# Diffusion Models and SDEs

**Lecture 2:**
**SDEs and how to manipulate them**

Time Reversal and Score-based modelling

Probability Flow ODE and Flow Matching

Conditioning SDEs via Doob's h-transform

# Score-based generative modelling

*Training:* learn score $s_t(x) := \nabla \log p_t(x)$ by

1. Sample from target $x_1 \sim p_1$
2. Run "forward" SDE to "noise" $x_1$ until it becomes "simple" $x_0 \sim p_0$
3. Minimize some loss $\propto \left\| \hat{s}_t(x) - s_t(x) \right\|^2$

*Inference:* sample using "reverse" SDE or prob-flow ODE

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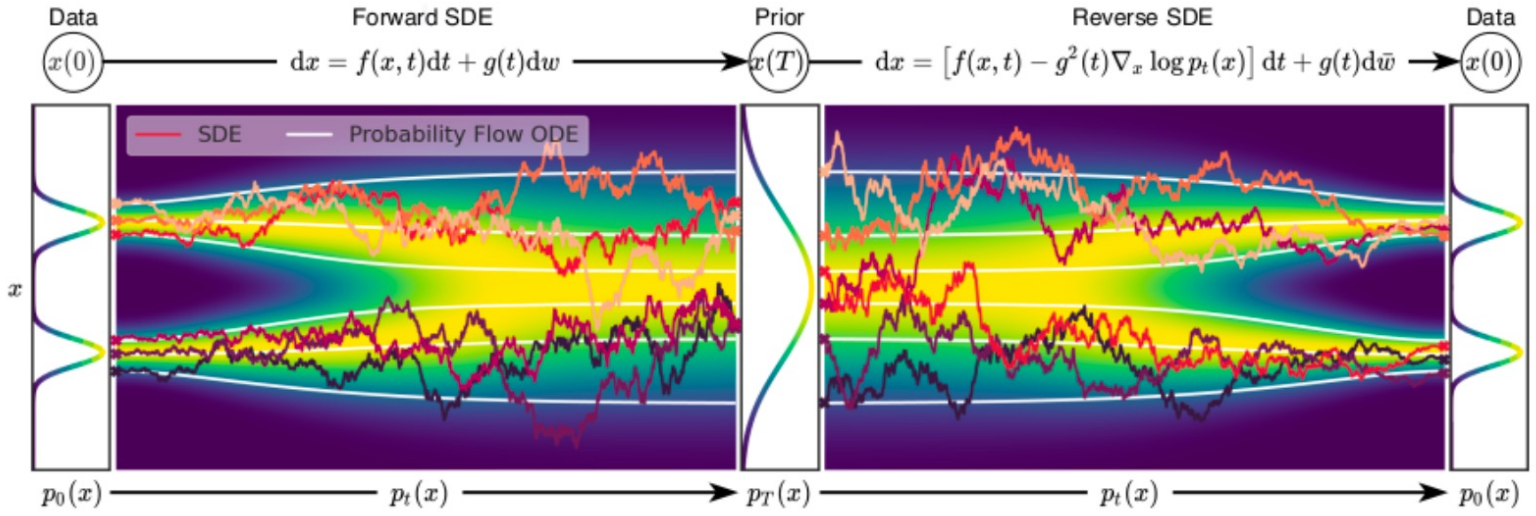


Figure 2 from Song et al. (2020)

# Time Reversal - Chain Rule

**A discrete time "heuristic" sketch**

Via the chain rule we can decompose the joint in either direction,

$$p_{t|t+\delta}(x|y)p_{t+\delta}(y) = p_{t+\delta|t}(y|x)p_t(x)$$

Now consider an EM approx transition density, for the forward kernel:

$$p_{t+\delta|t}(y|x) = \mathcal{N}(y|x + f^+(x)\delta, \delta\sigma^2)$$

$$p_{t|t+\delta}(x|y) = ?$$

# Time Reversal - Chain Rule

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$$p_{t|t+\delta}(x|y) = p_{t+\delta|t}(y|x)\frac{p_t(x)}{p_{t+\delta}(y)}$$

# Time Reversal - Chain Rule

**A discrete time "heuristic" sketch**

Via Taylors Theorem we can expand time t marginal around y:

$$p_{t|t+\delta}(x|y) = p_{t+\delta|t}(y|x)\frac{p_t(y)e^{(x-y)^\top \nabla_y \ln p_t(y)+\mathcal{O}(\delta^2)}}{p_{t+\delta}(y)}$$

Assuming $|\ln p_t(x) - \ln p_s(x)| = \mathcal{O}(|t-s|^2)$

$$p_{t|t+\delta}(x|y) = p_{t+\delta|t}(y|x)e^{(x-y)^\top \nabla_y \ln p_t(y)+\mathcal{O}(\delta^2)}$$

# Time Reversal - Chain Rule

**A discrete time "heuristic" sketch**

Regrouping and completing the square:

$$p_{t|t+\delta}(x|y) = \frac{e^{-\frac{||x-(y-f^+(y)\delta+\sigma^2\nabla_y \ln p_t(y)\delta||^2}{\sigma^2\delta}+\mathcal{O}(\delta^2)}}{\sqrt{2\pi}\delta^{d/2}\sigma^d}$$

Which corresponds to the Euler Maruyama discretization of the following SDE (seem familiar ?):

$$\mathrm{d}X_t = \left(-f^+(X_t, T-t) + \sigma^2 \nabla_{X_t} \ln p_{T-t}(X_t)\right)\mathrm{d}t + \sigma \mathrm{d}W_t$$

# Time Reversal - Chain Rule

**A discrete time “heuristic” sketch**

Inspecting the relationship between the drifts yields Nelsons duality formula:

$$f^{-}(x,t) + f^{+}(x, T-t) = \sigma^2 \nabla_x \ln p_{T-t}(x)$$

# Time Reversal - Chain Rule

**A discrete time “heuristic” sketch**

Inspecting the relationship between the drifts yields Nelsons duality formula:

$$f^{-}(x,t) + f^{+}(x, T-t) = \sigma^2 \nabla_x \ln p_{T-t}(x)$$

Looks slightly different to Song et al. 2021, why ?

# Time Reversal - Chain Rule

**Nelsons Relation – Semantics Clarification**

Looks slightly different to Song et al. 2020, why ?

Due to 2 equivalent ways of representing time reversals:

$$\mathrm{d}Y_t = f^{+}(Y_t, t)\mathrm{d}t + \sigma \mathrm{d}W_t$$

**Forward SDE (e.g. De Bortoli 2021)**

**- Travels forward in time**

$$\mathrm{d}\mathbf{X_t} = \mathbf{f}^{-}(\mathbf{X_t}, \mathbf{t})\mathrm{d}\mathbf{t} + \sigma \mathrm{d}\mathbf{W_t}$$

$$\mathbf{f}^{-}(\mathbf{x}, \mathbf{t}) + \mathbf{f}^{+}(\mathbf{x}, \mathbf{T} - \mathbf{t}) = \sigma^{\mathbf{2}} \nabla_{\mathbf{x}} \ln \mathbf{p}_{\mathbf{T}-\mathbf{t}}(\mathbf{x})$$

**- Flips / No longer the same joint**

$$\mathrm{Law}(\mathbf{x_t})_{\mathbf{t=0}}^{\mathbf{T}} = \mathrm{Law}(\mathbf{y}_{\mathbf{T}-\mathbf{t}})_{\mathbf{t=0}}^{\mathbf{T}}$$

**Backwards SDE (e.g. Song 2021)**

**- Travels Backwards in time**

$$\mathrm{d}\mathbf{X}_{\mathbf{t}}^{-} = \mathbf{f}^{-}(\mathbf{X}_{\mathbf{t}}^{-}, \mathbf{t})\mathrm{d}\mathbf{t} + \sigma \mathrm{d}\mathbf{W}_{\mathbf{t}}^{-}$$

$$\mathbf{f}^{-}(\mathbf{x}, \mathbf{t}) - \mathbf{f}^{+}(\mathbf{x}, \mathbf{t}) = \sigma^{\mathbf{2}} \nabla_{\mathbf{x}} \ln \mathbf{p_t}(\mathbf{x})$$

**- Encodes the same joint**

$$\mathrm{Law}(\mathbf{x_t})_{\mathbf{t=0}}^{\mathbf{T}} = \mathrm{Law}(\mathbf{y_t})_{\mathbf{t=0}}^{\mathbf{T}}$$

# Time Reversal – Generative Modelling

**Time reversing VP-SDE / OU Process [Song 2021, De Bortoli 2021]**

Consider the time homogenous VP-SDE (OU Process):

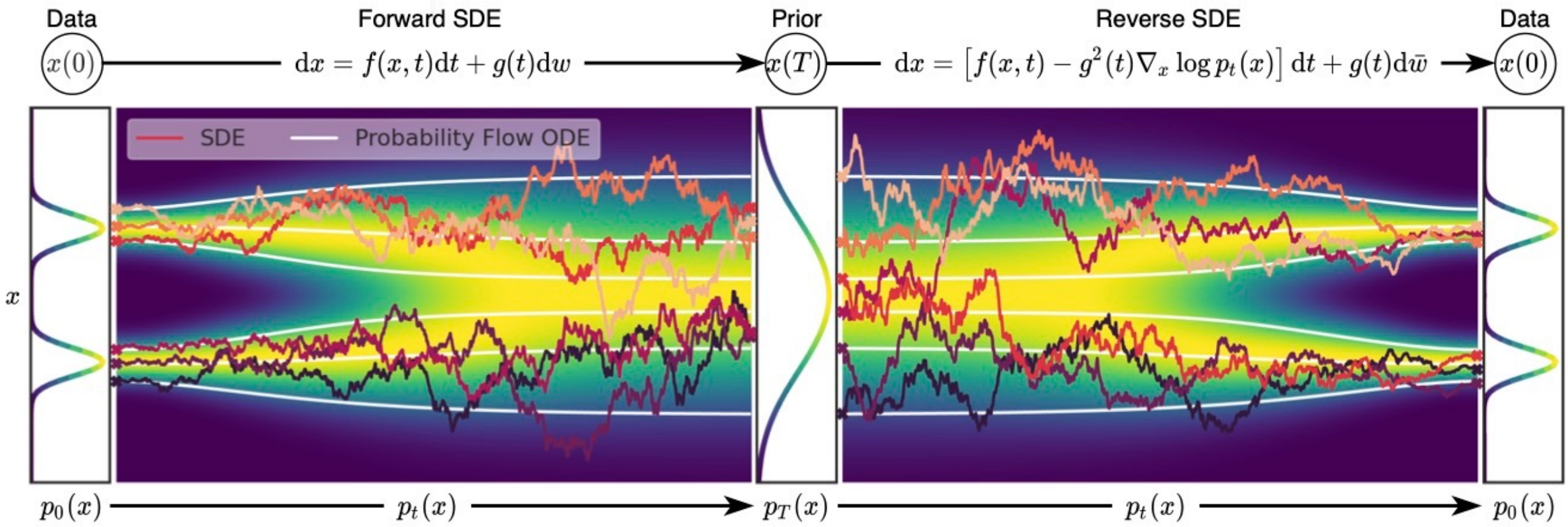
$$X_0 \sim p_{\text{data}}$$
$$\mathrm{d}X_t = -\beta X_t \mathrm{d}t + \sqrt{2\beta}\mathrm{d}W_t$$

Then its time reversal $(Y_t)_{t=0}^T \overset{d}{=} (X_{T-t})_{t=0}^T$ satisfies the score SDE [Song 2021]:

$$Y_0 \sim p_T \approx \mathcal{N}(0, I)$$
$$\mathrm{d}Y_t = \left(\alpha Y_t + 2\alpha \nabla_{Y_t} \ln p_{T-t}(Y_t)\right)\mathrm{d}t + \sqrt{2\alpha}\mathrm{d}B_t$$

Where $Y_T \sim p_{\text{data}}$ , thus we could instead sample approximately $Y_0 \sim \mathcal{N}(0, I)$ and have $\text{Law}Y_T \approx p_{\text{data}}$ following the mixing rate of the OU [De Bortoli 2021]

# Probability flow ODE



# Probability Flow ODE

Definition: Every stochastic process described by an SDE has a corresponding deterministic process described by an ODE that has the same marginal probability densities $\{\mathrm{p_t(x)}\}_{\mathrm{t=0}}^{\mathrm{T}}$. This process is called the *probability flow ODE*. For a general SDE of the form $\mathrm{dX_t} = \mu(\mathrm{X_t}, \mathrm{t})\mathrm{dt} + \sigma(\mathrm{X_t}, \mathrm{t})\mathrm{dW_t}$, the corresponding ODE is given by

$$\mathrm{dX_t} = \left[\mu(\mathrm{X_t}, \mathrm{t}) - \frac{1}{2}\nabla_{\mathrm{x}}[\sigma(\mathrm{X_t}, \mathrm{t})\sigma(\mathrm{X_t}, \mathrm{t})^{\mathrm{T}}] - \frac{1}{2}\sigma(\mathrm{X_t}, \mathrm{t})\sigma(\mathrm{X_t}, \mathrm{t})^{\mathrm{T}}\nabla_{\mathrm{x}}\log \mathrm{p_t(x)}\right]\mathrm{dt}$$

# Probability Flow ODE

$$\mathrm{d}\mathrm{X}_\mathrm{t} = \left[\mu(\mathrm{X}_\mathrm{t}, \mathrm{t}) - \frac{1}{2}\nabla_\mathrm{x}[\sigma(\mathrm{X}_\mathrm{t}, \mathrm{t})\sigma(\mathrm{X}_\mathrm{t}, \mathrm{t})^\mathrm{T}] - \frac{1}{2}\sigma(\mathrm{X}_\mathrm{t}, \mathrm{t})\sigma(\mathrm{X}_\mathrm{t}, \mathrm{t})^\mathrm{T}\nabla_\mathrm{x}\log \mathrm{p}_\mathrm{t}(\mathrm{x})\right]\mathrm{dt}$$

$$\mathrm{d}\mathrm{X}_\mathrm{t} = [\mu(\mathrm{X}_\mathrm{t}, \mathrm{t}) - \frac{1}{2}\sigma^2(\mathrm{t})\nabla_\mathrm{x}\log \mathrm{p}_\mathrm{t}(\mathrm{X}_\mathrm{t})]\mathrm{dt}$$

# Probability Flow ODE

FPE

$$\frac{\partial}{\partial t} p_t(x) = -\frac{\partial}{\partial x}[\mu(x,t)p_t(x)] + \frac{\partial}{\partial x}\frac{\partial}{\partial x}[\frac{1}{2}\sigma(x,t)\sigma(x,t)^T p_t(x)]$$

Product Rule

$$\frac{\partial}{\partial t} p_t(x) = -\frac{\partial}{\partial x}[\mu(x,t)p_t(x)] + \frac{1}{2}\frac{\partial}{\partial x}\left[\nabla_x[\sigma(x,t)\sigma(x,t)^T]p_t(x)\right] + \frac{1}{2}\frac{\partial}{\partial x}\left[\sigma(x,t)\sigma(x,t)^T \frac{\partial p_t(x)}{\partial x}\right]$$

Log Der. Trick

$$\frac{\partial}{\partial t} p_t(x) = -\frac{\partial}{\partial x}[\mu(x,t)p_t(x)] + \frac{1}{2}\frac{\partial}{\partial x}\left[\nabla_x[\sigma(x,t)\sigma(x,t)^T]p_t(x)\right] + \frac{1}{2}\frac{\partial}{\partial x}\left[\sigma(x,t)\sigma(x,t)^T p_t(x)\nabla_x \log p_t(x)\right]$$

# Probability Flow ODE

$$\frac{\partial}{\partial t} p_t(x) = -\frac{\partial}{\partial x}[\mu(x,t)p_t(x)] + \frac{1}{2}\frac{\partial}{\partial x}\left[\nabla_x[\sigma(x,t)\sigma(x,t)^T]p_t(x)\right] + \frac{1}{2}\frac{\partial}{\partial x}\left[\sigma(x,t)\sigma(x,t)^T p_t(x)\nabla_x \log p_t(x)\right]$$

Pull der. And p(x) out

$$\frac{\partial}{\partial t} p_t(x) = -\frac{\partial}{\partial x}\left[\mu(x,t) - \frac{1}{2}\nabla_x[\sigma(x,t)\sigma(x,t)^T] - \frac{1}{2}\sigma(x,t)\sigma(x,t)^T\nabla_x[\log p_t(x)]\right]$$

$$\frac{\partial}{\partial t} p_t(x) = -\frac{\partial}{\partial x}\tilde{\mu}(x,t)p_t(x)$$

# Generative Modelling

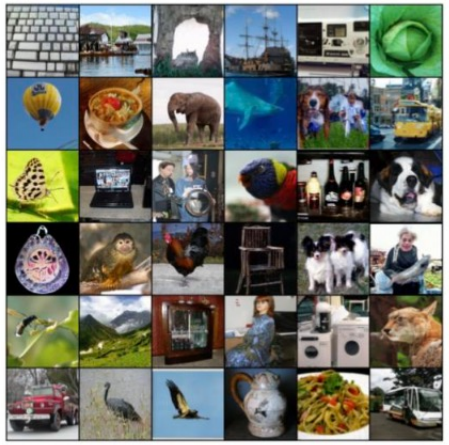
Given samples $x_1, \ldots, x_n$ with $x \sim p$

Infer $\hat{p}$ such that $\hat{p} \approx p$.

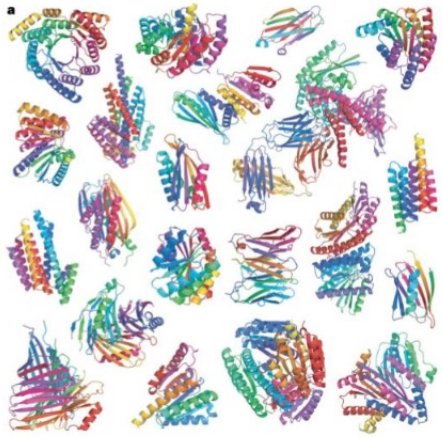
**Tasks**

Evaluate the likelihood of new data $\hat{p}(x)$

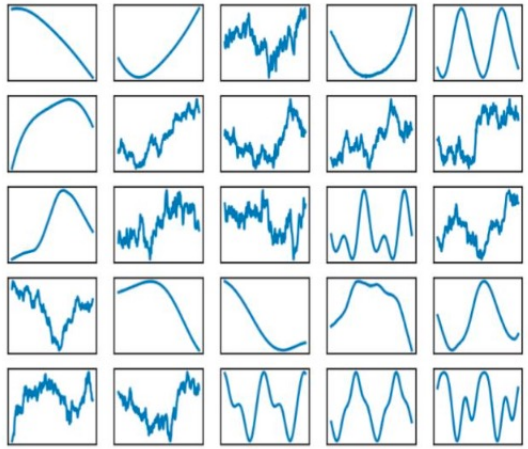
Sample $x \sim \hat{p}$



Images



Proteins



Functions

# Generative Modelling

$$\max_{\theta} \mathbb{E}_{\mathbf{x} \sim \mathbf{p}_{\text{data}}} \log \mathbf{p}_{\theta}(\mathbf{x})$$

# Generative Modelling

$$\max_{\theta} \mathbb{E}_{x \sim p_{data}} \log p_\theta(x)$$

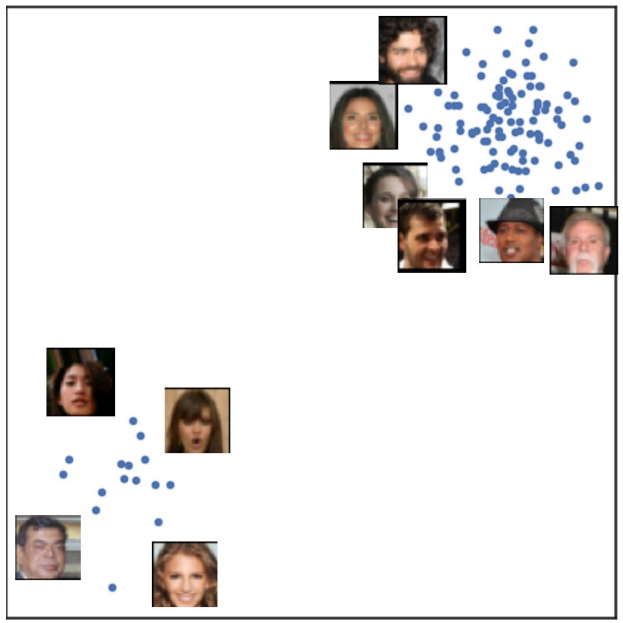
$$\begin{aligned} s_\theta(x) &= \nabla_x \log p_\theta(x) \\ &= \nabla_x \log \left(\frac{f_\theta(x)}{Z_\theta}\right) \\ &= \nabla_x \log f_\theta(x) - \underbrace{\nabla_x \log Z_\theta}_{=0} \\ &= \nabla_x \log f_\theta(x) \end{aligned}$$

# How to train and simulate?

$$\mathbb{E}_{p(\mathbf{x})}[\|\nabla_{\mathbf{x}} \log p(\mathbf{x}) - \mathbf{s}_\theta(\mathbf{x})\|_2^2]$$

$$\mathbb{E}_{p(\mathbf{x})}[\|\nabla_{\mathbf{x}} \log p(\mathbf{x}) - \mathbf{s}_\theta(\mathbf{x})\|_2^2] = \int p(\mathbf{x}) \|\nabla_{\mathbf{x}} \log p(\mathbf{x}) - \mathbf{s}_\theta(\mathbf{x})\|_2^2 \mathrm{d}\mathbf{x}.$$

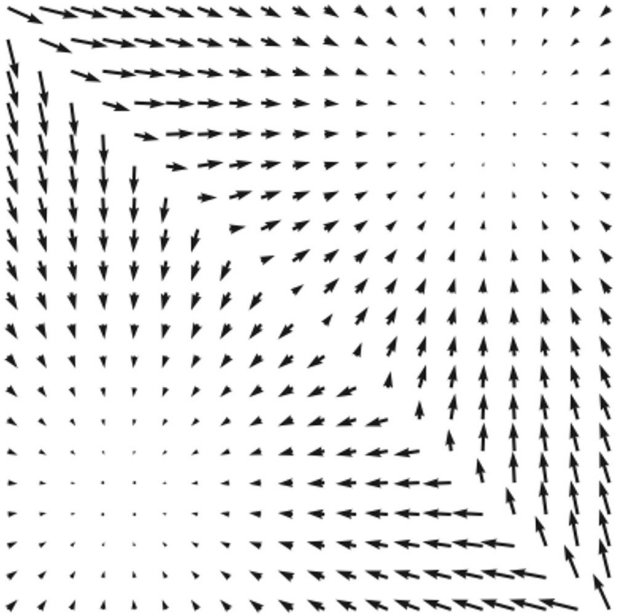
# Naïve Score Matching



Data samples

$$\{\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_N\} \overset{\text{i.i.d.}}{\sim} p(\mathbf{x})$$

score matching



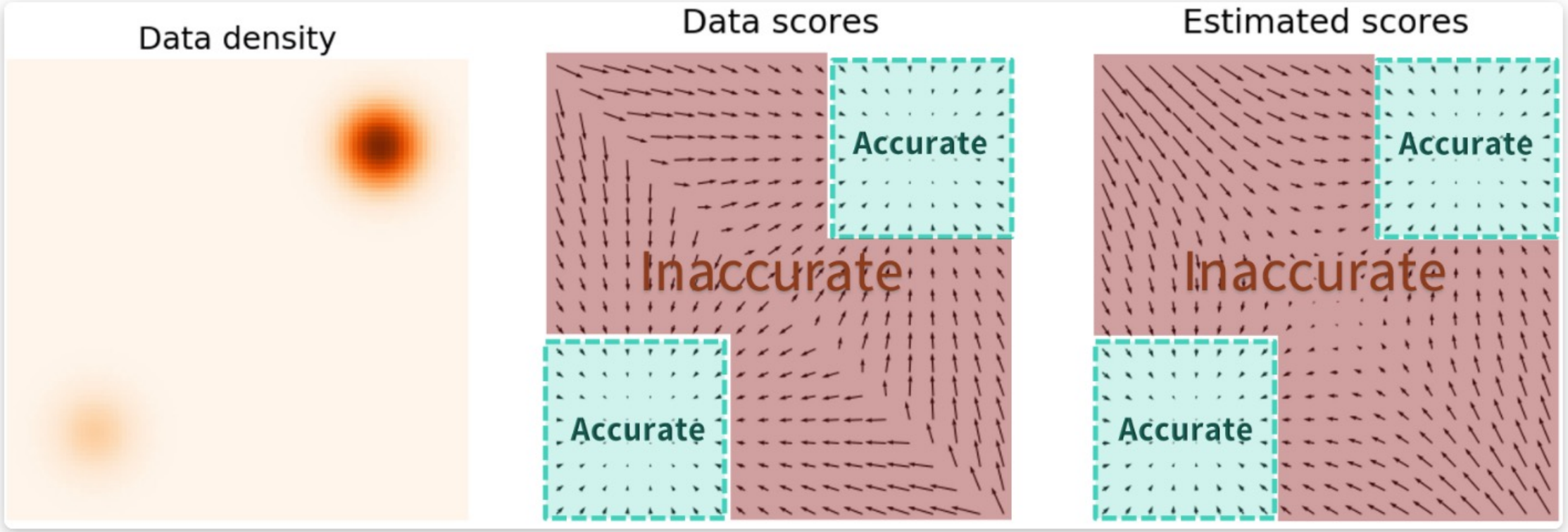
Scores

$$\mathbf{s}_\theta(\mathbf{x}) \approx \nabla_{\mathbf{x}} \log p(\mathbf{x})$$

Langevin dynamics

New samples

# Naïve Score Matching

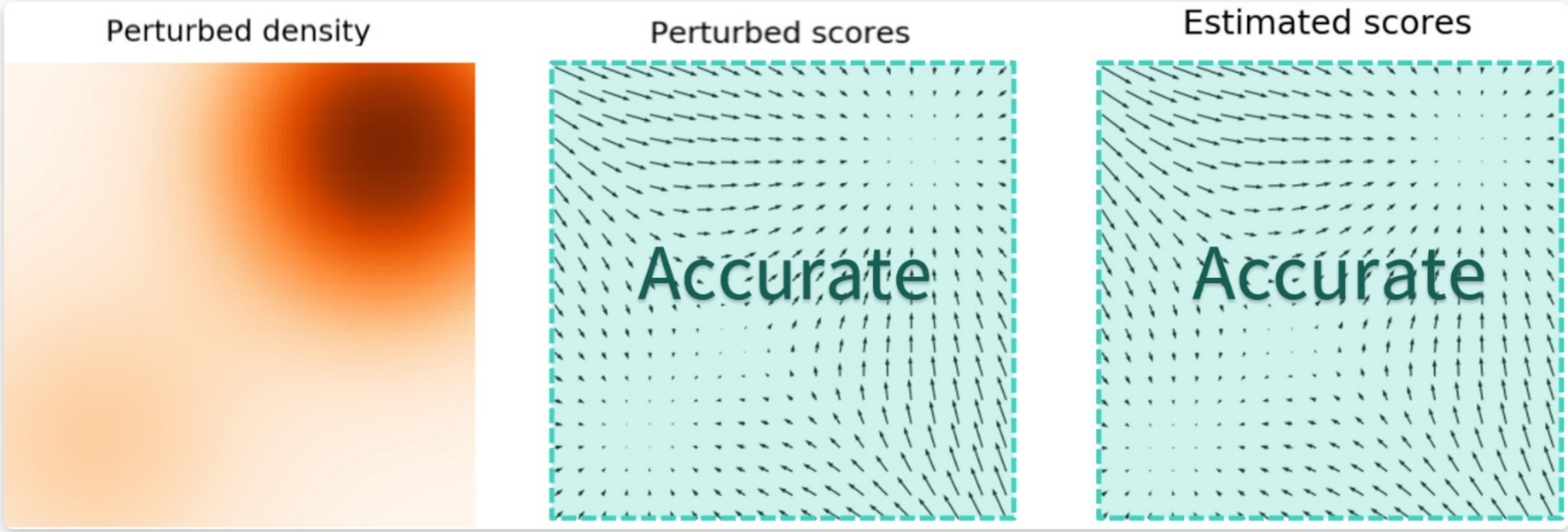


# How to train and simulate?

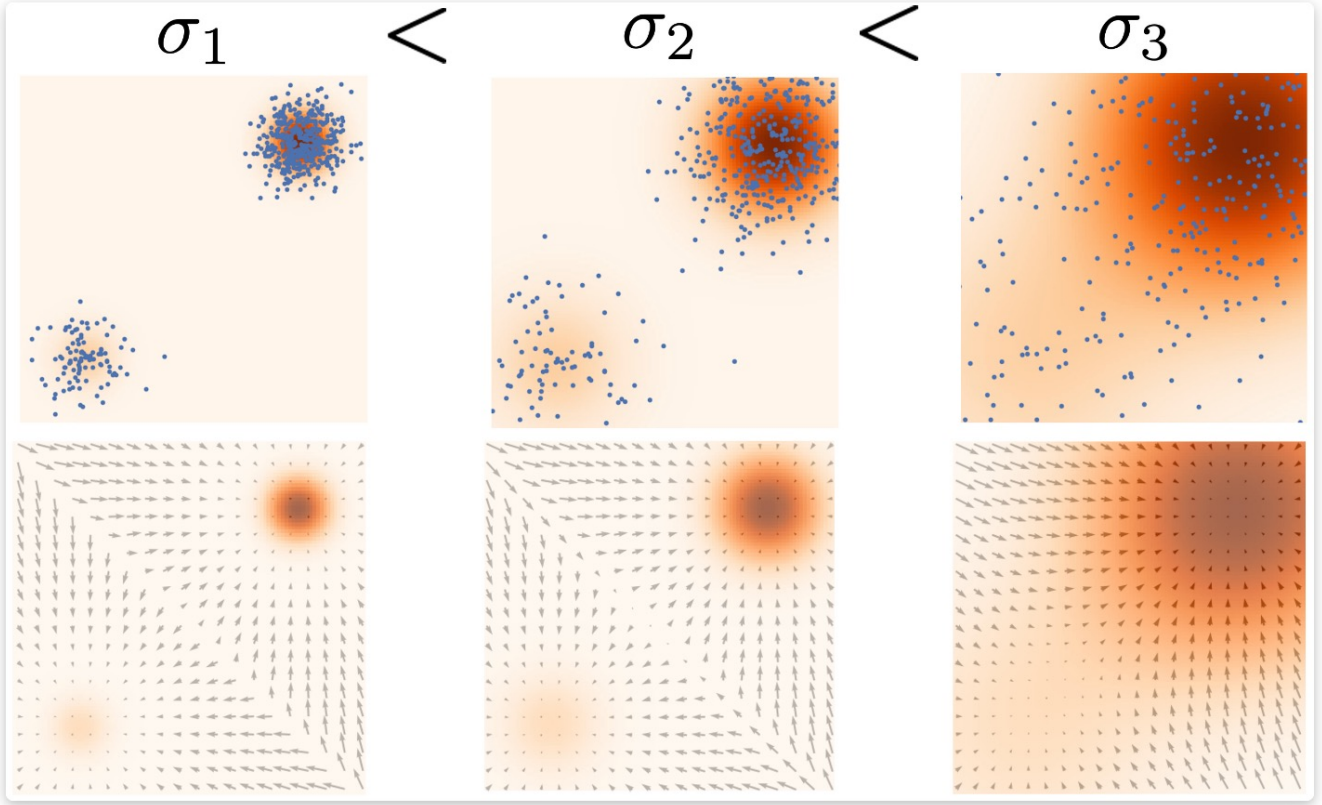
$$\mathbb{E}_{p(\mathbf{x})}[\|\nabla_{\mathbf{x}} \log p(\mathbf{x}) - \mathbf{s}_\theta(\mathbf{x})\|_2^2]$$

$$\mathbb{E}_{t\in\mathcal{U}(0,T)}\mathbb{E}_{p_t(\mathbf{x})}[\lambda(t)\|\nabla_{\mathbf{x}} \log p_t(\mathbf{x}) - \mathbf{s}_\theta(\mathbf{x}, t)\|_2^2],$$

# Denoising Score Matching



# Denoising Score Matching




We apply multiple scales of Gaussian noise to perturb the data distribution (**first row**), and jointly estimate the score functions for all of them (**second row**).

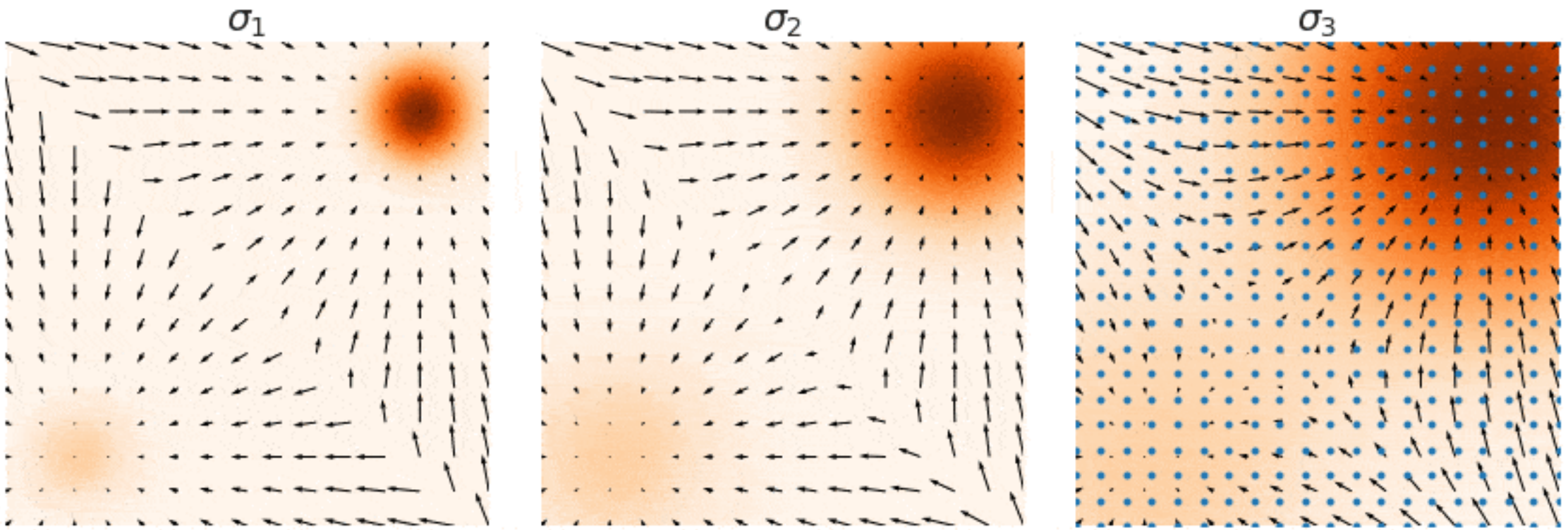
# How to train and simulate?

$$\mathbb{E}_{p(\mathbf{x})}[\|\nabla_{\mathbf{x}} \log p(\mathbf{x}) - \mathbf{s}_\theta(\mathbf{x})\|_2^2]$$

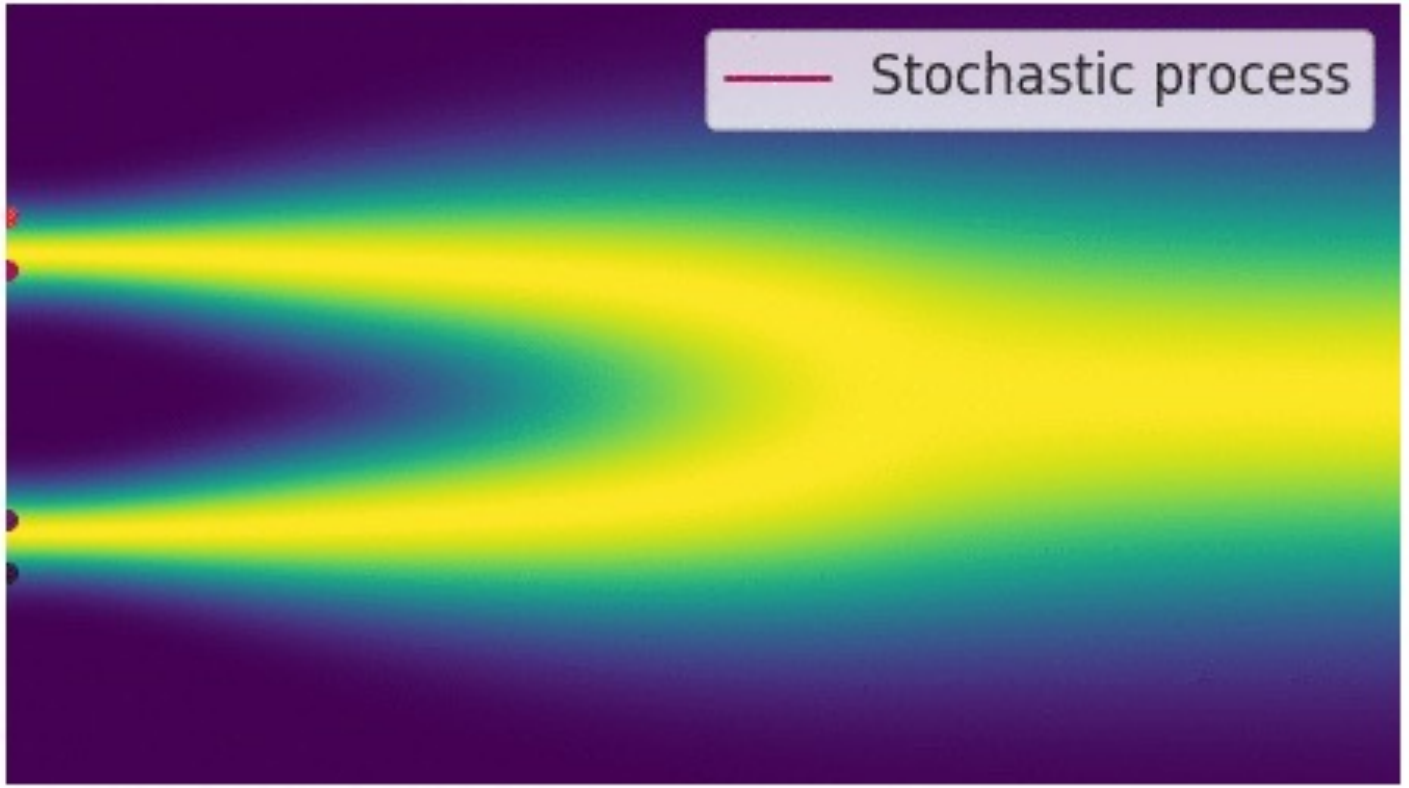
$$\mathbb{E}_{t\in\mathcal{U}(0,T)}\mathbb{E}_{p_t(\mathbf{x})}[\lambda(t)\|\nabla_{\mathbf{x}} \log p_t(\mathbf{x}) - \mathbf{s}_\theta(\mathbf{x}, t)\|_2^2],$$

$$\begin{aligned}
\Delta\mathbf{x} &\leftarrow [\mathbf{f}(\mathbf{x}, t) - g^2(t)\mathbf{s}_\theta(\mathbf{x}, t)]\Delta t + g(t)\sqrt{|\Delta t|}\mathbf{z}_t \\
\mathbf{x} &\leftarrow \mathbf{x} + \Delta\mathbf{x} \\
t &\leftarrow t + \Delta t,
\end{aligned}$$

# Denoising Score Matching



# Denoising Score Matching



# Conditional Flow Matching

**Diffusion Process**

$$d\mathbf{x}_t = f_t(\mathbf{x}_t)dt + g_t(\mathbf{x}_t)d\mathbf{w}$$

**Closed-form conditional probability**

$$p(\mathbf{x}_t \mid \mathbf{x}_0)$$

**Training**

$$\left\| s_\theta(\mathbf{x}_t) - \nabla \log p_t(\mathbf{x}_t \mid \mathbf{x}_0) \right\|^2$$

**Sampling**

$$\dot{\mathbf{x}}_t = f_t(\mathbf{x}_t) - \frac{1}{2} g_t^2 s_\theta(\mathbf{x}_t)$$

# Key Equations for Score-based Modelling

"Forward" SDE

$$\mathrm{d}\overrightarrow{x}_t = f(\overrightarrow{x}_t, t)\,\mathrm{d}t + g(t)\,\mathrm{d}W \quad \text{with} \quad \overrightarrow{x}_0 \sim p_1$$

"Reverse" SDE

$$\mathrm{d}\overleftarrow{x}_t = \left(f(\overleftarrow{x}_t, t) - g(t)^2 \nabla \log p_t(\overleftarrow{x}_t)\right)\mathrm{d}t + g(t)\,\mathrm{d}W \quad \text{with} \quad \overleftarrow{x}_0 \sim p_0$$

Probability flow ODE

$$\mathrm{d}x_t = \left[f(x_t, t) - \frac{1}{2} g(t)^2 \nabla \log p_t(x_t)\right]\mathrm{d}t \quad \text{with} \quad x_0 \sim p_0$$

# Score-based generative modelling

*Training:* learn score $s_t(x) := \nabla \log p_t(x)$ by

1. Sample from target $x_1 \sim p_1$
2. Run "forward" SDE to "noise" $x_1$ until it becomes "simple" $x_0 \sim p_0$
3. Minimize some loss $\propto \left\| \hat{s}_t(x) - s_t(x) \right\|^2$

*Inference:* sample using "reverse" SDE or prob-flow ODE

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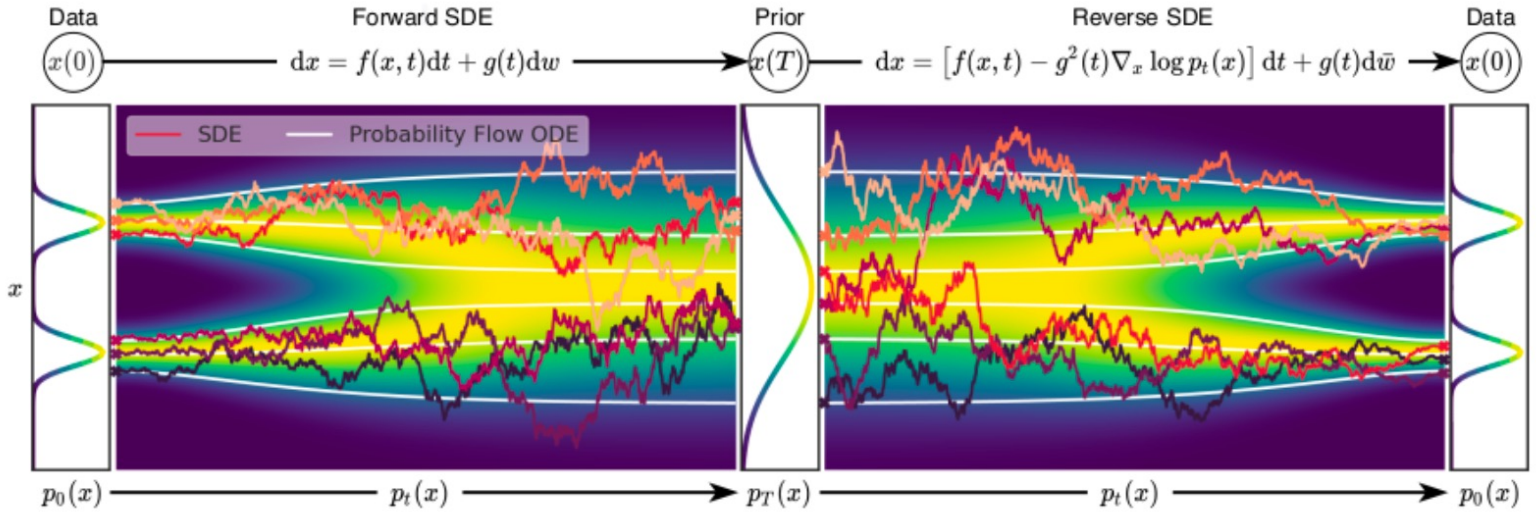


Figure 2 from Song et al. (2020)

# Conditional Flow Matching

**Diffusion Process**

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**Closed-form conditional probability**

$$p(\mathbf{x}_t \mid \mathbf{x}_0)$$

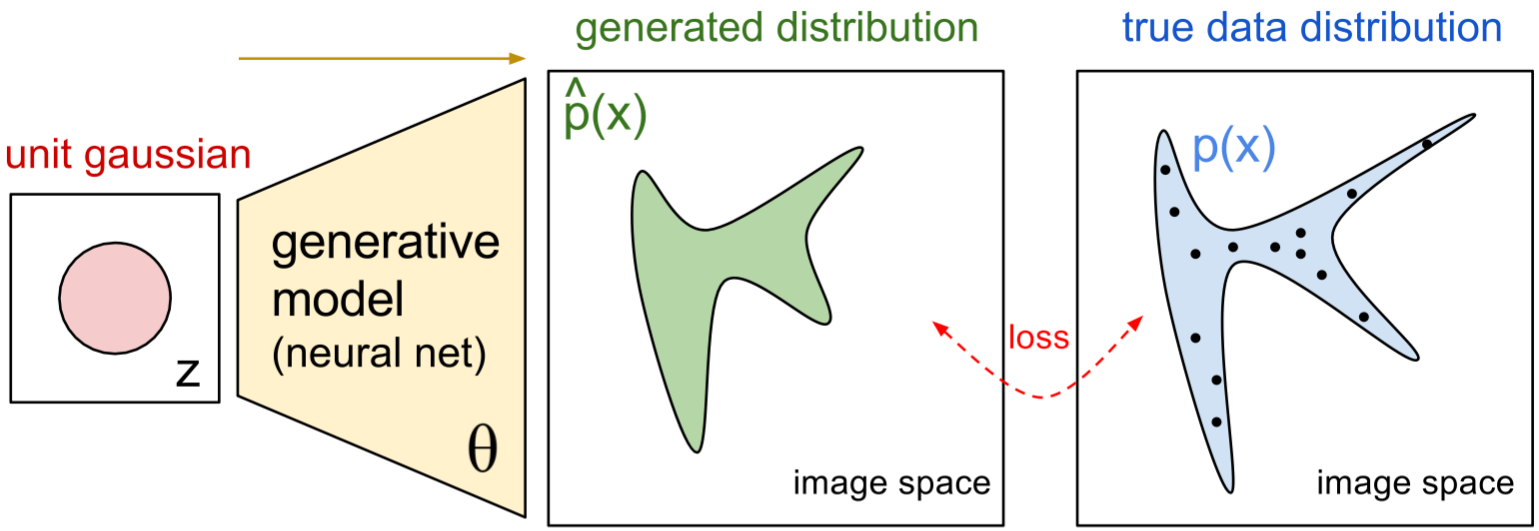
**Training**

$$\left\| s_\theta(\mathbf{x}_t) - \nabla \log p_t(\mathbf{x}_t \mid \mathbf{x}_0) \right\|^2$$

**Sampling**

$$\dot{\mathbf{x}}_t = f_t(\mathbf{x}_t) - \frac{1}{2} g_t^2 s_\theta(\mathbf{x}_t)$$

# Normalising Flows




Let $p_0$ be a simple distribution on $\mathbb{R}^d$ and $\phi : \mathbb{R}^d \to \mathbb{R}^d$ a transformation (diffeomorphism).

Let $p_1$ be the distribution of moving the samples of $p_0$ along $x_1 = \phi(x_0)$.

$$p_1(x_1) = p_0(x_0) \left| \frac{\partial \phi}{\partial x_0}(x_0) \right|^{-1}, \quad \text{where} \quad x_0 = \phi^{-1}(x_1)$$

# Normalising Flows

Parameterise the transformation by a deep neural network $\hat{\phi}$.

Maximum log likelihood objective:

$$\mathbb{E}_{x\sim\mathcal{D}}\left[\log p_1(x)\right] = \mathbb{E}\left[\log p_0(x_0) - \log\left|\frac{\partial\hat{\phi}}{\partial x_0}(x_0)\right|\right], \quad \text{where} \quad x_0 = \hat{\phi}^{-1}(x)$$

**Challenges** Requires computation of inverse $\phi^{-1}$ and the determinant of Jacobian $\left|\frac{\partial\phi}{\partial z}\right|$

# Continuous Normalising Flows (CNFs)

Use multiple 'residual' transformations

$$x = (u_N \circ u_{N-1} \ldots \circ u_1)(x_0).$$

For $N \to \infty$, the flow $\phi_t$ describes the position of a starting point $x_0$ along the vector field $u_t$, defined via an ODE

$$\frac{\mathrm{d}x_t}{\mathrm{d}t} = u_t(x_t),$$

where $x_t = \phi_t(x_0)$ and $u_t : \mathbb{R}^d \to \mathbb{R}^d$ is the tangent field of the flow.

The transformation is then the solution to

$$x \triangleq \phi_1(x_0) = x_0 + \int_0^1 u_t(x_t)\mathrm{d}t.$$

# Continuous change-in-variables

Fokker–Planck equation without the diffusion term:

$$\log p_t(x) = \log p_0(x_0) - \int_0^t (\nabla \cdot u_t)(x_t) \mathrm{d}t$$

Maximum likelihood training of Continuous Normalising Flows require:

- expensive numerical ODE simulations
- estimators for the divergence.

# Flow Matching

Integral-free approach to training CNF models

Supervised regression objective

Let $u_t$ be a vector field that generates $p_t$, then we parameterise a neural net $\hat{u} : \mathbb{R}_+ \times \mathbb{R}^{\mathbb{d}} \to \mathbb{R}^{\mathbb{d}}$ and want to learn it using

$$\mathcal{L} = \mathbb{E}_{t, p_t(x)} \left[ \| \hat{u}(t, x) - u_t(x) \|^2 \right]$$

**Challenges:**

How do we ensure $p_1 \approx p$

What should $p_0$ be?

What is $u_t$?

# Many names – same idea

## FLOW MATCHING FOR GENERATIVE MODELING

**Yaron Lipman**[1,2] **Ricky T. Q. Chen**[1] **Heli Ben-Hamu**[2] **Maximilian Nickel**[1] **Matt Le**[1]
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## BUILDING NORMALIZING FLOWS WITH STOCHASTIC INTERPOLANTS

**Michael S. Albergo**
Center for Cosmology and Particle Physics
New York University
New York, NY 10003, USA
albergo@nyu.edu

**Eric Vanden-Eijnden**
Courant Institute of Mathematical Sciences
New York University
New York, NY 10012, USA
eve2@cims.nyu.edu

# Many names – same idea

## FLOW MATCHING

**Yaron Lipman**[1,2] **Ricky T. Q.**
[1]Meta AI (FAIR) [2]Weizmann I

## BUILDING NORMA INTERPOLANTS

**Michael S. Albergo**
Center for Cosmology and Particle Physics
New York University
New York, NY 10003, USA
albergo@nyu.edu

## Flow Straight and Fast:
## Learning to Generate and Transfer Data with Rectified Flow

Xingchao Liu*
University of Texas at Austin
xcliu@utexas.edu

Chengyue Gong*
University of Texas at Austin
cygong@cs.utexas.edu

Qiang Liu
University of Texas at Austin
lqiang@cs.utexas.edu

**Eric Vanden-Eijnden**
Courant Institute of Mathematical Sciences
New York University
New York, NY 10012, USA
eve2@cims.nyu.edu

# Many names – same idea

## FLOW MATCHING

**Yaron Lipman**[1,2] **Ricky T. Q.**
[1]Meta AI (FAIR) [2]Weizmann I

## BUILDING NORMA INTERPOLANTS

**Michael S. Albergo**
Center for Cosmology and Particle Ph
New York University
New York, NY 10003, USA
albergo@nyu.edu

## Flow Straight and Fast:
## Learning to Generate and Transfer Data with Rectified Flow

Xingchao Liu*
University of Texas at Austin
xcliu@utexas.edu

Chengyue Gong*
University of Texas at Austin
cygong@cs.utexas.edu

Qiang Liu
University of Texas at Austin
lqiang@cs.utexas.edu

## Action Matching:
## Learning Stochastic Dynamics from Samples

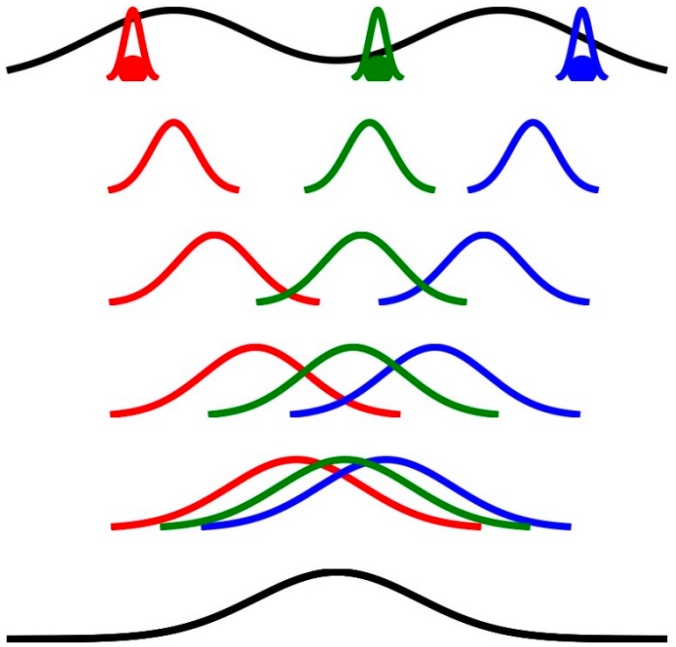
**Kirill Neklyudov** [1] **Rob Brekelmans** [1] **Daniel Severo** [1 2] **Alireza Makhzani** [1 2]

# Conditional Flow Matching

**Target probability path:** as mixture of simpler probability paths
$p_t = \int p_t(\cdot|x_1)p(x_1)\mathrm{d}x_1$

**Conditional probability path** $p_t(\cdot|x_1)$ s.t. $p_1(\cdot|x_1) = \delta_{x_1}$ and $p_0(\cdot|x_1) = p_0$

**Recover data distribution**
$p_1(x) = \int p_1(x|x_1)q(x_1)\mathrm{d}x_1 = \int \delta_{x_1}(x)q(x_1)\mathrm{d}x_1 = q_1(x)$

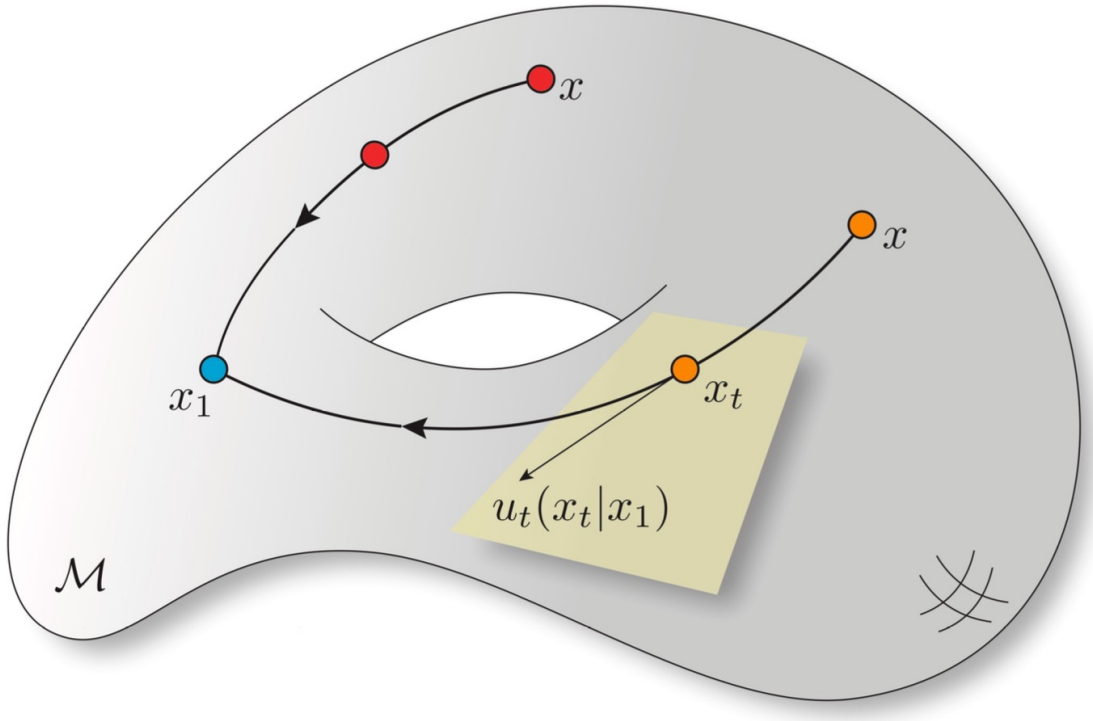


# Conditional Flows

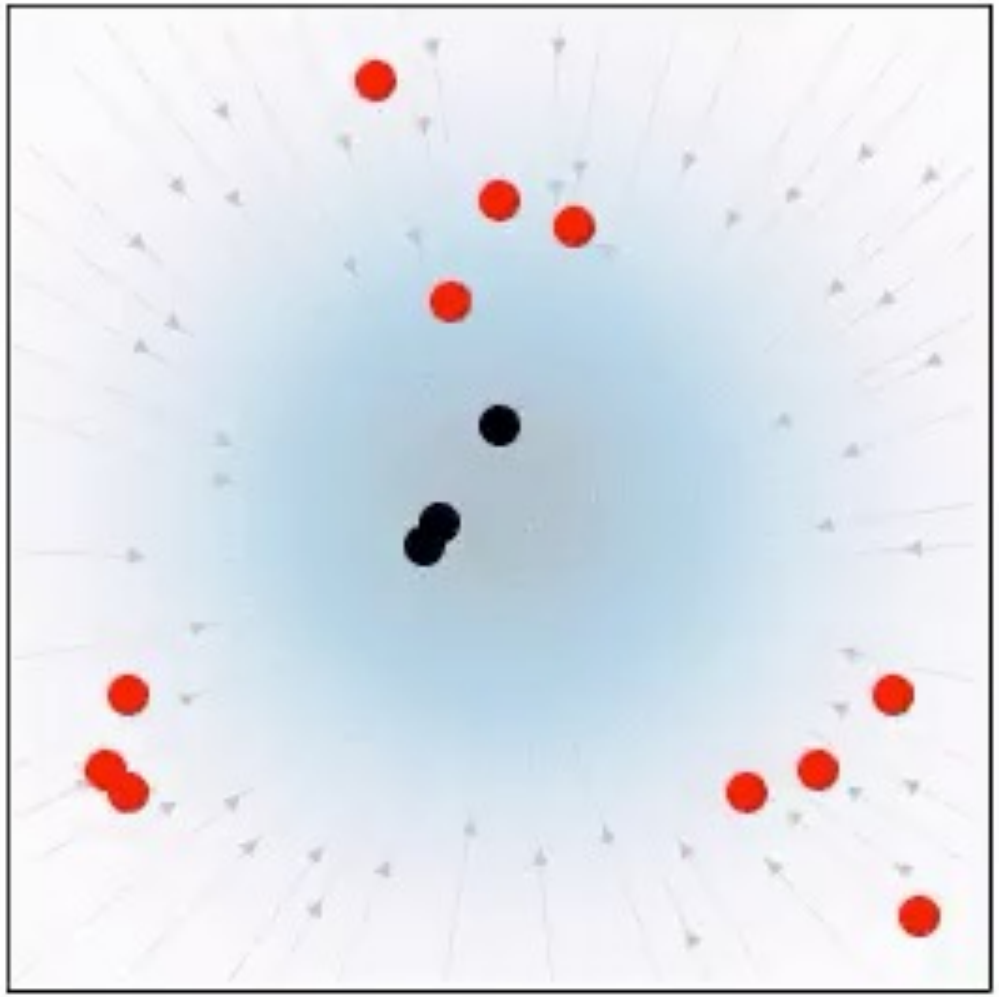
**Conditional vector field** $u_t(\cdot|x_1)$ inducing conditional probability path $p_t(\cdot|x_1)$

**Marginal vector field** $u_t$ via *marginalising* over the *conditional* vector field $u_t(\cdot|x_1)$

$$u_t(x) = \int u_t(x|x_1)p_t(x_1|x)dx_1 = \int u_t(x|x_1)\frac{p_t(x|x_1)q(x_1)}{p_t(x)}dx_1 = \mathbb{E}_{x_0,x_t\sim q_1 p_{t|1}}[u_t(x_t|x_1)]$$



# Conditional Flows



# (Conditional) Flow Matching: Training

**(Exact) flow matching**: $\mathcal{L}_{\mathrm{FM}}(\theta) = \mathbb{E}_{t x_t \sim \mathcal{U}[0,1] p_t}[\|u_\theta(t, x_t) - u_t(x_t)\|^2]$ with $u_t(x) = \mathbb{E}_{x_0, x_t \sim q_1 p_{t|1}}[u_t(x_t|x_1)]$

Akin to score matching, one can actually move the expectation outside the $\ell^2$ norm

**Conditional flow matching**:
$\mathcal{L}_{\mathrm{CFM}}(\theta) = \mathbb{E}_{t, x_0, x_t \sim \mathcal{U}[0,1] q_1 p_{t|1}}[\|u_\theta(t, x_t) - u_t(x_t|x_1)\|^2]$

$\nabla_\theta \mathcal{L}_{\mathrm{FM}}(\theta) = \nabla_\theta \mathcal{L}_{\mathrm{CFM}}(\theta)$

Sampling $x_t$ and evaluating $u(x_t|x_1)$ is available in closed form.

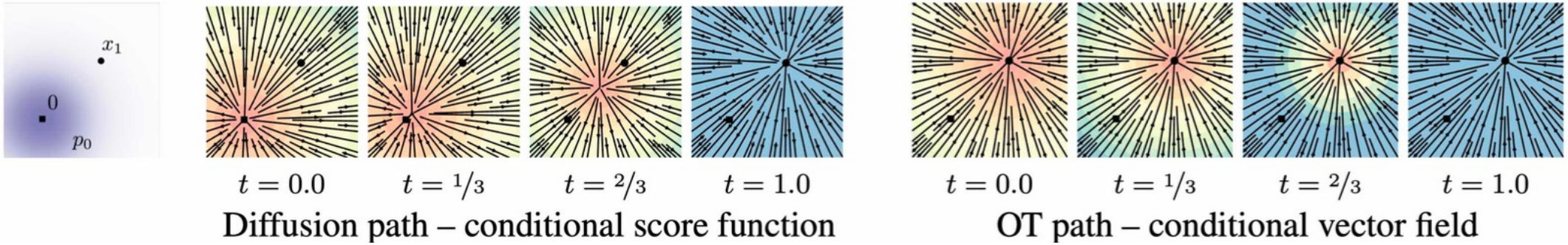
# Gaussian Probability Paths

**Conditional Probability path**: $p_t(x|x_1) = \mathrm{N}(\mu_t(x_1), \sigma_t(x_1)^2\mathrm{I})$

**Conditional vector field**: $u_t(x|x_1) = \frac{\sigma_t'(x_1)}{\sigma_t(x_1)}(x - \mu_t(x_1)) + \mu_t'(x_1)$

**Example: Linear interpolation**

- $\mu_t \triangleq tx_1$ and $\sigma_t \triangleq 1 - t \Rightarrow p_t(x|x_1) = \mathrm{N}(x|tx_1, (1-t)^2)$
- $u_t(x|x_1) = \frac{1}{1-t}(x_1 - x)$



# Flow Matching vs. Diffusion

**Algorithm 1:** Flow Matching training.

**Input** : dataset $q$, noise $p$
Initialize $v^\theta$
**while** *not converged* **do**
  $t \sim \mathcal{U}([0,1])$ ▷ sample time
  $x_1 \sim q(x_1)$ ▷ sample data
  $x_0 \sim p(x_0)$ ▷ sample noise
  $x_t = \Psi_t(x_0|x_1)$ ▷ conditional flow
  Gradient step with $\nabla_\theta \|v_t^\theta(x_t) - \dot{x}_t\|^2$
**Output:** $v^\theta$

**Algorithm 2:** Diffusion training.

**Input** : dataset $q$, noise $p$
Initialize $s^\theta$
**while** *not converged* **do**
  $t \sim \mathcal{U}([0,1])$ ▷ sample time
  $x_1 \sim q(x_1)$ ▷ sample data
  $x_t = p_t(x_t|x_1)$ ▷ sample conditional prob
  Gradient step with
  $\nabla_\theta \|s_t^\theta(x_t) - \nabla_{x_t} \log p_t(x_t|x_1)\|^2$
**Output:** $v^\theta$

$p_t(x_t \mid x_1)$ general
$p(x_0)$ is general

$p_t(x_t \mid x_1)$ closed-form from of SDE $dx_t = f_t dt + g_t dw$

- *Variance Exploding*: $p_t(x \mid x_1) = \mathcal{N}(x \mid x_1, \sigma_{1-t}^2 I)$
- *Variance Preserving*: $p_t(x \mid x_1) = \mathcal{N}(x \mid \alpha_{1-t} x_1, (1 - \alpha_{1-t}^2) I)$

$$\alpha_t = e^{-\frac{1}{2}T(t)}$$

$p(x_0)$ is Gaussian
$p_0(\cdot \mid x_1) \approx p$

# Conditional Flow Matching

## "So, what's the difference between FMs and SBDMs?"

| | Learn | ODE inference | SDE inference | Exact endpoints |
|---|---|---|---|---|
| FM | $u(t, x)$ | ✓ | ×[1] | ✓ |
| SBDM | $s(t, x)$ | ✓ | ✓ | ×[2] |

Which is "better"? 🤦

Note: unclear whether "exact endpoint" and "normalisable guarantee" matters in practice

# Score-based modelling

**Diffusion Process**

$$d\mathbf{x}_t = f_t(\mathbf{x}_t)dt + g_t(\mathbf{x}_t)d\mathbf{w}$$

**Closed-form conditional probability**

$$p(\mathbf{x}_t \mid \mathbf{x}_0)$$

**Training**

$$\left\| s_\theta(\mathbf{x}_t) - \nabla \log p_t(\mathbf{x}_t \mid \mathbf{x}_0) \right\|^2$$

**Sampling**

$$\dot{\mathbf{x}}_t = f_t(\mathbf{x}_t) - \frac{1}{2} g_t^2 s_\theta(\mathbf{x}_t)$$

# Conditional Flow Matching

**General conditional probability path**

$$p(\mathbf{x}_t \mid \mathbf{x}_0) = \mathcal{N}(\mu_t(\mathbf{x}_0), \sigma_t^2(\mathbf{x}_0) I)$$

**Training**

$$\left\| v_\theta(\mathbf{x}_t) - u_t(\mathbf{x}_t \mid \mathbf{x}_0) \right\|^2$$

**Sampling**

$$\dot{\mathbf{x}}_t = v_\theta(\mathbf{x}_t)$$