Flow and Diffusion Models

Lecture 04

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Roadmap

1. Flow models: ODEs, flows, simulation, sampling algorithm
2. Diffusion models: SDEs, Brownian motion, Euler–Maruyama, sampling algorithm
3. Constructing training targets: probability paths, continuity / Fokker–Planck

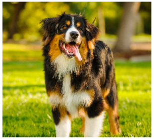
Flow and Diffusion Models

Turn noise into data

Initial distribution: p_{init} **Default:** $p_{\text{init}} = \mathcal{N}(0, I_d)$

A generative model converts samples from a initial distribution (e.g. Gaussian) into samples from the data distribution:

$x \sim p_{\text{init}}$ → Generative Model → $z \sim p_{\text{data}}$



Generative modeling viewpoint

Sampling goal:

$$X_1 \sim p_{\text{data}} \quad \text{by transforming} \quad X_0 \sim p_{\text{init}} \;\; (\text{e.g. } \mathcal{N}(0, I_d)).$$

Key idea: obtain the transformation by simulating

- an **ODE** (flow models), or
- an **SDE** (diffusion models).

ODEs and vector fields

A trajectory is a map

$$X : [0, 1] \to \mathbb{R}^d, \qquad t \mapsto X_t.$$

A (time-dependent) vector field:

$$u : \mathbb{R}^d \times [0, 1] \to \mathbb{R}^d, \qquad (x, t) \mapsto u_t(x).$$

ODE with initial condition:

$$\frac{d}{dt} X_t = u_t(X_t), \qquad X_0 = x_0.$$

Flows

The *flow* map answers: where do we go starting from x_0?

$$\phi : \mathbb{R}^d \times [0,1] \to \mathbb{R}^d, \qquad (x_0, t) \mapsto \phi_t(x_0),$$

defined by

$$\frac{d}{dt}\phi_t(x_0) = u_t(\phi_t(x_0)), \qquad \phi_0(x_0) = x_0.$$

Trajectory recovery: $X_t = \phi_t(X_0)$.

Existence and uniqueness

Theorem (Flow existence and uniqueness, Picard–Lindelöf Theorem)

If $u_t : \mathbb{R}^d \to \mathbb{R}^d$ is continuously differentiable with bounded derivative, then the ODE has a unique solution given by a flow ϕ_t. Moreover, ϕ_t is a diffeomorphism for all t. More generally, this is true if the vector field is Lipschitz.

Remark

Key takeaway: In the cases of practical interest for machine learning, unique solutions to ODE/flows exist.

Example (Linear vector fields)

Let $u_t(x) = -\theta x$ with $\theta > 0$, and the ODE be given:

$$\frac{d}{dt}\phi_t(x_0) = u_t(\phi_t(x_0)), \qquad \phi_0(x_0) = x_0.$$

Then the flow is given by:

$$\phi_t(x_0) = e^{-\theta t}\, x_0.$$

Simulating an ODE: Euler method

If ϕ_t is not available in closed form, simulate:

$$X_{t+h} = X_t + h\, u_t(X_t), \qquad t = 0, h, 2h, \ldots, 1-h, \qquad h = \frac{1}{n}.$$

(Heun's method is a simple higher-order alternative.)

Key Idea

A *flow model* uses a neural vector field:

$$X_0 \sim p_{\text{init}}, \qquad \frac{d}{dt} X_t = u_t^\theta(X_t), \qquad u^\theta : \mathbb{R}^d \times [0,1] \to \mathbb{R}^d.$$

Training goal (later): choose θ so that

$$X_1 \sim p_{\text{data}}.$$

Sampling from a flow model with Euler method

Algorithm 1: Sampling from a flow model with Euler method.

Input: Neural network vector field u_t^θ, number of steps n

Set $t = 0$;

Set step size $h = \frac{1}{n}$;

Draw a sample $X_0 \sim p_{\text{init}}$;

for $i = 1, \ldots, n$ **do**

  $X_{t+h} \leftarrow X_t + h\, u_t^\theta(X_t)$;

  Update $t \leftarrow t + h$;

return X_1;

A toy example

Toy example

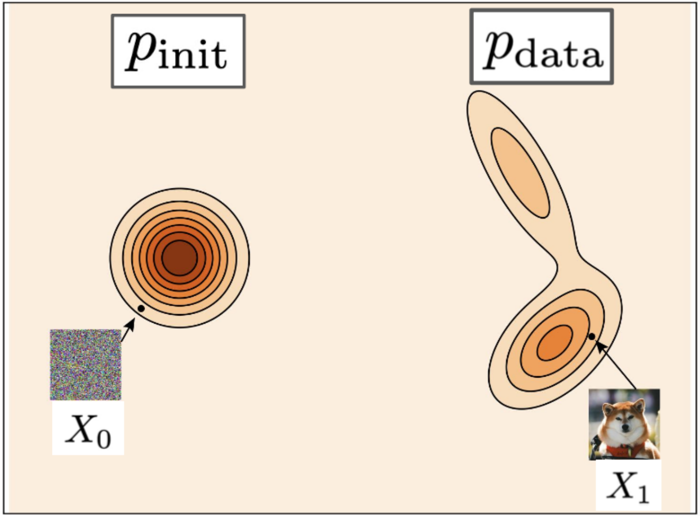


Figure credit:
Yaron Lipman

SDEs and stochastic trajectories

An SDE produces a stochastic process $(X_t)_{0\leq t\leq 1}$:

$$X_t \text{ is random for each } t.$$

Different simulations yield different sample paths.

Brownian motion

A Brownian motion W_t satisfies:

- $W_0 = 0$ and paths are continuous;
- **Normal increments:** $W_t - W_s \sim \mathcal{N}\big(0, (t-s)I_d\big)$;
- **Independent increments.**

Discrete simulation ($h = 1/n$):

$$W_{t+h} = W_t + \sqrt{h}\,\varepsilon_t, \qquad \varepsilon_t \sim \mathcal{N}(0, I_d).$$

From ODEs to SDEs

Heuristic increment form:

$$X_{t+h} = X_t + h\, u_t(X_t) + \sigma_t \big(W_{t+h} - W_t\big) + hR_t(h).$$

Symbolic SDE notation:

$$dX_t = u_t(X_t)\, dt + \sigma_t\, dW_t, \qquad X_0 = x_0.$$

SDE existence and uniqueness

Theorem (SDE solution existence and uniqueness)

If u_t is continuously differentiable with bounded derivative and σ_t is continuous, then

$$dX_t = u_t(X_t)\,dt + \sigma_t\,dW_t, \qquad X_0 = x_0$$

has a unique solution process $(X_t)_{0 \le t \le 1}$.

Remark

Key takeaway: In the cases of practical interest for machine learning, unique solutions to SDEs exist.

Example: Ornstein–Uhlenbeck

Example (Ornstein–Uhlenbeck process)

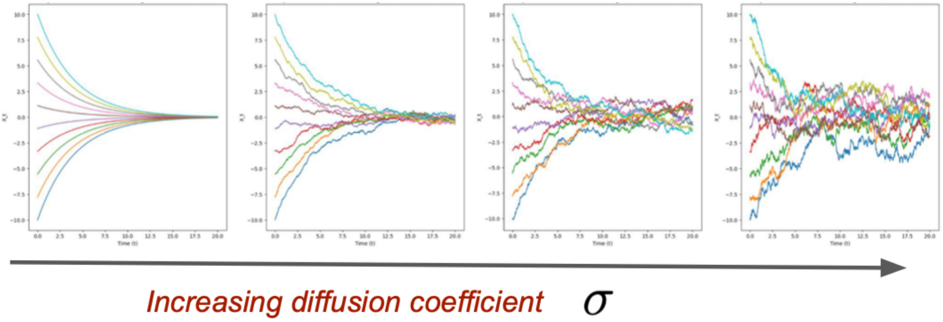
For $\theta > 0$ and constant $\sigma \geq 0$:

$$dX_t = -\theta X_t \, dt + \sigma \, dW_t.$$

Drift pulls toward 0; diffusion injects noise. For $\sigma = 0$, recovers the deterministic linear flow.

Ornstein–Uhlenbeck Processes: Sample Paths

$$\mathrm{d}X_t = -\theta X_t \mathrm{d}t + \sigma dW_t$$



Simulating an SDE: Euler–Maruyama

Euler–Maruyama update ($h = 1/n$):

$$X_{t+h} = X_t + h\, u_t(X_t) + \sigma_t \sqrt{h}\, \varepsilon_t, \qquad \varepsilon_t \sim \mathcal{N}(0, I_d).$$

Key Idea

A *diffusion model*:

$$X_0 \sim p_{\text{init}}, \qquad dX_t = u_t^\theta(X_t)\, dt + \sigma_t\, dW_t,$$

where u_t^θ is neural and σ_t is a fixed schedule. Goal: $X_1 \sim p_{\text{data}}$ after training.

Sampling from a diffusion model with Euler–Maruyama method

Algorithm 2: Sampling from a Diffusion Model with Euler–Maruyama method.

Input: Neural network u_t^θ, number of steps n, diffusion coefficient σ_t

Set $t = 0$;

Set step size $h = \frac{1}{n}$;

Draw a sample $X_0 \sim p_{\mathrm{init}}$;

for $i = 1, \ldots, n$ **do**

  Draw a sample $\varepsilon \sim \mathcal{N}(0, I_d)$;

  $X_{t+h} \leftarrow X_t + h\, u_t^\theta(X_t) + \sigma_t \sqrt{h}\, \varepsilon$;

  Update $t \leftarrow t + h$;

return X_1;

SDE generative model summary

Summary (Diffusion vs. flow)

A diffusion model consists of:

$$u^\theta : \mathbb{R}^d \times [0,1] \to \mathbb{R}^d, \qquad \sigma : [0,1] \to [0,\infty).$$

Sampling:

- $X_0 \sim p_{\text{init}}$
- simulate $dX_t = u_t^\theta(X_t)\, dt + \sigma_t\, dW_t$
- hope (after training) $X_1 \sim p_{\text{data}}$

If $\sigma_t \equiv 0$, the diffusion model reduces to a flow model.

Constructing the Training Target

Summary: Flow and Diffusion

Flow Model

Initialize: $X_0 \sim p_{\text{init}},$

ODE: $\mathrm{d}X_t = u_t^\theta(X_t)\mathrm{d}t$

E.g. Gaussian

Neural network vector field

Diffusion coeff.

Diffusion Model

Initialize: $X_0 \sim p_{\text{init}},$

SDE: $\mathrm{d}X_t = u_t^\theta(X_t)\mathrm{d}t + \sigma_t \mathrm{d}W_t$

To get samples, simulate ODE/SDE from t=0 to t=1 and return X_1

Next step: Training the model

With random θ, simulating gives "non-sense".

Therefore we need to train u_t^θ such that

$$\underbrace{X_0 \sim p_{\text{init}}}_{\substack{\text{start with initial}\\ \text{initial distribution}}}, \qquad \underbrace{\frac{d}{dt}X_t = u_t^\theta(X_t)}_{\substack{\text{follow along}\\ \text{the vector field } u_t^\theta}} \quad \Longrightarrow \quad \underbrace{X_1 \sim p_{\text{data}}}_{\substack{\text{end with data}\\ \text{distribution}}}.$$

Next step: Training the model

With random θ, simulating gives "non-sense".

Therefore we need to train u_t^θ such that

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Train via (e.g.) MSE:

$$L(\theta) = \| \underbrace{u_t^\theta(x)}_{\substack{\text{neural network}\\ \text{vector field}}} - \underbrace{u_t^{\text{target}}(x)}_{\text{training target}} \|^2.$$

No label :($\rightarrow$ We have to derive a training target:

1. choose a probability path $(p_t)_{t\in[0,1]}$ from p_{init} to p_{data};
2. derive u_t^{target} that realizes this path.

Constructing the Training Target

Goal: Derive a formula for a training target for training our models

A Lookhead: Key concepts and formulas

You will see the following concepts. Make sure you understand the formulas and the ideas behind them:

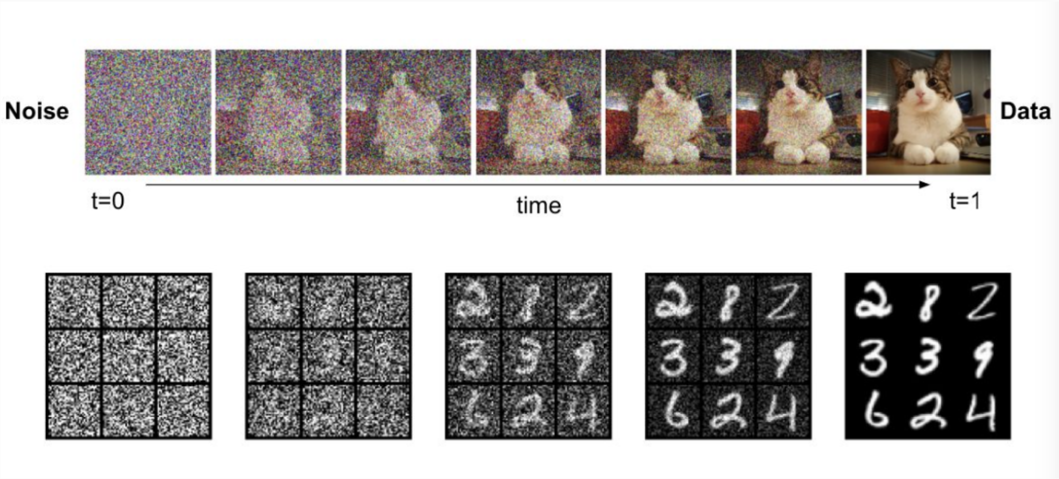
Conditional Probability Path	**Conditional** Vector Field	**Conditional** Score Function
Marginal Probability Path	**Marginal** Vector Field	**Marginal** Score Function

Remark

Key terminology:

1. **Conditional** = "Per single data point"
2. **Marginal** = "Across distribution of data points"

(Marginal) Probability paths: the path from noise to data



Conditional and marginal probability paths

A conditional path $p_t(x \mid z)$ satisfies:

$$p_0(\cdot \mid z) = p_{\text{init}}, \qquad p_1(\cdot \mid z) = \delta_z.$$

Induced marginal path:

$$p_t(x) = \int p_t(x \mid z)\, p_{\text{data}}(z)\, dz,$$

so

$$p_0 = p_{\text{init}}, \qquad p_1 = p_{\text{data}}.$$

Conditional and marginal probability paths

A conditional path $p_t(x \mid z)$ satisfies:

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Induced marginal path:

$$p_t(x) = \int p_t(x \mid z)\, p_{\text{data}}(z)\, dz,$$

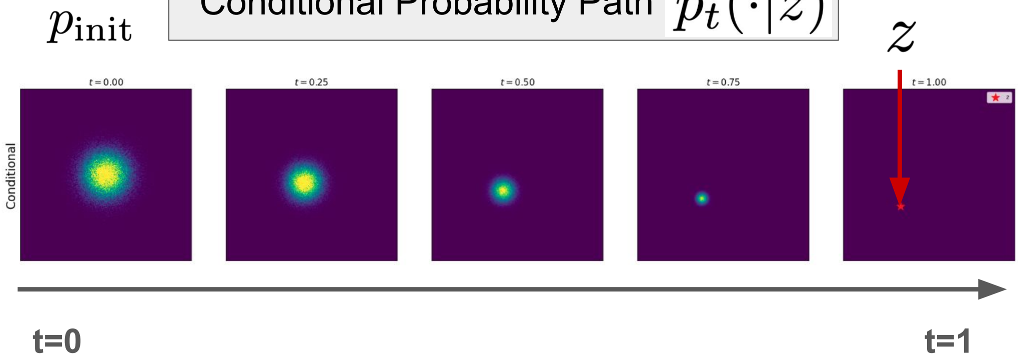
so

$$p_0 = p_{\text{init}}, \qquad p_1 = p_{\text{data}}.$$

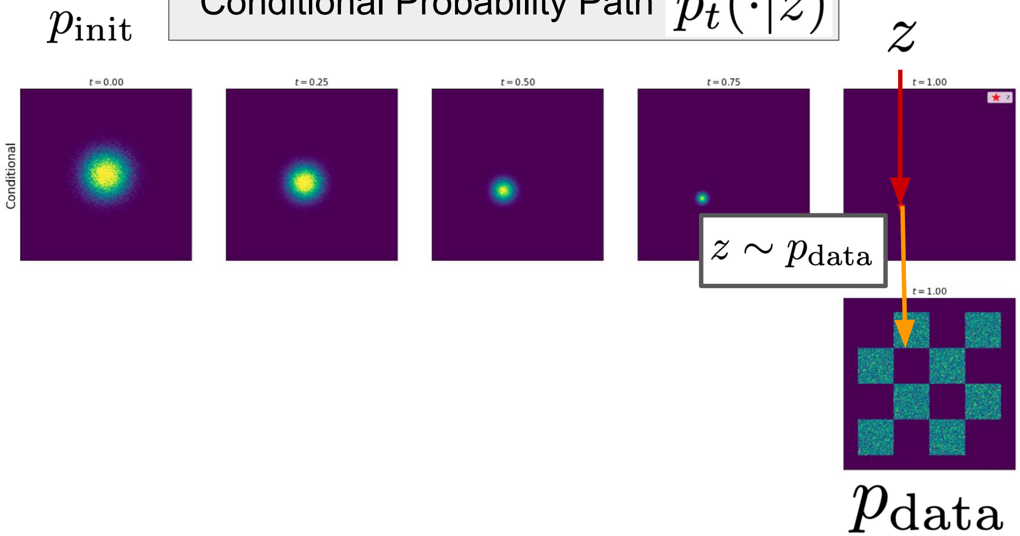
Sampling from the marginal:

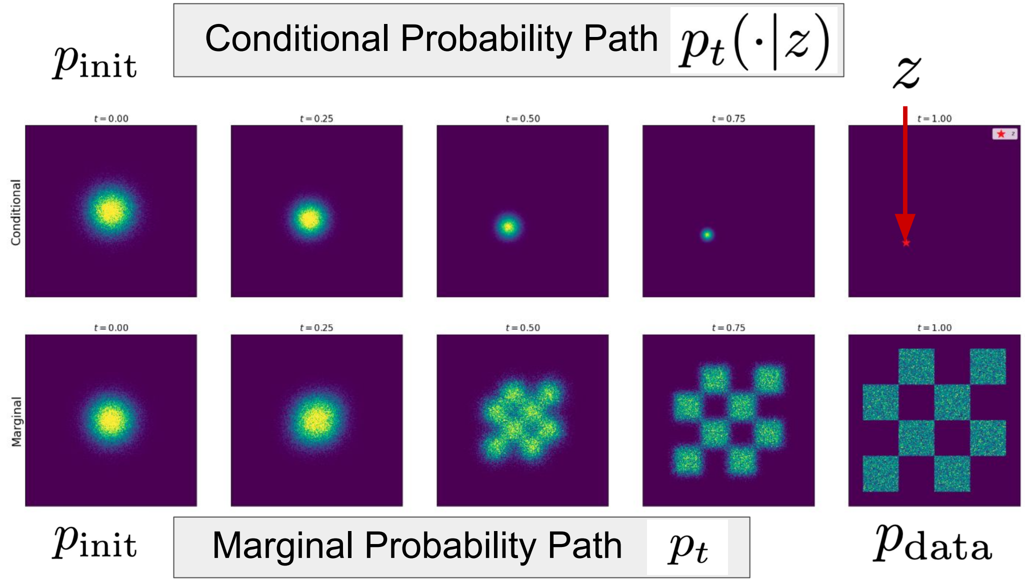
$$z \sim p_{\text{data}},\; x|z \sim p_t(x|z) \implies x \sim p_t.$$

Conditional Probability Path $p_t(\cdot|z)$



Conditional Probability Path $p_t(\cdot|z)$





Conditional Probability Path $p_t(\cdot|z)$
p_{init}
z
$t = 0.00$
$t = 0.25$
$t = 0.50$
$t = 0.75$
$t = 1.00$
Conditional
Marginal
p_{init}
Marginal Probability Path p_t
p_{data}

Gaussian conditional probability path

Example (Gaussian conditional probability path)

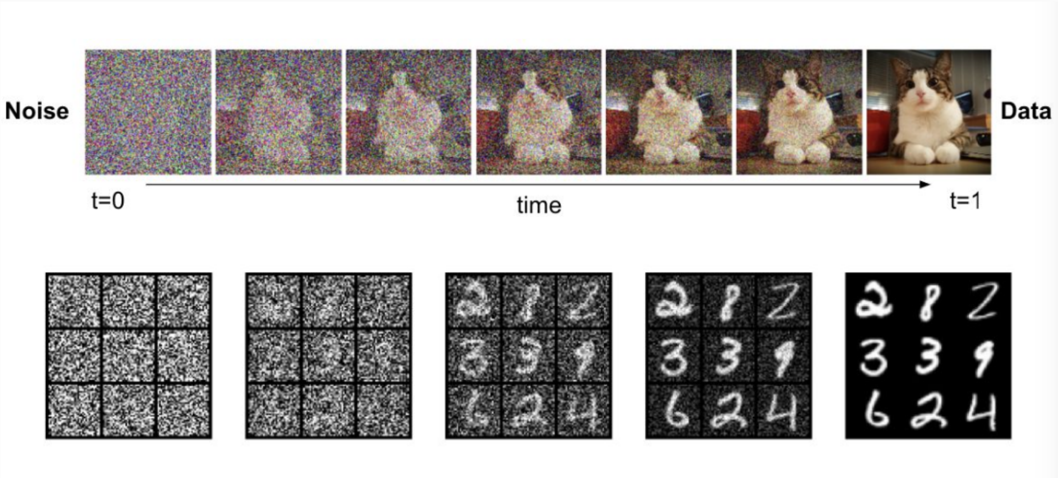
Schedulers α_t, β_t with $\alpha_0 = 0, \alpha_1 = 1, \beta_0 = 1, \beta_1 = 0$:

$$p_t(\cdot \mid z) = \mathcal{N}(\alpha_t z, \beta_t^2 I_d).$$

Sampling from the marginal:

$$z \sim p_{\text{data}}, \ \varepsilon \sim \mathcal{N}(0, I_d) \implies x = \alpha_t z + \beta_t \varepsilon \sim p_t.$$

Interpolation between Gaussian noise and data

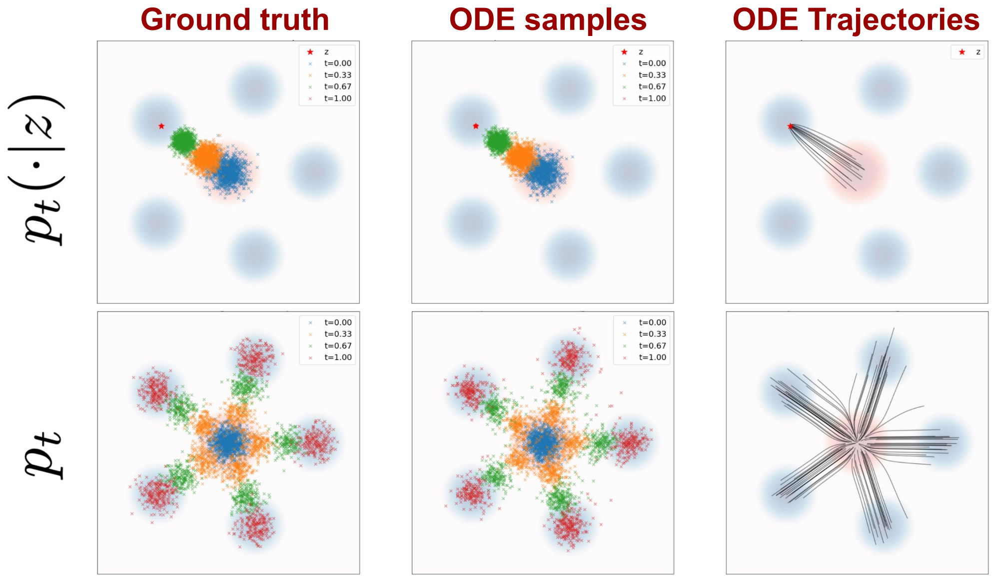


Conditional Prob. Path

	Notation	Key property	Gaussian example
Conditional Probability Path	$p_t(\cdot\|z)$	Interpolates p_{init} and a data point z	$\mathcal{N}(\alpha_t z, \beta_t^2 I_d)$
Conditional Vector Field			
Conditional Score Function			

Marginal Prob. Path

	Notation	Key property	Formula
Marginal Probability Path	p_t	Interpolates p_{init} and p_{data}	$\int p_t(x\|z)p_{\text{data}}(z)\mathrm{d}z$
Marginal Vector Field			
Marginal Score Function			


Ground truth
ODE samples
ODE Trajectories
$p_t(\cdot|z)$
p_t
z
t=0.00
t=0.33
t=0.67
t=1.00

Marginalization trick (flow target)

Theorem (Marginalization trick)

Assume conditional drift $u_t^{target}(\cdot \mid z)$ *yields*

$$X_0 \sim p_{init}, \quad \frac{d}{dt}X_t = u_t^{target}(X_t \mid z) \implies X_t \sim p_t(\cdot \mid z).$$

Define

$$u_t^{target}(x) = \int u_t^{target}(x \mid z) \frac{p_t(x \mid z) p_{data}(z)}{p_t(x)} \, dz.$$

Then

$$X_0 \sim p_{init}, \quad \frac{d}{dt}X_t = u_t^{target}(X_t) \implies X_t \sim p_t,$$

hence $X_1 \sim p_{data}$.

Target ODE for Gaussian paths

Example (Target ODE for Gaussian probability paths)

For $p_t(\cdot \mid z) = \mathcal{N}(\alpha_t z, \beta_t^2 I_d)$ with $\dot{\alpha}_t = \partial_t \alpha_t$, $\dot{\beta}_t = \partial_t \beta_t$:

$$u_t^{\text{target}}(x \mid z) = \left(\dot{\alpha}_t - \frac{\dot{\beta}_t}{\beta_t}\alpha_t\right) z + \frac{\dot{\beta}_t}{\beta_t} x.$$

Also, conditional flow map:

$$\phi_t^{\text{target}}(x \mid z) = \alpha_t z + \beta_t x.$$

Continuity Equation

Randomly initialized ODE

Given: $X_0 \sim p_{\text{init}}, \quad \frac{\mathrm{d}}{\mathrm{d}t} X_t = u_t(X_t)$

Follow probability path:

$$X_t \sim p_t \quad (0 \leq t \leq 1)$$

Marginals are p_t

equivalent

Continuity equation holds

$$\frac{\mathrm{d}}{\mathrm{d}t} p_t(x) = -\mathrm{div}(p_t u_t)(x)$$

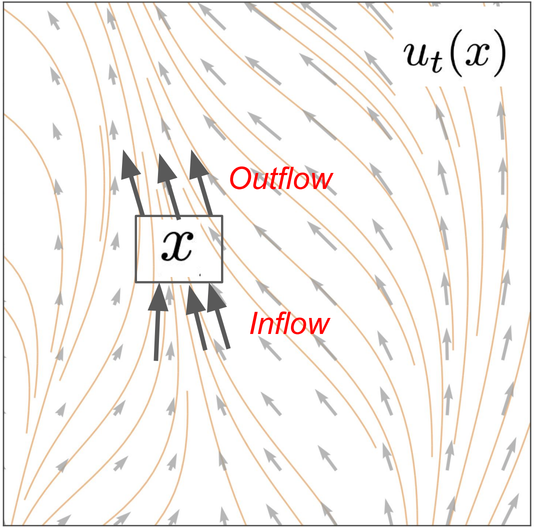
PDE holds

Continuity Equation

$$\frac{\mathrm{d}}{\mathrm{d}t} p_t(x) = -\mathrm{div}(p_t u_t)(x)$$

Change of probability mass at x

Outflow - inflow of probability mass from u



Gaussian Conditional Probability Path And Conditional Vector Field

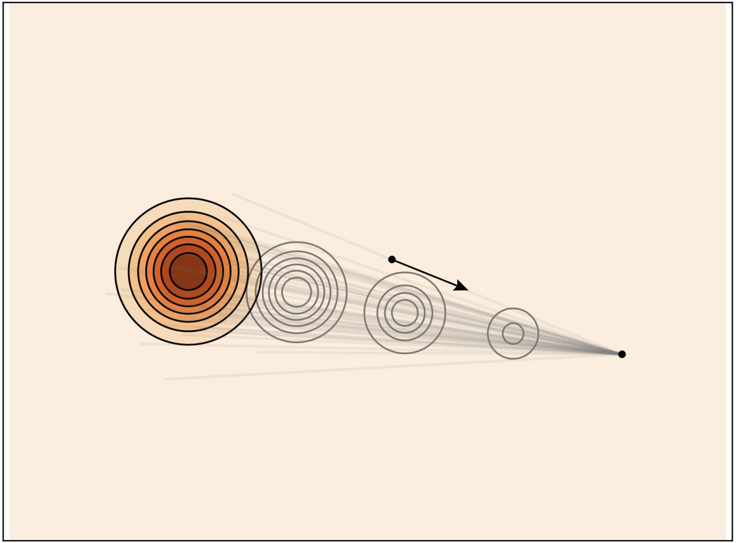


Figure credit: Yaron Lipman

Toy example

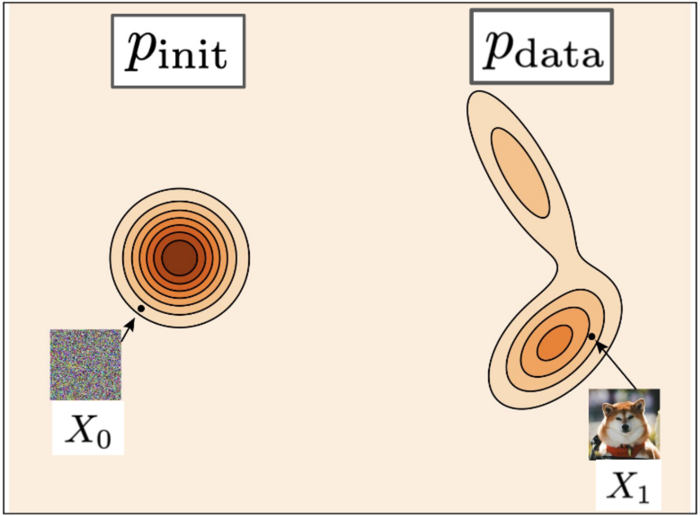


Figure credit:
Yaron Lipman

Proof idea: marginalization trick (one-slide sketch)

- Start from $p_t(x) = \int p_t(x \mid z) p_{\text{data}}(z)\, dz$.
- Differentiate in t and use conditional continuity:

$$\partial_t p_t(x \mid z) = -\operatorname{div}\big(p_t(\cdot \mid z)\, u_t^{\text{target}}(\cdot \mid z)\big)(x).$$

- Swap integral and divergence, then factor $p_t(x)$ to obtain

$$\partial_t p_t(x) = -\operatorname{div}\big(p_t(x)\, u_t^{\text{target}}(x)\big),$$

with u_t^{target} given by the Theorem.

Conditional Prob. Path, Vector Field, and Score

	Notation	Key property	Gaussian example
Conditional Probability Path	$p_t(\cdot\|z)$	Interpolates p_{init} and a data point z	$\mathcal{N}(\alpha_t z, \beta_t^2 I_d)$
Conditional Vector Field	$u_t^{\text{target}}(x\|z)$	ODE follows conditional path	$\left(\dot{\alpha}_t - \frac{\dot{\beta}_t}{\beta_t}\alpha_t\right) z + \frac{\dot{\beta}_t}{\beta_t} x$
Conditional Score Function			

Marginal Prob. Path, Vector Field, and Score

	Notation	Key property	Formula
Marginal Probability Path	p_t	Interpolates p_{init} and p_{data}	$\int p_t(x\|z)p_{\mathrm{data}}(z)\mathrm{d}z$
Marginal Vector Field	$u_t^{\mathrm{target}}(x)$	ODE follows marginal path	$\int u_t^{\mathrm{target}}(x\|z)\frac{p_t(x\|z)p_{\mathrm{data}}(z)}{p_t(x)}\mathrm{d}z$
Marginal Score Function			

Flow matching loss

The Flow Matching loss is a mean squared error between the neural network and the marginal vector field:

$$L_{\text{fm}}(\theta) = \mathbb{E}_{t\sim\text{Unif},x\sim p_t}[\|u_t^\theta(x) - u_t^{\text{target}}(x)\|^2]$$

Training a Flow Model Consists of Learning the Marginal Vector Field (How? Next lecture!)

SDE and Diffusion Target Derivation

SDE extension trick (diffusion target)

Define the marginal score $\nabla \log p_t(x)$.

Theorem (SDE extension trick)

For diffusion coefficient $\sigma_t \geq 0$, the SDE

$$dX_t = \left(u_t^{target}(X_t) + \frac{\sigma_t^2}{2}\nabla \log p_t(X_t)\right) dt + \sigma_t \, dW_t, \quad X_0 \sim p_{init},$$

follows the same marginal path $X_t \sim p_t$ (hence $X_1 \sim p_{data}$).

Score marginalization + Gaussian score

Score marginalization identity:

$$\nabla \log p_t(x) = \int \nabla \log p_t(x \mid z) \, \frac{p_t(x \mid z) p_{\text{data}}(z)}{p_t(x)} \, dz.$$

Example (Gaussian score)

If $p_t(x \mid z) = \mathcal{N}(x; \alpha_t z, \beta_t^2 I_d)$, then

$$\nabla \log p_t(x \mid z) = -\frac{x - \alpha_t z}{\beta_t^2}.$$

Langevin dynamics

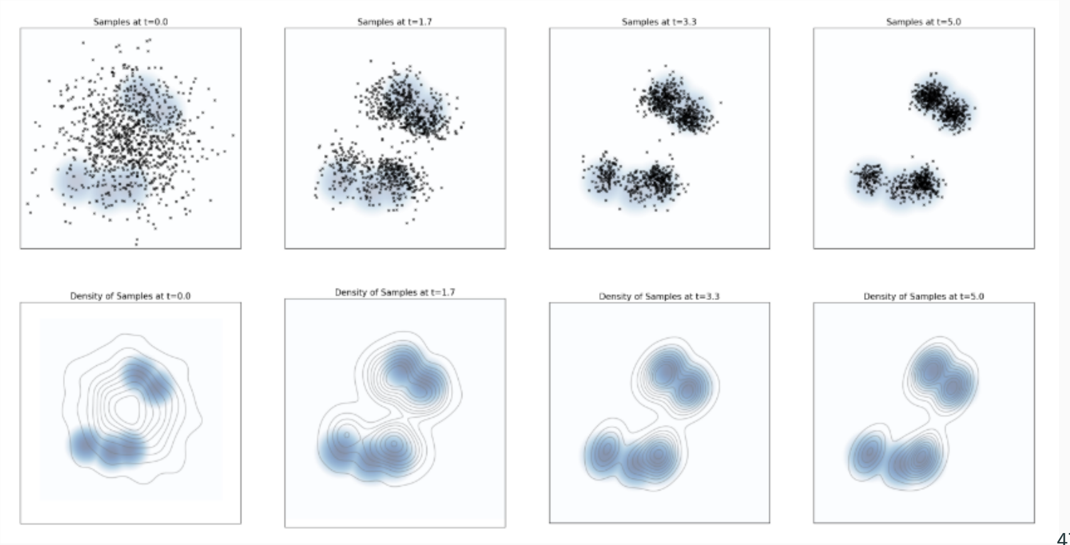
Remark (Langevin dynamics)

For a static target $p_t = p$ and $u_t^{\text{target}} = 0$:

$$dX_t = \frac{\sigma_t^2}{2} \nabla \log p(X_t)\, dt + \sigma_t\, dW_t.$$

Under mild conditions, p is stationary and the dynamics converge to p from broad initializations.

Langevin dynamics: sample paths



Fokker-Planck equation

Randomly initialized SDE

Given: $X_0 \sim p_{\text{init}}, \qquad \mathrm{d}X_t = u_t(X_t)\mathrm{d}t + \sigma_t \mathrm{d}W_t$

Follow probability path:

$$X_t \sim p_t \quad (0 \leq t \leq 1)$$

Marginals are p_t

equivalent

Fokker-Planck equation holds

$$\frac{\mathrm{d}}{\mathrm{d}t} p_t(x) = -\mathrm{div}(p_t u_t)(x) + \frac{\sigma_t^2}{2} \Delta p_t(x)$$

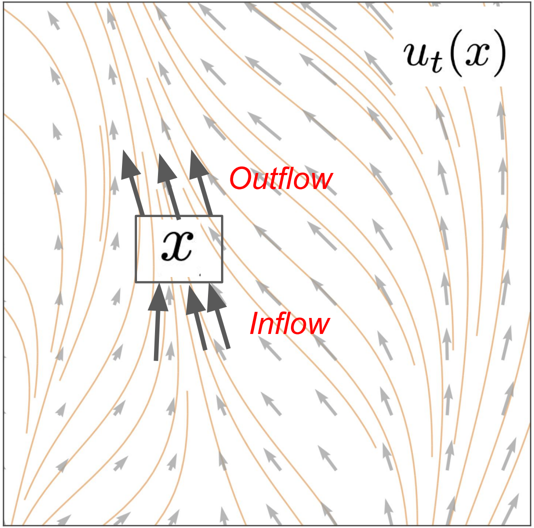
Continuity equ. *Heat equ.*

Continuity Equation

$$\frac{\mathrm{d}}{\mathrm{d}t}p_t(x) = -\mathrm{div}(p_t u_t)(x)$$

Change of probability mass at x

Outflow - inflow of probability mass from u

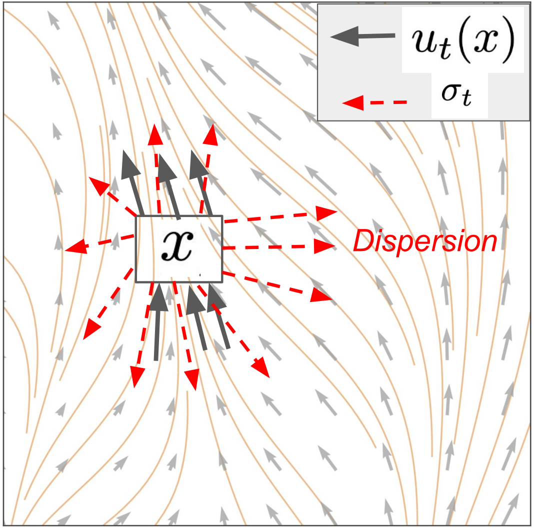


Fokker-Planck Equation

$$\frac{\mathrm{d}}{\mathrm{d}t} p_t(x) = -\mathrm{div}(p_t u_t)(x) + \frac{\sigma_t^2}{2} \Delta p_t(x)$$

Change of probability mass at x

Heat dispersion



Proof idea: SDE extension trick (one-slide sketch)

- Start from continuity equation for the flow target:

$$\partial_t p_t = -\operatorname{div}(p_t u_t^{\text{target}}).$$

- Add/subtract $\frac{\sigma_t^2}{2}\Delta p_t$ and rewrite

$$\Delta p_t = \operatorname{div}(\nabla p_t) = \operatorname{div}\left(p_t \nabla \log p_t\right).$$

- Conclude Fokker–Planck holds with drift

$$u_t = u_t^{\text{target}} + \frac{\sigma_t^2}{2}\nabla \log p_t,$$

which proves Theorem **??**.

Score matching loss

The Score Matching loss is a mean squared error between the neural network and the marginal score function:

$$L_{\mathrm{sm}}(\theta) = \mathbb{E}_{z\sim p_{\mathrm{data}}, x\sim p_t(\cdot|z)}[\|s_t^\theta(x) - \nabla \log p_t(x)\|^2]$$

To train a diffusion model, we need to train the score network by minimizing the score matching loss (How? Next class!)

Summary: training target derivation

Summary (Derivation of the training target)

Flow target:

$$u_t^{\text{target}}(x) = \int u_t^{\text{target}}(x \mid z)\, \frac{p_t(x \mid z) p_{\text{data}}(z)}{p_t(x)}\, dz.$$

Diffusion extension:

$$dX_t = \left(u_t^{\text{target}}(X_t) + \frac{\sigma_t^2}{2} \nabla \log p_t(X_t)\right) dt + \sigma_t\, dW_t.$$

Gaussian path (key formulas):

$$p_t(x \mid z) = \mathcal{N}(x; \alpha_t z, \beta_t^2 I_d), \quad u_t^{\text{target}}(x \mid z) = \left(\dot{\alpha}_t - \frac{\dot{\beta}_t}{\beta_t}\alpha_t\right) z + \frac{\dot{\beta}_t}{\beta_t} x,$$

$$\nabla \log p_t(x \mid z) = -\frac{x - \alpha_t z}{\beta_t^2}.$$

Conditional Prob. Path, Vector Field, and Score

	Notation	Key property	Gaussian example
Conditional Probability Path	$p_t(\cdot\|z)$	Interpolates p_{init} and a data point z	$\mathcal{N}(\alpha_t z, \beta_t^2 I_d)$
Conditional Vector Field	$u_t^{\text{target}}(x\|z)$	ODE follows conditional path	$\left(\dot{\alpha}_t - \frac{\dot{\beta}_t}{\beta_t}\alpha_t\right) z + \frac{\dot{\beta}_t}{\beta_t} x$
Conditional Score Function	$\nabla \log p_t(x\|z)$	Gradient of log-likelihood	$-\frac{x - \alpha_t z}{\beta_t^2}$

Marginal Prob. Path, Vector Field, and Score

	Notation	Key property	Formula
Marginal Probability Path	p_t	Interpolates p_{init} and p_{data}	$\int p_t(x\|z)p_{\text{data}}(z)\mathrm{d}z$
Marginal Vector Field	$u_t^{\text{target}}(x)$	ODE follows marginal path	$\int u_t^{\text{target}}(x\|z)\frac{p_t(x\|z)p_{\text{data}}(z)}{p_t(x)}\mathrm{d}z$
Marginal Score Function	$\nabla \log p_t(x)$	Can be used to convert ODE target to SDE	$\int \nabla \log p_t(x\|z)\frac{p_t(x\|z)p_{\text{data}}(z)}{p_t(x)}\mathrm{d}z$

Today was the **technically most challenging lecture**!

The next lectures will **be much much easier**!

Make sure you **understand the formulas** for:

Conditional **Probability Path**	**Conditional** **Vector Field**	**Conditional** **Score Function**
Marginal **Probability Path**	**Marginal** **Vector Field**	**Marginal** **Score Function**

These 6 formulas is all we need for training!