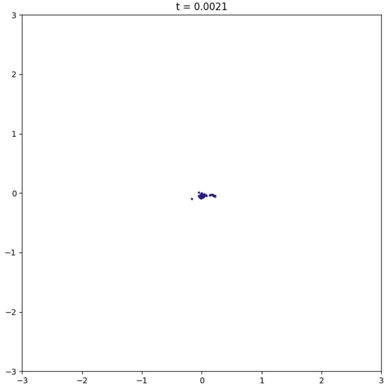

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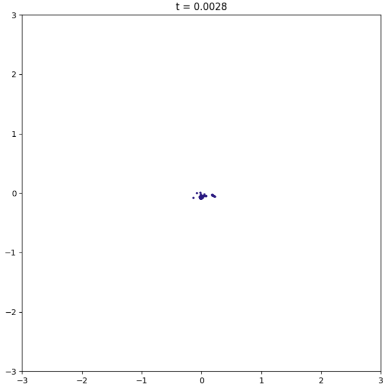

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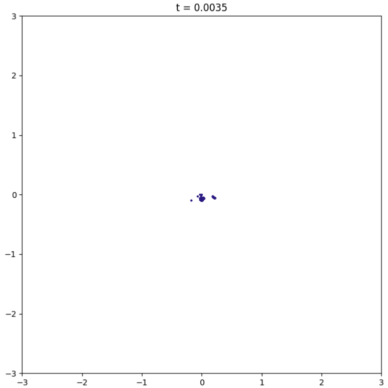

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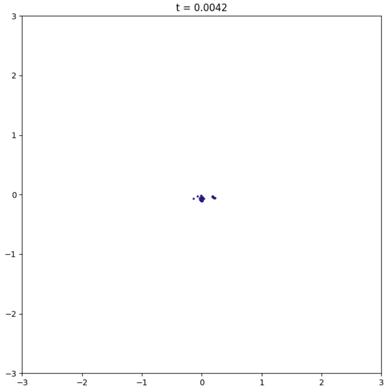

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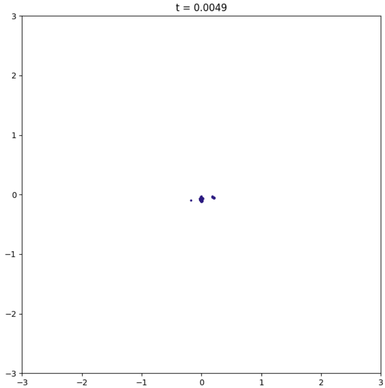

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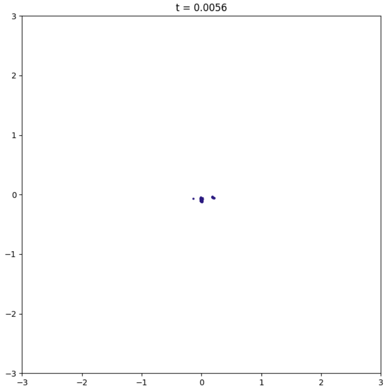

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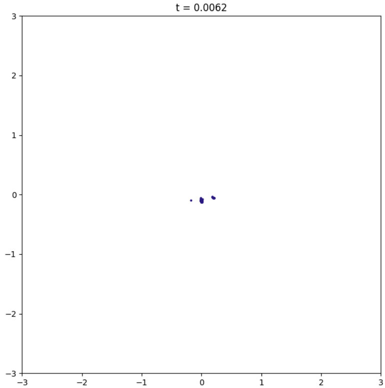

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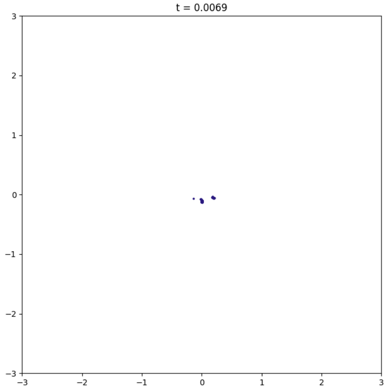

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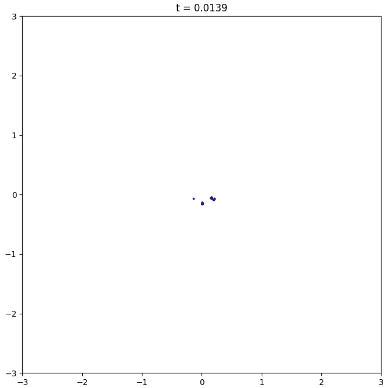

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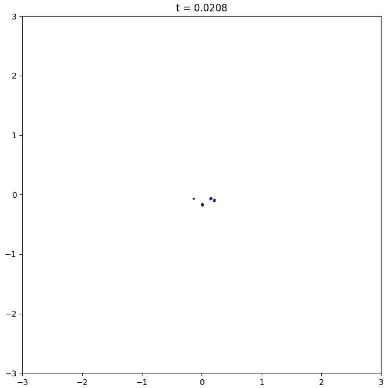

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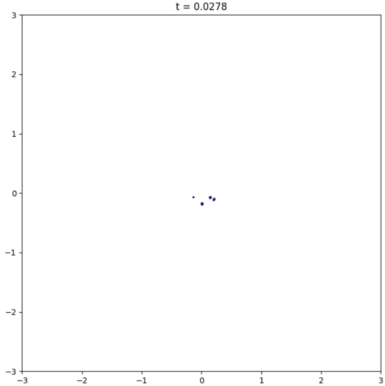

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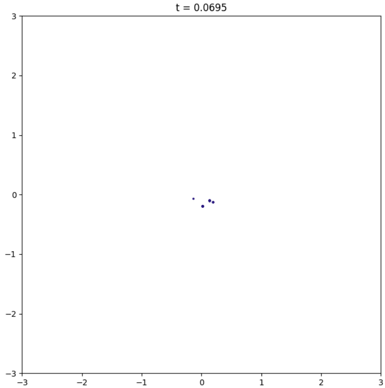

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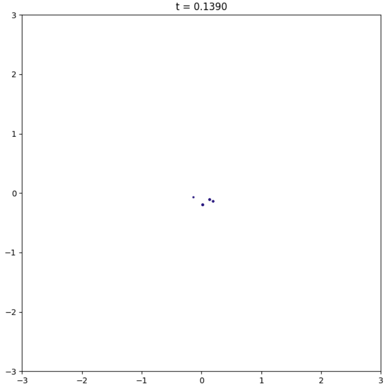

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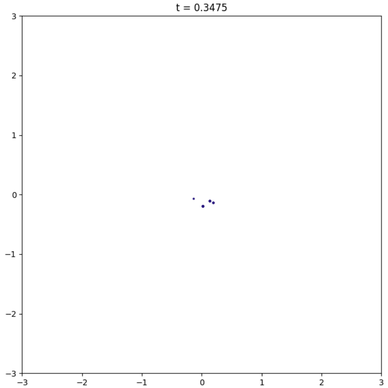

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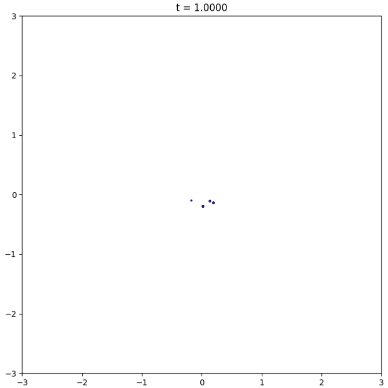


Deterministic Continuous Transformations

What just happened!!?

Deterministic Continuous Transformations

What just happened!!?

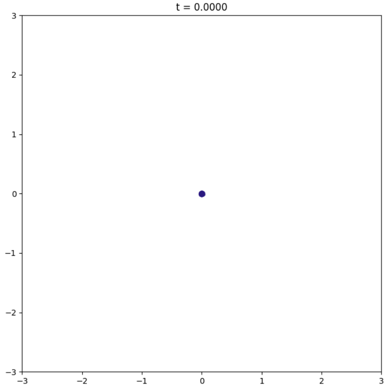
How to fix it?

Stochastic Continuous Transformations

Transport maps do not have to be deterministic!

Example: Brownian Motion

$$dX_t = dW_t$$



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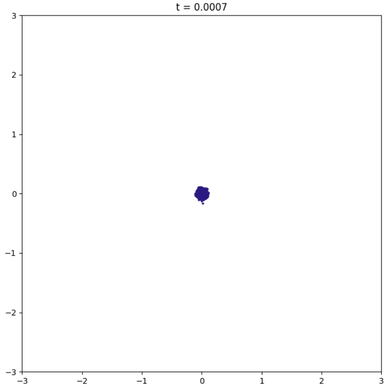

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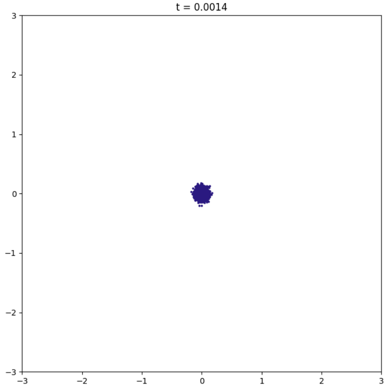

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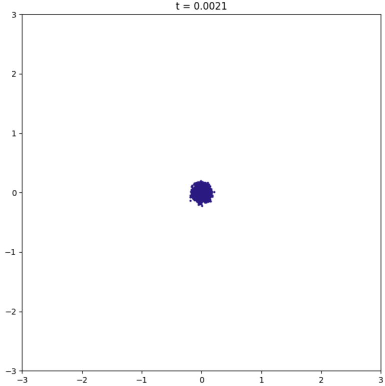

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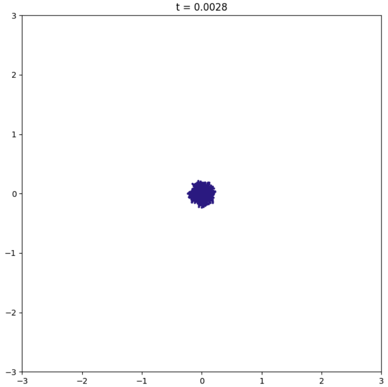

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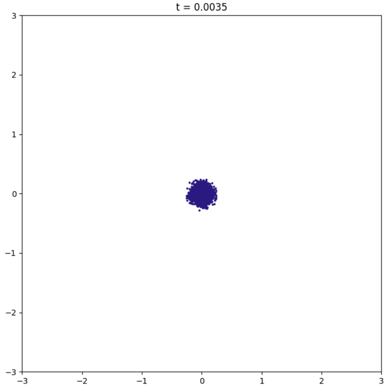

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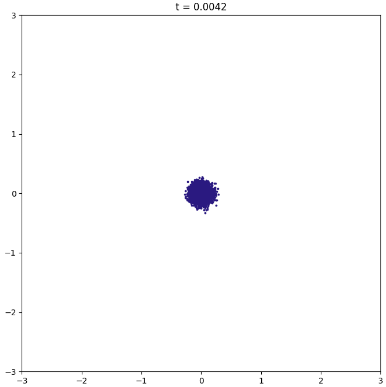

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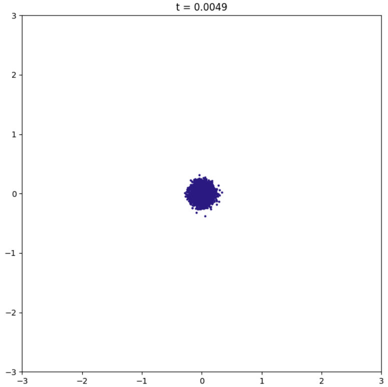

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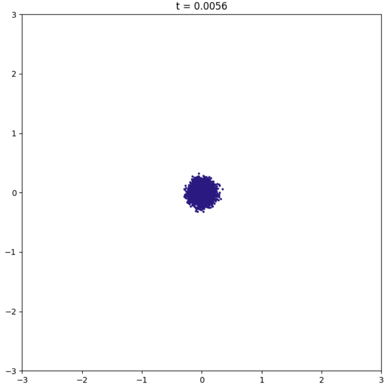

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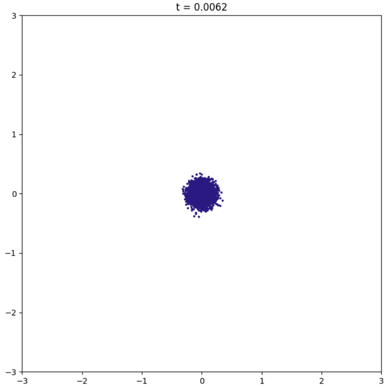

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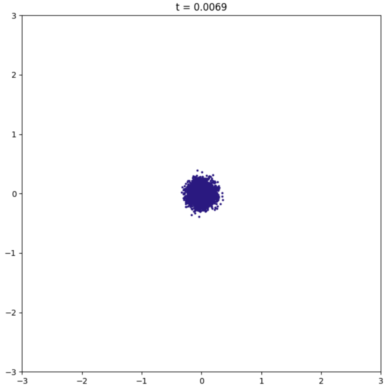

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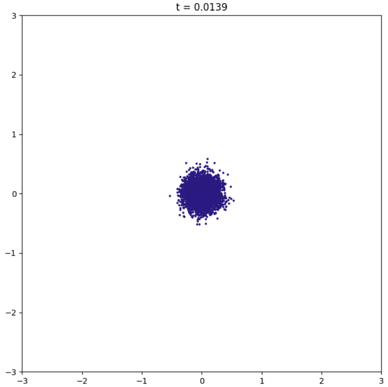

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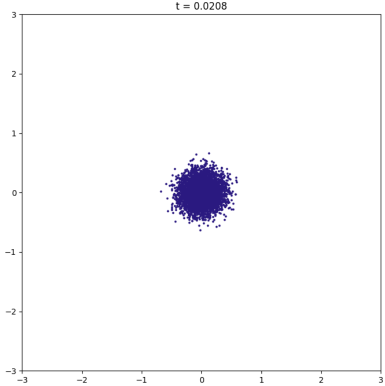

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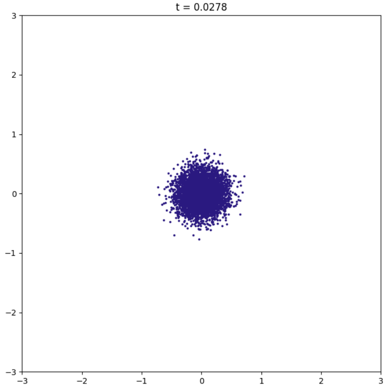

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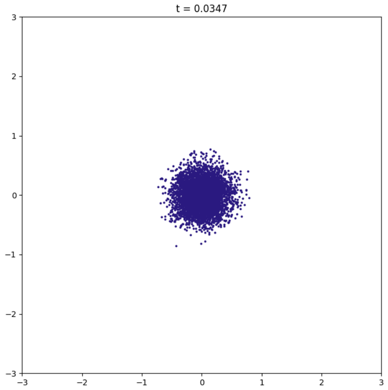

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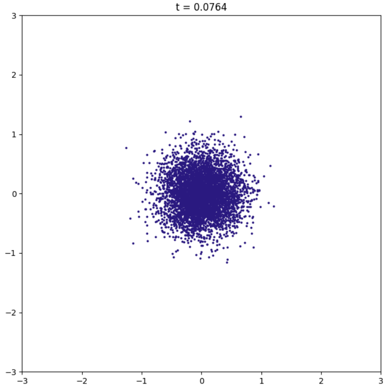

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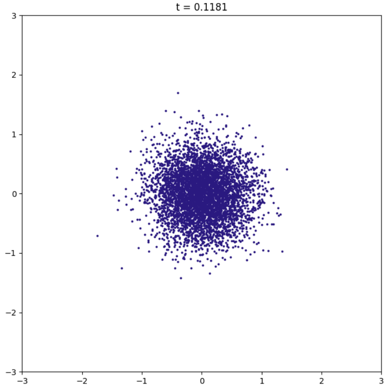

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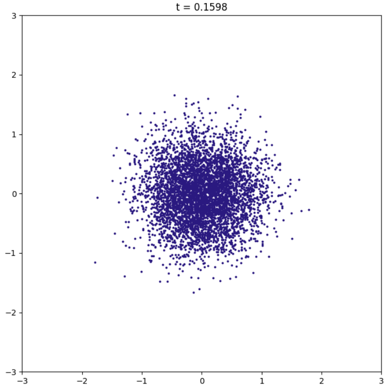

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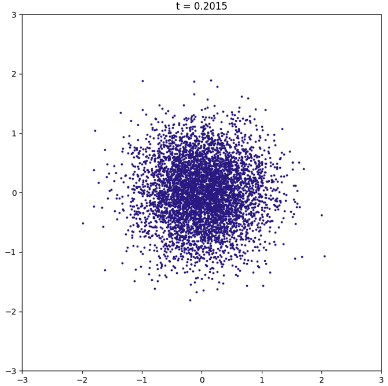

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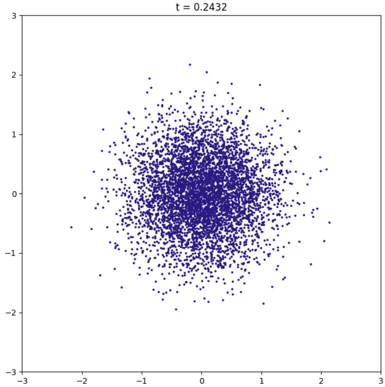

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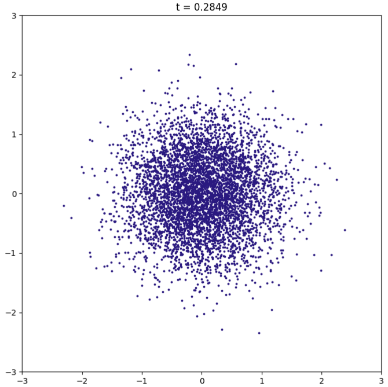

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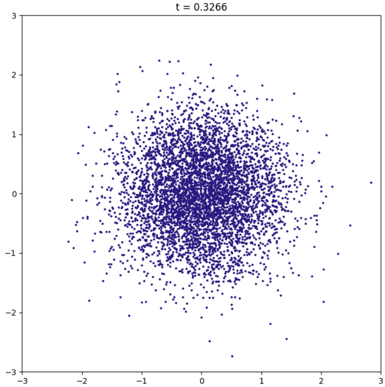

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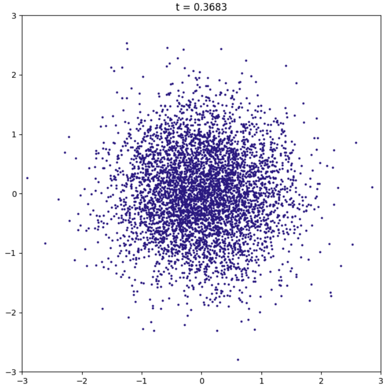

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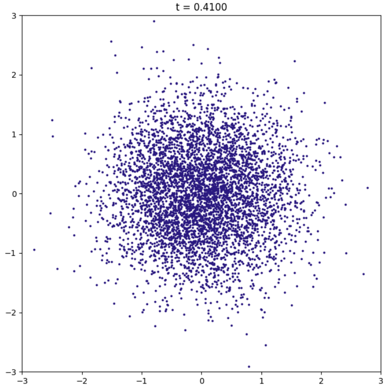

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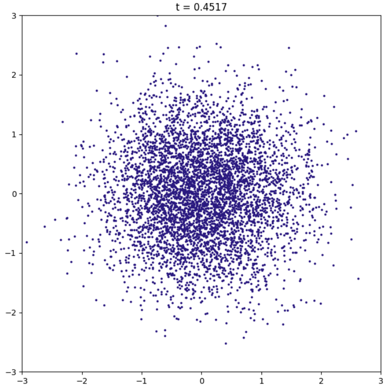

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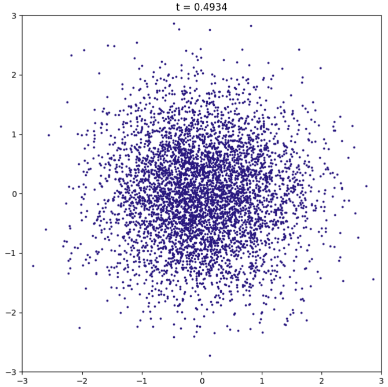

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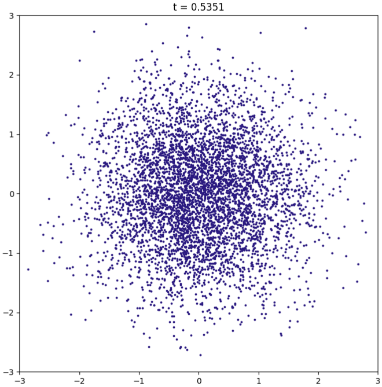

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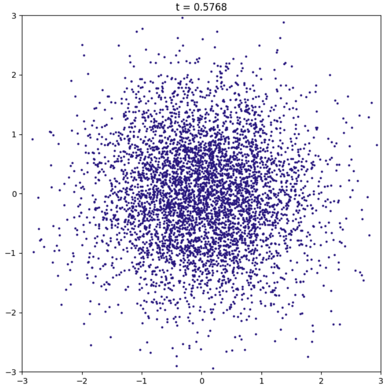

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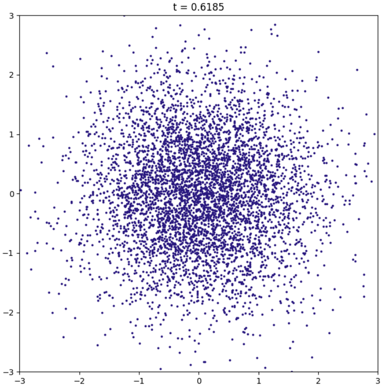

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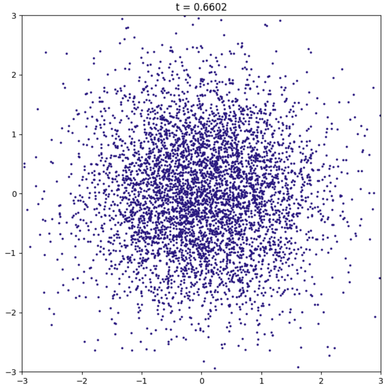

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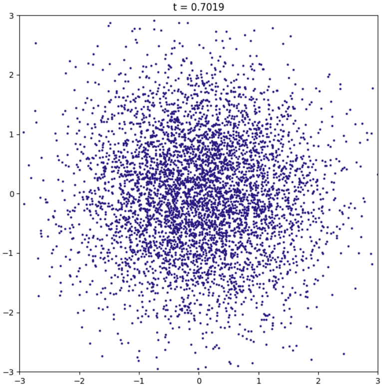

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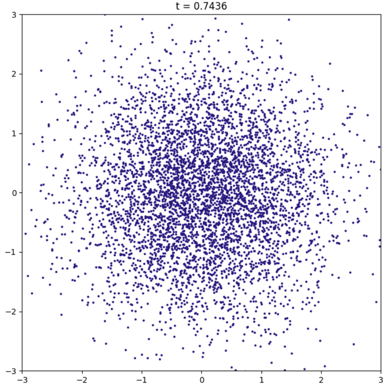

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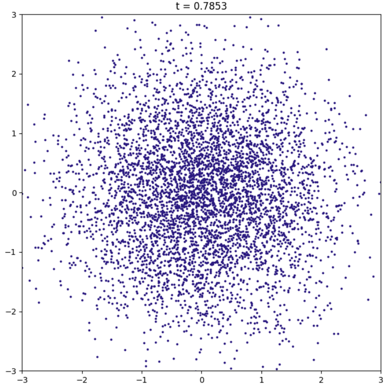

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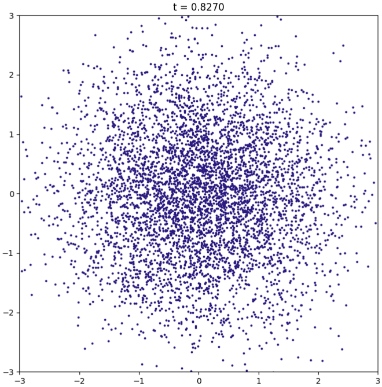

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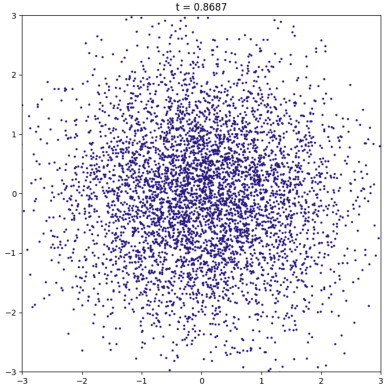

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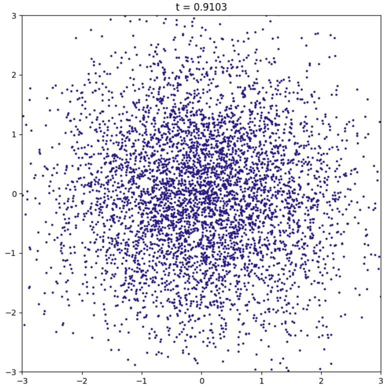

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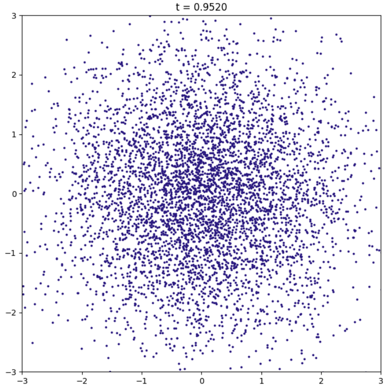

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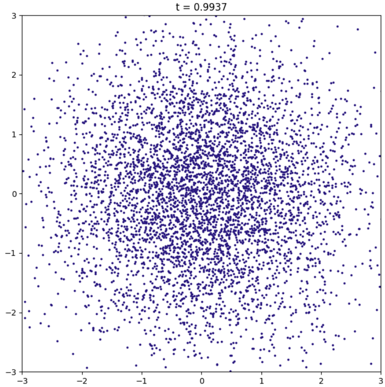

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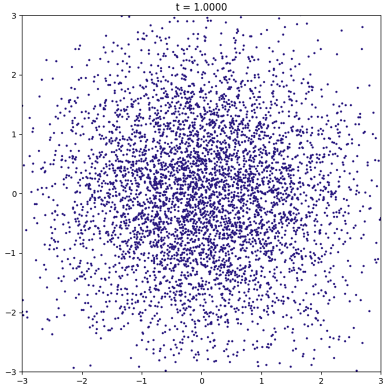

Stochastic Continuous Transformations

"Change of variables" for stochastic maps !!???

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Fokker-Planck Equation!

Stochastic Continuous Transformations

An even more general framework?

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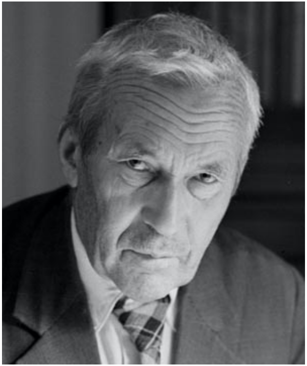

Now we get back to this one

Example: Overdamped Langevin Dynamics

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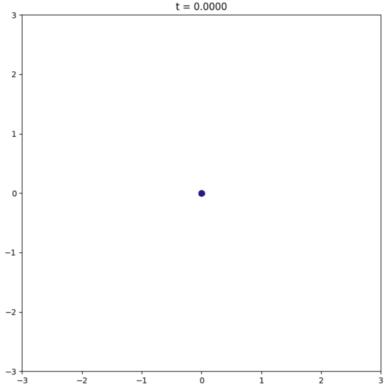

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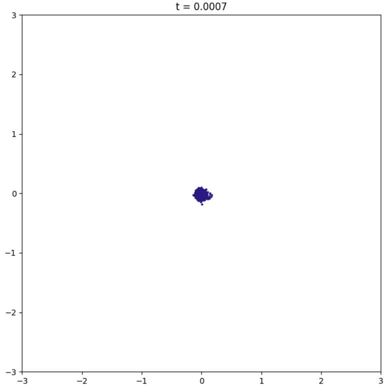

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Probabilistic Modeling with Flows

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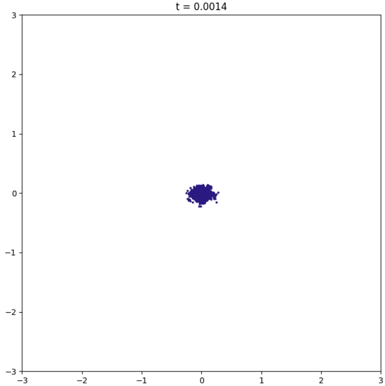

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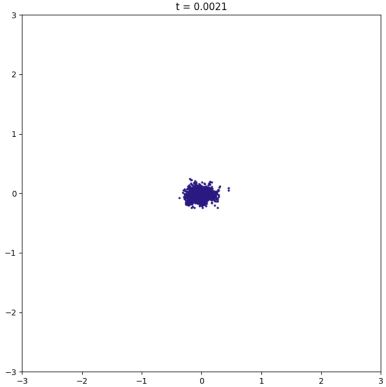

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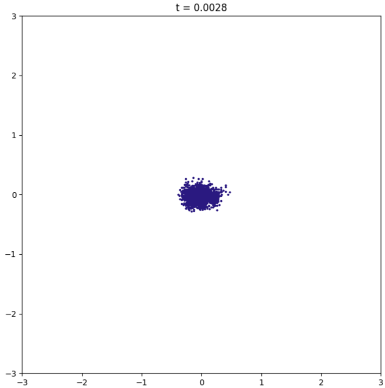

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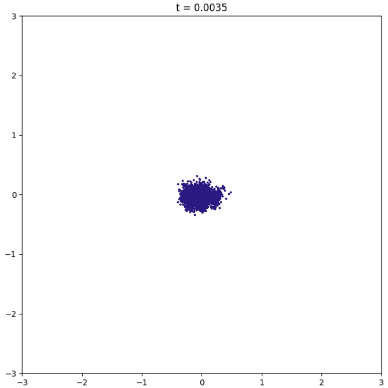

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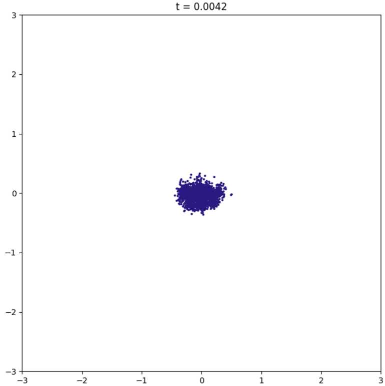

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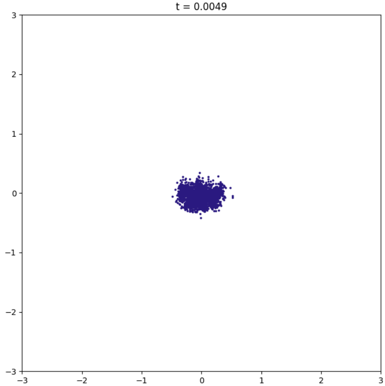

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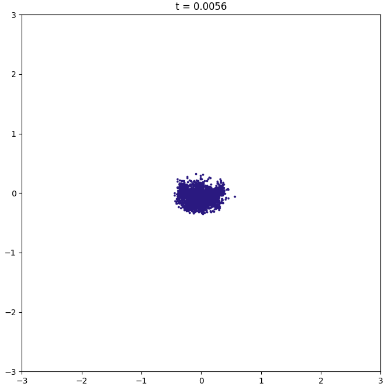

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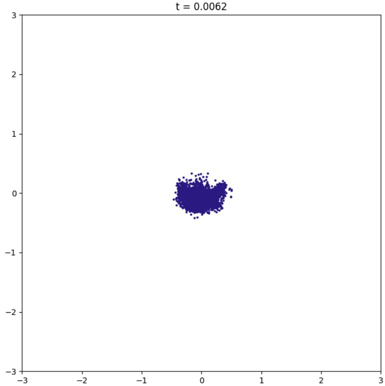

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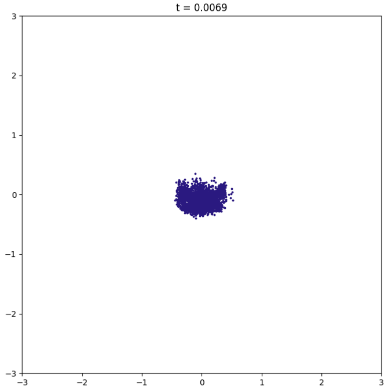

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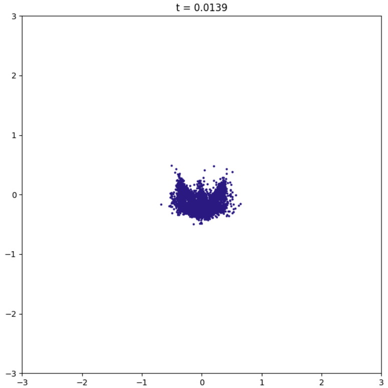

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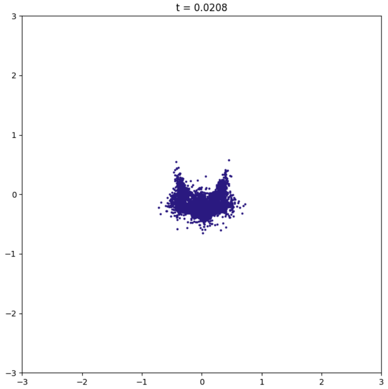

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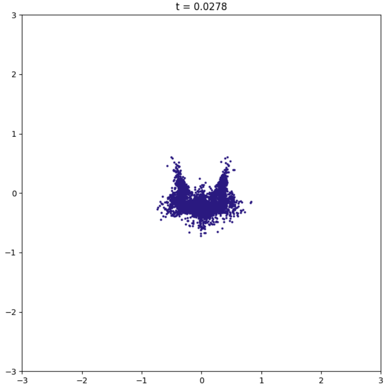

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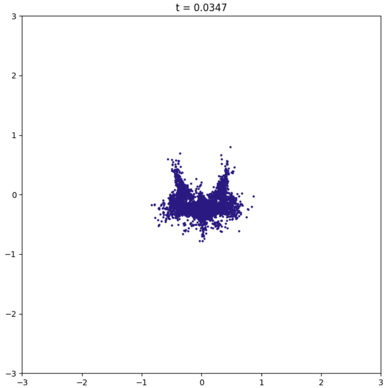

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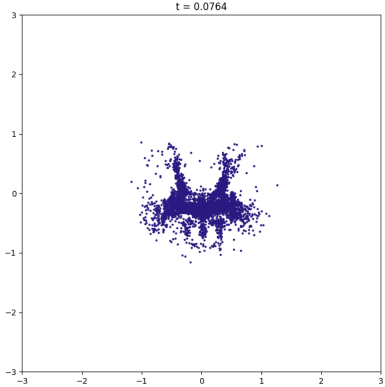

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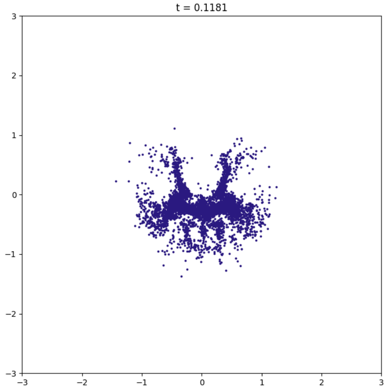

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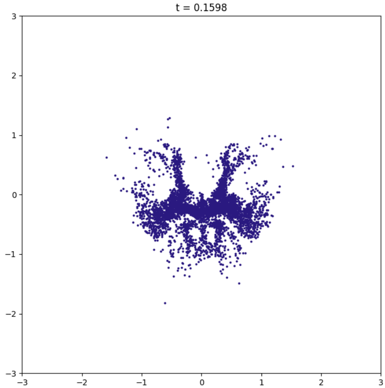

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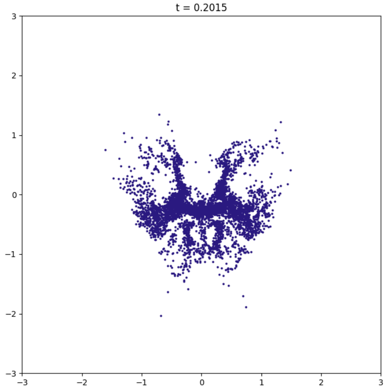

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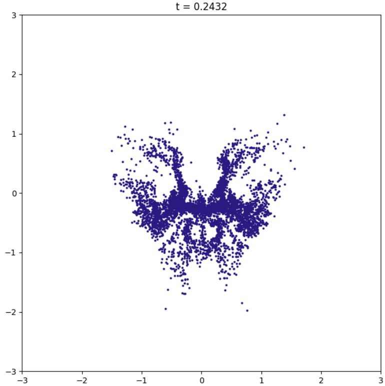

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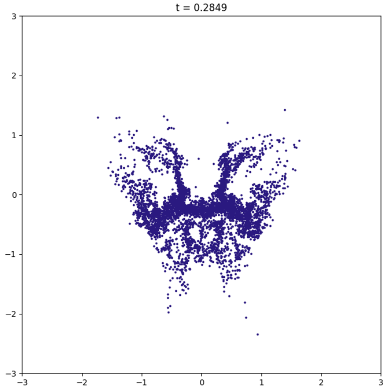

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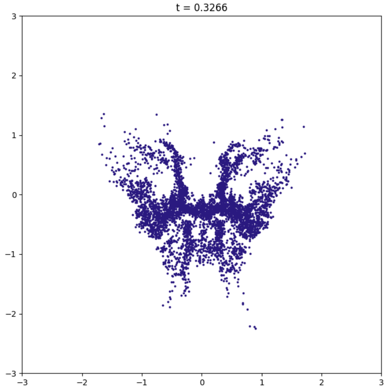

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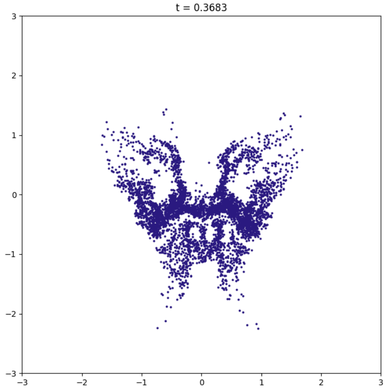

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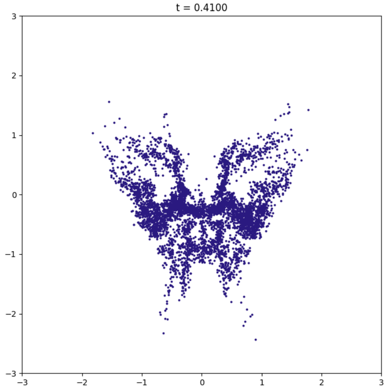

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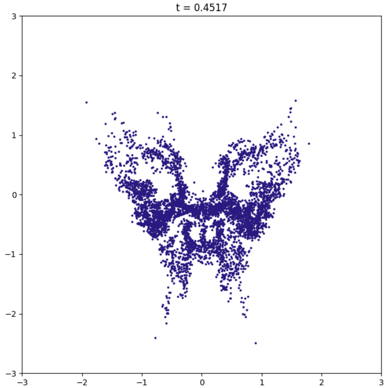
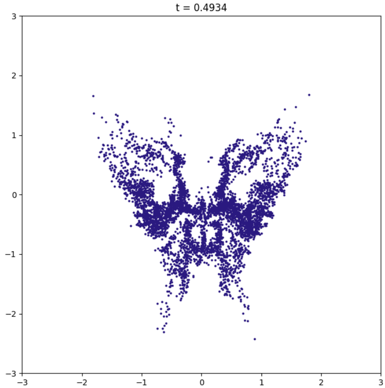


Probabilistic Modeling with Flows

Example: Overdamped Langevin Dynamics

$$dX_t = \tau \nabla_x U(X_t)dt + \sqrt{2\tau}dW_t$$



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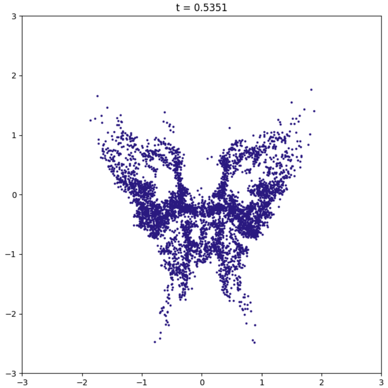

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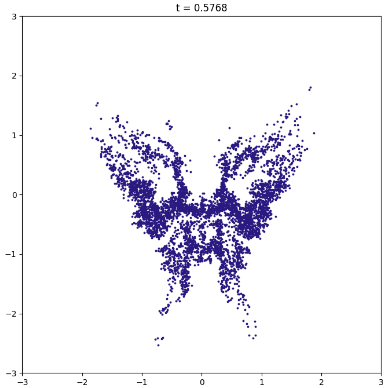

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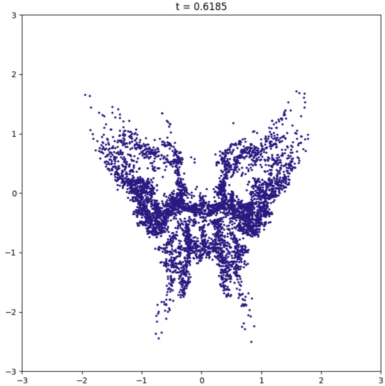

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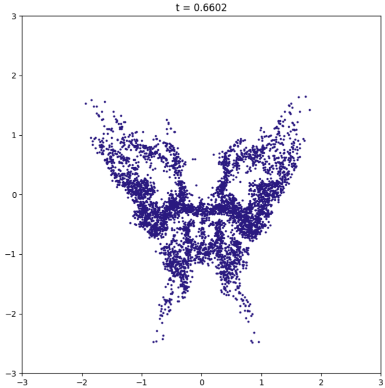

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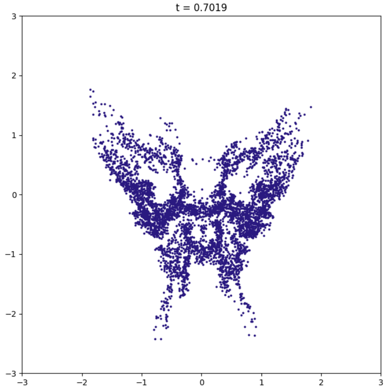

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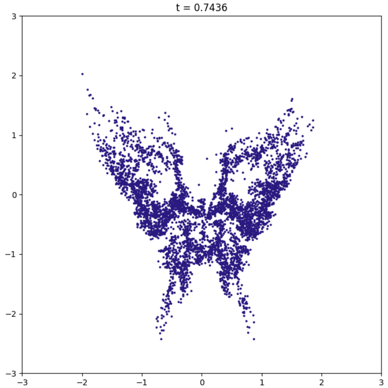

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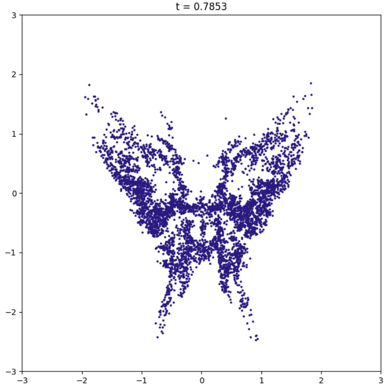

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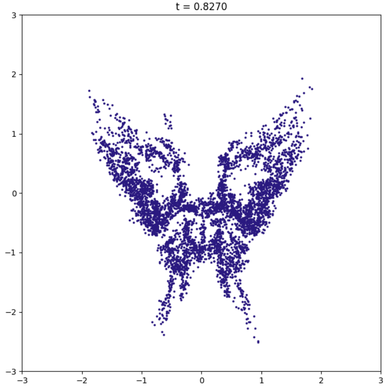

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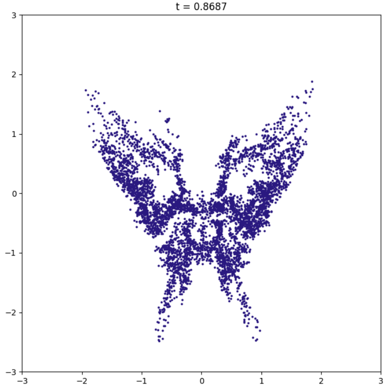

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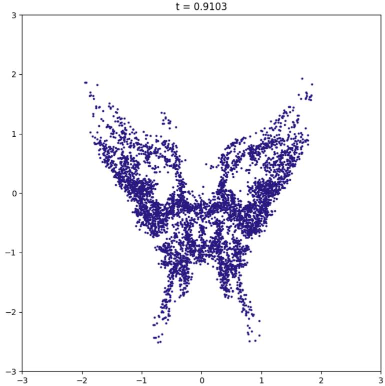

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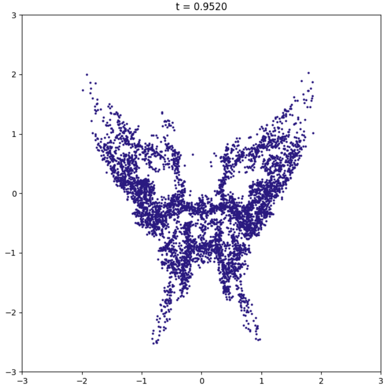

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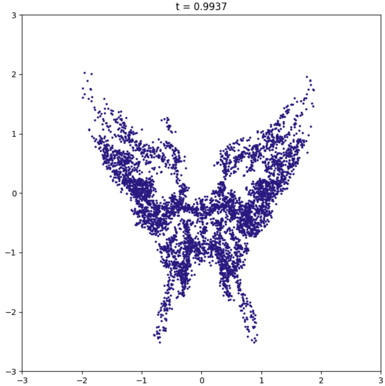

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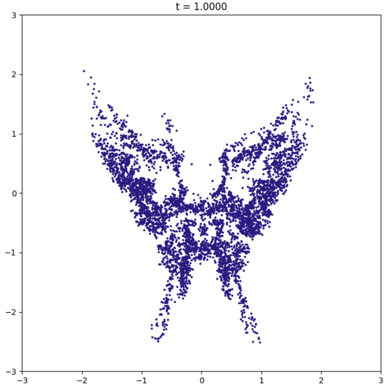
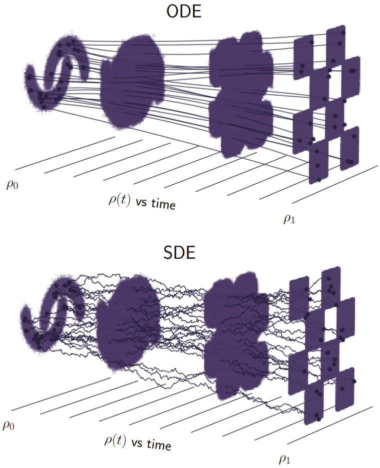


Is there any way to train a parameterized ODE/SDE!?

Stochastic Interpolants



Stochastic Interpolants: A Unifying Framework for Flows and Diffusions, arXiv:2303.08797 [cs.LG]

Stochastic Interpolants

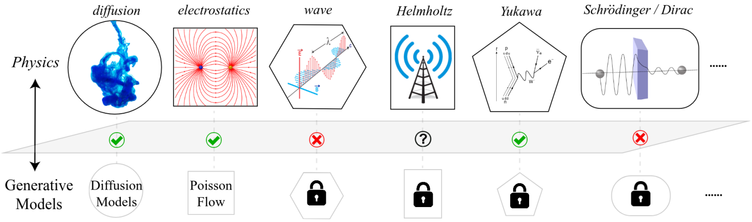
Without latent variable $x_t = (1 - t)x_0 + tx_1$

Stochastic Interpolants: A Unifying Framework for Flows and Diffusions, arXiv:2303.08797 [cs.LG]

Different Approaches to Study Generative Flows

Kolmogorv, Einstein, Feynman, Schrödinger, Smoluchowski, Pontryagin, Fokker, Planck, Monge, Kantorovich, ...

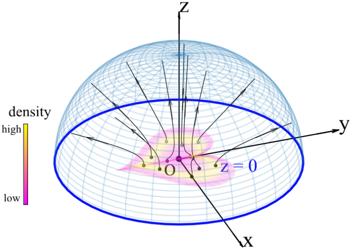
A Physics-Inspired Approach

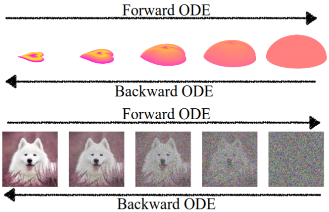


GenPhys: From Physical Processes to Generative Models, arXiv:2304.02637[cs.LG]

Example: Poisson Flow Generative Models

$$dX_t = E(x)\,dt$$





Poisson Flow Generative Models, arXiv:2209.11178[cs.LG]

A Game-Theoretic Approach

Generative modeling is more than designing particle dynamics!

A Game-Theoretic Approach

	Mean-field game (11)			
Model	$\mathcal{M}(\rho)$	$\mathcal{I}(\rho)$	$L(x, v)$	**Dynamics**
Continuous normalizing flow	$\mathcal{D}_{KL}(\rho \Vert \rho_{ref})$	0	0	$dx = v\,dt$
Score-based generative modeling	$-\mathbb{E}_\rho\left[\log \pi\right]$	0	$\frac{\lvert v\rvert^2}{2} - \nabla \cdot f$	$dx = (f + \sigma v)\,dt + \sigma\,dW_t$
Score-based probability flow	$-\frac{1}{2}\mathbb{E}_\rho\left[\log \pi\right]$	$\mathbb{E}_\rho\left[\frac{\lvert\sigma\nabla \log \rho\rvert^2}{8}\right]$	$\frac{\lvert v\rvert^2}{2} - \frac{\nabla \cdot f}{2}$	$dx = (f + \sigma v)\,dt$
Wasserstein gradient flow (WGF) $(\epsilon \to 0)$	$\mathcal{F}(\rho)e^{-T/\epsilon}$	$\frac{e^{-t/\epsilon}}{\epsilon}\mathcal{F}(\rho)$	$\frac{e^{-t/\epsilon}}{2}\lvert v\rvert^2$	$dx = v\,dt$
OT-Flow	$\mathcal{D}_{KL}(\rho \Vert \rho_{ref})$	0	$\frac{1}{2}\lvert v\rvert^2$	$dx = v\,dt$
Boltzmann generator	$\lambda\mathcal{D}_{KL}(\pi \Vert \rho) + (1-\lambda)\mathcal{D}_{KL}(\rho \Vert \pi)$	0	0	$dx = v\,dt$
Schrödinger bridge	$\rho = \pi$	0	$\frac{1}{2}\lvert v\rvert^2$	$dx = \sigma v\,dt + \sigma\,dW_t$
Generalized Schrödinger bridge	$\rho = \pi$	$\mathcal{I}(x, \rho)$	$\frac{1}{2}\lvert v\rvert^2$	$dx = \sigma v\,dt + \sigma\,dW_t$

A mean-field games laboratory for generative modeling, arXiv:2304.13534 [stat.ML]

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