

Generative AI With Stochastic Differential Equations: Course Notes

Peter Holderrieth and Ezra Erives

| | | |
|-----|---|----|
| 1 | Introduction | 2 |
| 1.1 | Overview | 2 |
| 1.2 | Course Overview | 2 |
| 1.3 | Generative Modeling As Sampling | 3 |
| 2 | Flow and Diffusion Models | 6 |
| 2.1 | Flow Models | 6 |
| 2.2 | Stochastic Differential Equations (SDEs) | 9 |
| 3 | Constructing the Training Target | 13 |
| 3.1 | Conditional and Marginal Probability Path | 14 |
| 3.2 | Conditional and Marginal Vector Fields | 15 |
| 3.3 | Conditional and Marginal Score Functions | 19 |
| 4 | Training the Generative Model | 24 |
| 4.1 | Flow Matching | 24 |
| 4.2 | Score matching | 28 |
| 4.3 | Optional: A Guide to the Diffusion Model Literature | 32 |
| 5 | References | 35 |
| A | A Reminder on Probability Theory | 37 |
| A.1 | Random vectors | 37 |
| A.2 | Conditional densities and expectations | 37 |
| B | A Proof of the Fokker-Planck equation | 39 |

1 Introduction

Creating noise from data is easy; creating data from noise is generative modeling.

Song et al. [17]

1.1 Overview

In recent years, we all have witnessed a tremendous revolution in artificial intelligence (AI). Image generators like *Stable Diffusion* can generate photorealistic and artistic images across a diverse range of styles, video models like *Sora* can generate highly realistic movie clips, and large language models like *ChatGPT* can generate seemingly human-level responses to text prompts. At the heart of this revolution lies a new ability of AI systems: the ability to *generate* objects. While previous generations of AI systems were mainly used to *predict* things, these new AI system are creative: they create, dream or come up with new objects based on user-specified input. Such **generative AI** systems are at the core of this recent AI revolution.

The goal of this class is to teach you two of the most widely used generative AI algorithms: **denoising diffusion models** and **flow matching**. These models are the backbone of the best image, audio, or video generation models (e.g. Stable Diffusion, Sora) - and most recently became the state-of-the-art in scientific applications such as protein structures (e.g. AlphaFold3 is a diffusion model). Without a doubt, understanding these models is truly an extremely useful skill to have.

All of these generative models generate objects by iteratively converting *noise* into *data*. This evolution from noise to data is constructed via a **ordinary or stochastic differential equation (SDEs)**. Flow matching and denoising diffusion models are a family of techniques that allow us to (1) construct, (2) train, and (3) simulate, such SDEs at large scale with deep neural networks. While these models are rather simple to implement, the technical nature of SDEs can make these models difficult to understand. In this class, our goal is to equip you with the necessary mathematical toolbox about differential equations to allow you to systematically understand these models and provide a self-contained introduction to these algorithms. While this will provide you with a systematic understanding of generative models, it is the instructors' firm belief that true learning requires *getting your hands dirty*, i.e. to code. Accordingly, this course involves a hands-on coding component, which will allow you to implement and experiment with concepts taught in class, and which will culminate in the design of your very own generative model built from scratch. Therefore, the goal of this class is to give a systematic and principled understanding of *why* and *how* flow and diffusion models work. Finally, we believe that flow and diffusion models are not only very useful but also very beautiful concepts. Therefore, most importantly, we hope that this class will be a lot of fun to you.

1.2 Course Overview

We give a brief overview over of this document.

- 1. Section, From generation to sampling:** We will conclude this section by briefly formalizing what it means to “generate” an image, video, protein, etc. We will translate the problem of e.g., “how to generate an image

of a dog?" into the more precise problem of sampling from a probability distribution.

2. **Section, Flow and Diffusion Models:** Next, we explain the machinery of generation. As you can guess by the name of this class, this machinery consists of simulating ordinary and stochastic differential equations. We provide an introduction to differential equations and explain how to construct them with neural networks.
3. **Section, Finding a training target:** To train our generative model, we must first pin down precisely what it is that our model is supposed to approximate. In other words, what's the ground truth? We will introduce the celebrated *Fokker-Planck equation*, a fundamental result from stochastic calculus which governs the evolution of a distribution under the flow of an ODE or SDE, and which will allow us to formalize the notion of ground truth.
4. **Section, Training algorithm:** This section formulates a *training objective*, allowing us to approximate the training target, or ground truth, of the previous section. With this, we are ready to provide a minimal implementation of flow matching and denoising diffusion models.
5. **Section, Building an image generator:** We next focus on using our algorithms to build a conditional image generator. In order to do so, we need to discuss two crucial design choices: (1) neural network architectures and (2) how to condition on a specific prompt (e.g. "generate an image of a cat").
6. **Section, Advanced topics:** Finally, we discuss some advanced topics. We discuss distillation (making diffusion models faster), reward-finetuning (aligning with human feedback) as well as building diffusion-like models for other data types such as data on manifolds.

Required background. Due to the technical nature of this subject, we recommend some base level of mathematical maturity, and in particular some familiarity with probability theory. For this reason, we included a brief reminder section on probability theory in appendix A. Don't worry if some of the concepts there are unfamiliar to you. We are always happy to explain them after class.

1.3 Generative Modeling As Sampling

Let's begin by thinking about various data types, or *modalities*, that we might encounter, and how we will go about representing them numerically:

1. **Image:** Consider images with $H \times W$ pixels where H describes the height and W the width of the image, each with three color channels (RGB). For every pixel and every color channel, we are given an intensity value in \mathbb{R} . Therefore, an image can be represented by an element $z \in \mathbb{R}^{H \times W \times 3}$.
2. **Video:** A video is simply a series of images in time. If we have T time points or *frames*, a video would therefore be represented by an element $z \in \mathbb{R}^{T \times H \times W \times 3}$.
3. **Molecular structure:** A naive way would be to represent the structure of a molecule by a matrix $z \in \mathbb{R}^{N \times 3}$ where n is the number of atoms in the molecule and each $z^i \in \mathbb{R}^3$ describes the location of that atom. Of course, there are other, more sophisticated ways of representing such a molecule.

In all of the above examples, the object that we want to generate can be mathematically represented as a vector (potentially after flattening). Therefore, throughout this document, we will have:

Key Idea 1 (Objects as Vectors)

We identify the objects being generated as vectors $z \in \mathbb{R}^d$.

A notable exception to the above is text data, which is typically modeled as a discrete object via autoregressive language models (such as *ChatGPT*). While flow and diffusion models for discrete data have been developed, this course focuses exclusively on applications to continuous data.

Generation as Sampling. Let us think for a second what it means to generate something. For example, let's say we want to generate an image of a dog. Naturally, there are *many* possible images of dogs that we would be happy with. In particular, there is no one single "best" image of a dog. Rather, there is a spectrum of images that fit better or worse. In machine learning, it is common to think of this diversity of possible images as a *probability distribution*. We call it the **data distribution** and denote it as p_{data} . In the example of dog images, this distribution would therefore give higher likelihood to images that look more like a dog. Therefore, how "good" an image/video/molecule fits is replaced by how "likely" it is under the data distribution p_{data} . With this, we can mathematically express the task of generation as sampling from the (unknown) distribution p_{data} :

Key Idea 2 (Generation as Sampling)

Generating an object z is modeled as sampling from the data distribution $z \sim p_{\text{data}}$.

A **generative model** is a machine learning model that allows us to generate samples from p_{data} . In machine learning, we require data to train models. In generative modeling, we usually assume access to a finite number of examples sampled independently from p_{data} , which together serve as a proxy for the true distribution.

Key Idea 3 (Dataset)

A dataset consists of a finite number of samples $z_1, \dots, z_N \sim p_{\text{data}}$.

For images, we might construct a dataset by compiling publicly available images from the internet. For videos, we might similarly use YouTube as a database. For protein structures, we can use experimental data bases from sources such as the Protein Data Bank (PDB) that collected scientific measurements over decades. As the size of our dataset grows very large, it becomes an increasingly better representation of the underlying distribution p_{data} .

Conditional Generation. In many cases, we want to generate an object *conditioned* on some data y . For example, we might want to generate an image conditioned on y = "a dog running down a hill covered with snow with mountains in the background". We can rephrase this as sampling from a *conditional distribution*:

Key Idea 4 (Conditional Generation)

Conditional generation involves sampling from $z \sim p_{\text{data}}(\cdot|y)$, where y is a conditioning variable.

We call $p_{\text{data}}(\cdot|y)$ the **conditional data distribution**. The conditional generative modeling task typically involves learning to condition on an arbitrary, rather than fixed, choice of y . Using our previous example, we might

alternatively want to condition on a different text prompt, such as $y =$ “a photorealistic image of a cat blowing out birthday candles”. We therefore seek a single model which may be conditioned on any such choice of y . It turns out that techniques for unconditional generation are readily generalized to the conditional case. Therefore, for the first 3 sections, we will focus almost exclusively on the unconditional case (keeping in mind that conditional generation is what we’re building towards).

From Noise to Data. So far, we have discussed the *what* of generative modeling: generating samples from p_{data} . Here, we will briefly discuss the *how*. For this, we assume that we have access to some **initial distribution** p_{init} that we can easily sample from, such as the Gaussian $p_{\text{init}} = \mathcal{N}(0, I_d)$. The goal of a generative modeling is then to transform samples from $x \sim p_{\text{init}}$ into samples from p_{data} . We note that p_{init} does not have to be so simple as a Gaussian. As we shall see, there are interesting use cases for leveraging this flexibility. Despite this, we will stick with the name p_{init} , because in the majority of applications we take it to be a simple Gaussian.

Summary We summarize our discussion so far as follows:

Summary 1 (Generation as Sampling)

We summarize the findings of this section:

1. In this class, we consider the task of generating objects that are represented as vectors $z \in \mathbb{R}^d$ such as images, videos, or molecular structures.
2. Generation is the task of generating samples from a probability distribution p_{data} having access to a dataset of samples $z_1, \dots, z_N \sim p_{\text{data}}$ during training.
3. Conditional generation assumes that we condition the distribution on a label y and we want to sample from $p_{\text{data}}(\cdot|y)$ having access to data set of pairs $(z_1, y), \dots, (z_N, y)$ during training.
4. Our goal is to train a generative model to transform samples from a simple distribution p_{init} (e.g. a Gaussian) into samples from p_{data} .

2 Flow and Diffusion Models

In the previous section, we formalized generative modeling as sampling from a data distribution p_{data} . Further, we saw that sampling could be achieved via the transformation of samples from a simple distribution p_{init} , such as the Gaussian $\mathcal{N}(0, I_d)$, to samples from the target distribution p_{data} . In this section, we describe how the desired transformation can be obtained as the simulation of a suitably constructed differential equation. For example, flow matching and diffusion models involve simulating *ordinary differential equations* (ODEs) and *stochastic differential equations* (SDEs), respectively. Therefore, the goal of this section to construct the generative model used throughout this document: (1) Define what an ODE/SDE is and (2) Define how to parameterize an ODE/SDE in a neural network. This leads to the definition of a flow and diffusion model and the fundamental algorithms to sample from such models. In later sections, we then explain how to train these models.

2.1 Flow Models

We start by defining **ordinary differential equations (ODEs)**. A solution to an ODE is defined by a **trajectory**, i.e. a function of the form

$$X : [0, 1] \rightarrow \mathbb{R}^d, \quad t \mapsto X_t,$$

that maps from time t to some location in space \mathbb{R}^d . Every ODE is defined by a **vector field** u , i.e. a function of the form

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

i.e. for every time t and location x we get a vector $u_t(x) \in \mathbb{R}^d$ specifying a velocity in space (see fig. 1). An ODE imposes a condition on a trajectory: we want a trajectory X that “follows along the lines” of the vector field u_t , starting at the point x_0 . We may formalize such a trajectory as being the solution to the equation:

$$\frac{d}{dt} X_t = u_t(X_t) \tag{ODE} \quad (1a)$$

$$X_0 = x_0 \tag{initial conditions} \quad (1b)$$

Equation (1a) requires that the derivative of X_t is specified by the direction given by u_t . Equation (1b) requires that we start at x_0 at time $t = 0$. We may now ask: if we start at $X_0 = x_0$ at $t = 0$, where are we at time t (what is X_t)? This question is answered by a function called the **flow**, which is a solution to the ODE

$$\psi : \mathbb{R}^d \times [0, 1] \mapsto \mathbb{R}^d, \quad (x_0, t) \mapsto \psi_t(x_0) \tag{2a}$$

$$\frac{d}{dt} \psi_t(x_0) = u_t(\psi_t(x_0)) \tag{flow ODE} \quad (2b)$$

$$\psi_0(x_0) = x_0 \tag{flow initial conditions} \quad (2c)$$

For a given initial condition x_0 , a trajectory of the ODE is recovered via $X_t = \psi_t(X_0)$. Therefore, vector fields, ODEs, and flows are, intuitively, three descriptions of the same object: **vector fields define ODEs whose solutions are flows**. As with every equation, we should ask ourselves about an ODE: Does a solution exist and if so, is it

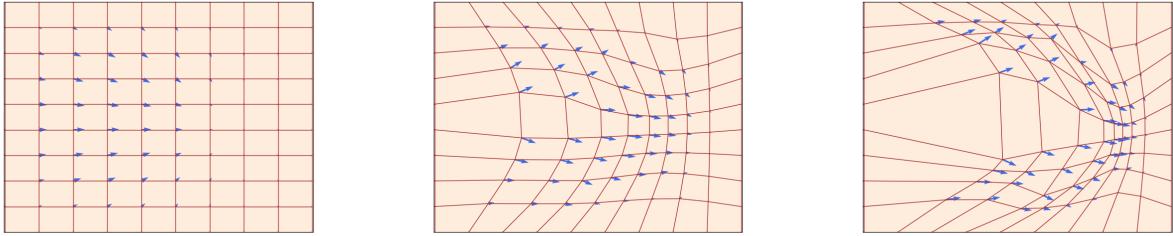


Figure 1: A flow $\psi_t : \mathbb{R}^d \rightarrow \mathbb{R}^d$ (red square grid) is defined by a velocity field $u_t : \mathbb{R}^d \rightarrow \mathbb{R}^d$ (visualized with blue arrows) that prescribes its instantaneous movements at all locations (here, $d = 2$). We show three different times t . As one can see, a flow is a diffeomorphism that "warps" space. Figure from [9].

unique? A fundamental result in mathematics is "yes!" to both, as long we impose weak assumptions on u_t :

Theorem 2 (Flow existence and uniqueness)

If $u : \mathbb{R}^d \times [0, 1] \rightarrow \mathbb{R}^d$ is continuously differentiable with a bounded derivative, then the ODE in (2) has a unique solution given by a flow ψ_t . In this case, ψ_t is a **diffeomorphism** for all t , i.e. ψ_t is continuously differentiable with a continuously differentiable inverse ψ_t^{-1} .

Note that the assumptions required for the existence and uniqueness of a flow are almost always fulfilled in machine learning, as we use neural networks to parameterize $u_t(x)$ and they always have bounded derivatives. Therefore, theorem 2 should not be a concern for you but rather good news: **flows exist and are unique solutions to ODEs in our cases of interest.** A proof can be found in [13, 3].

Example 3 (Linear Vector Fields)

Let us consider a simple example of a vector field $u_t(x)$ that is a simple linear function in x , i.e. $u_t(x) = -\theta x$ for $\theta > 0$. Then the function

$$\psi_t(x) = \exp(-\theta t) x \quad (3)$$

defines a flow ψ solving the ODE in eq. (2). You can check this yourself by checking that $\psi_0(x) = x$ and computing

$$\frac{d}{dt} \psi_t(x) \stackrel{(3)}{=} \frac{d}{dt} (\exp(-\theta t) x) \stackrel{(i)}{=} -\theta \exp(-\theta t) x \stackrel{(3)}{=} -\theta \psi_t(x) = u_t(\psi_t(x)),$$

where in (i) we used the chain rule. In fig. 3, we visualize a flow of this form converging to 0 exponentially.

Simulating an ODE. In general, it is not possible to compute the flow ψ_t explicitly if u_t is not as simple as a linear function. In these cases, one uses **numerical methods** to simulate ODEs. Fortunately, this is a classical and well researched topic in numerical analysis, and a myriad of powerful methods exist [6]. One of the simplest and

most intuitive methods is the **Euler method**. In the Euler method, we initialize with $X_0 = x_0$ and update via

$$X_{t+h} = X_t + hu_t(X_t) \quad (t = 0, h, 2h, 3h, \dots, 1-h) \quad (4)$$

where $h = n^{-1} > 0$ is a step size hyperparameter with $n \in \mathbb{N}$. For most of this class, Euler method will be good enough. To give you a taste of a more complex method, let us consider **Heun's method** defined via the update rule

$$\begin{aligned} X'_{t+h} &= X_t + hu_t(X_t) && \blacktriangleright \text{ initial guess of new state} \\ X_{t+h} &= X_t + \frac{h}{2}(u_t(X_t) + u_{t+h}(X'_{t+h})) && \blacktriangleright \text{ update with average } u \text{ at current and guessed state} \end{aligned}$$

Intuitively, the Heun's method is as follows: it takes a first guess X'_{t+h} of what the next step could be but corrects the direction initially taken via an updated guess. We will mainly use the Euler method in this class.

Flow models. We can now construct a generative model via an ODE. Remember that our goal was to convert a simple distribution p_{init} into a complex distribution p_{data} . The simulation of an ODE is thus a natural choice for this transformation. A **flow model** is described by the ODE

$$\begin{aligned} X_0 &\sim p_{\text{init}} && \text{(random initialization)} \\ \frac{d}{dt} X_t &= u_t^\theta(X_t) && \text{(ODE)} \end{aligned}$$

where the vector field u_t^θ is a neural network u_t^θ with parameters θ . For now, we will speak of u_t^θ as being a generic neural network; i.e. a continuous function $u_t^\theta : \mathbb{R}^d \times [0, 1] \rightarrow \mathbb{R}^d$ with parameters θ . Later, we will discuss particular choices of neural network architectures. Our goal is to make the endpoint X_1 of the trajectory have distribution p_{data} , i.e.

$$X_1 \sim p_{\text{data}} \Leftrightarrow \psi_1^\theta(X_0) \sim p_{\text{data}}$$

where ψ_t^θ describes the flow induced by u_t^θ . Note however: although it is called *flow model*, **the neural network is the vector field (not the flow)**. In order to compute the flow, we need to simulate the ODE. In algorithm 1, we summarize the procedure how to sample from a flow model.

Algorithm 1 Sampling from a Flow Model with Euler method

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

- 1: Set $t = 0$
 - 2: Set step size $h = \frac{1}{n}$
 - 3: Draw a sample $X_0 \sim p_{\text{init}}$
 - 4: **for** $i = 1, \dots, n - 1$ **do**
 - 5: $X_{t+h} = X_t + hu_t^\theta(X_t)$
 - 6: Update $t \leftarrow t + h$
 - 7: **end for**
 - 8: **return** X_1
-

2.2 Stochastic Differential Equations (SDEs)

Stochastic differential equations (SDEs) extend the deterministic trajectories from ODEs with *stochastic* trajectories. A stochastic trajectory is commonly called a **stochastic process** $(X_t)_{0 \leq t \leq 1}$ and is given by

$$X_t \text{ is a random variable for every } 0 \leq t \leq 1$$

$$X : [0, 1] \rightarrow \mathbb{R}^d, \quad t \mapsto X_t \text{ is a random trajectory for every draw of } X$$

In particular, when we simulate the same stochastic process twice, we might get different outcomes because the dynamics are designed to be random.

Brownian Motion. SDEs are constructed via a *Brownian motion* - a fundamental stochastic process that came out of the study physical diffusion processes. You can think of a Brownian motion as a continuous random walk. Let us first define what a Brownian motion is. A **Brownian motion**

$W = (W_t)_{0 \leq t \leq 1}$ is a stochastic process such that $W_0 = 0$, the trajectories $t \mapsto W_t$ are continuous, and the following two conditions hold:

1. **Normal increments:** $W_t - W_s \sim \mathcal{N}(0, (t-s)I_d)$ for all $0 \leq s < t$, i.e. increments have a Gaussian distribution with variance increasing linearly in time (I_d is the identity matrix).
2. **Independent increments:** For any $0 \leq t_0 < t_1 < \dots < t_n = 1$, the increments $W_{t_1} - W_{t_0}, \dots, W_{t_n} - W_{t_{n-1}}$ are independent random variables.

Brownian motion is also called a **Wiener process**, which is why we denote it with a "W".¹ We can easily simulate a Brownian motion approximately with step size $h > 0$ by setting $W_0 = 0$ and updating

$$W_{t+h} = W_t + \sqrt{h}\epsilon_t, \quad \epsilon_t \sim \mathcal{N}(0, I_d) \quad (t = 0, h, 2h, \dots, 1-h) \quad (5)$$

In fig. 2, we plot a few example trajectories of a Brownian motion. Brownian motion is as central to the study of stochastic processes as the Gaussian distribution is to the study of probability distributions. From finance to statistical physics to epidemiology, the study of Brownian motion has far reaching applications beyond machine learning. In finance, for example, Brownian motion is used to model the price of complex financial instruments. Also as a mathematical construction, Brownian motion is fascinating: For example, while the paths of a Brownian motion are continuous (so that you could draw it without ever lifting a pen), they are infinitely long (so that you would never stop drawing).

From ODEs to SDEs. The idea of an SDE is to extend the deterministic dynamics of an ODE by adding stochastic dynamics driven by a Brownian motion. Because everything is stochastic, there is *no derivative* anymore. Hence,

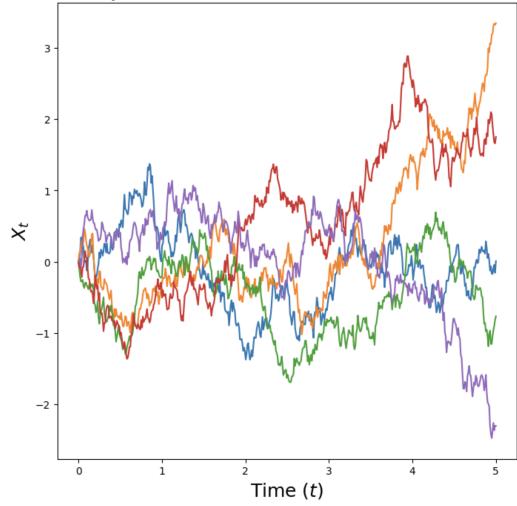


Figure 2: Sample trajectories of a Brownian motion W_t in dimension $d = 1$ simulated using eq. (5).

¹Nobert Wiener was a famous mathematician who taught at MIT. You can still see his portraits hanging at the MIT math department.

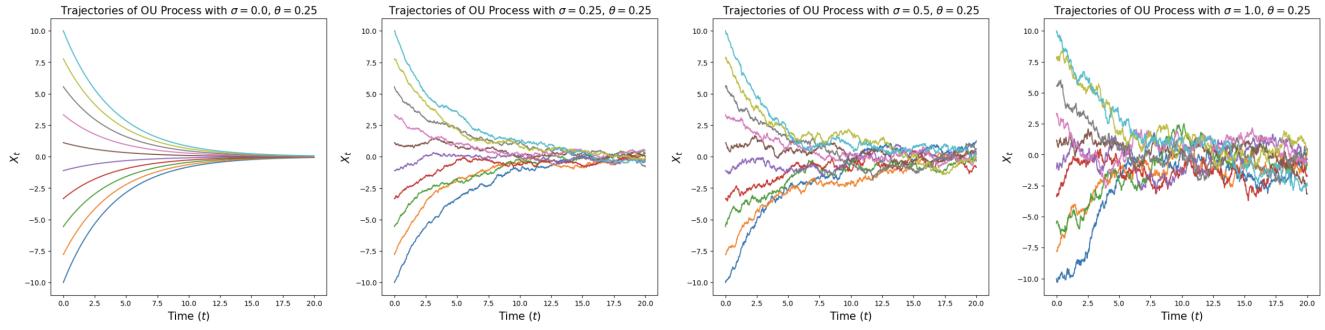


Figure 3: Illustration of Ornstein-Uhlenbeck processes (eq. (8)) in dimension $d = 1$ for $\theta = 0.25$ and various choices of σ (increasing from left to right). For $\sigma = 0$, we recover a flow (smooth, deterministic trajectories) that converges to the origin as $t \rightarrow \infty$. For $\sigma > 0$ we have random paths which converge towards the Gaussian $\mathcal{N}(0, \frac{\sigma^2}{2\theta})$ as $t \rightarrow \infty$.

we need to find an **equivalent formulation of ODEs that does not use derivatives**. For this, let us therefore rewrite trajectories $(X_t)_{0 \leq t \leq 1}$ of an ODE as follows:

$$\begin{aligned} \frac{d}{dt} X_t &= u_t(X_t) && \blacktriangleright \text{ expression via derivatives} \\ \stackrel{(i)}{\Leftrightarrow} \quad \frac{1}{h} (X_{t+h} - X_t) &= u_t(X_t) + R_t(h) \\ \Leftrightarrow \quad X_{t+h} &= X_t + h u_t(X_t) + h R_t(h) && \blacktriangleright \text{ expression via infinitesimal updates} \end{aligned}$$

where $R_t(h)$ describes a negligible function for small h , i.e. such that $\lim_{h \rightarrow 0} R_t(h) = 0$, and in (i) we simply use the definition of derivatives. The derivation above simply restates what we already know: A trajectory $(X_t)_{0 \leq t \leq 1}$ of an ODE takes, at every timestep, a small step in the direction $u_t(X_t)$. We may now amend the last equation to make it stochastic: A trajectory $(X_t)_{0 \leq t \leq 1}$ of an SDE takes, at every timestep, a small step in the direction $u_t(X_t)$ *plus* some contribution from a Brownian motion:

$$X_{t+h} = X_t + \underbrace{h u_t(X_t)}_{\text{deterministic}} + \underbrace{\sigma_t (W_{t+h} - W_t)}_{\text{stochastic}} + \underbrace{h R_t(h)}_{\text{error term}} \quad (6)$$

where $\sigma_t \geq 0$ describes the **diffusion coefficient** and $R_t(h)$ describes a stochastic error term such that the standard deviation $\mathbb{E}[\|R_t(h)\|^2]^{1/2} \rightarrow 0$ goes to zero for $h \rightarrow 0$. The above describes a **stochastic differential equation (SDE)**. It is common to denote it in the following symbolic notation:

$$dX_t = u_t(X_t) dt + \sigma_t dW_t \quad (\text{SDE}) \quad (7a)$$

$$X_0 = x_0 \quad (\text{initial condition}) \quad (7b)$$

However, always keep in mind that the "d X_t "-notation above is a purely informal notation of eq. (6). Unfortunately, SDEs do not have a flow map ϕ_t anymore. This is because the value X_t is not fully determined by $X_0 \sim p_{\text{init}}$ anymore as the evolution itself is stochastic. Still, in the same way as for ODEs, we have:

Theorem 4 (SDE solution existence and uniqueness)

If $u : \mathbb{R}^d \times [0, 1] \rightarrow \mathbb{R}^d$ is continuously differentiable with a bounded derivative and σ_t is continuous, then the SDE in (7) has a solution given by the unique stochastic process $(X_t)_{0 \leq t \leq 1}$ satisfying eq. (6).

If this was a stochastic calculus class, we would spend several lectures proving this theorem and constructing SDEs with full mathematical rigor, i.e. constructing a Brownian motion from first principles and constructing the process X_t via *stochastic integrals*. As we focus on machine learning in this class, we refer to a proof to [12]. Finally, note that every ODE is also an SDE - simply with a vanishing diffusion coefficient $\sigma_t = 0$. Therefore, for the remainder of this class, **when we speak about SDEs, we always include ODEs**.

Example 5 (Ornstein-Uhlenbeck Process)

Let us consider a constant diffusion coefficient $\sigma_t = \sigma \geq 0$ and a constant linear drift $u_t(x) = -\theta x$ for $\theta > 0$ resulting in the SDE:

$$dX_t = -\theta X_t dt + \sigma dW_t \quad (8)$$

A solution $(X_t)_{0 \leq t \leq 1}$ to the above SDE is known as an **Ornstein-Uhlenbeck process**. We visualize it in fig. 3. The vector field $-\theta x$ pushes the process back to its center 0 (as I always go the inverse direction of where I am), while the diffusion coefficient σ always adds more noise. This process converges towards a Gaussian distribution $\mathcal{N}(0, \sigma^2)$ if we simulate it for $t \rightarrow \infty$. Note that for $\sigma = 0$, we have a flow with linear vector field that we have studied in eq. (3).

Simulating an SDE. If you struggle with the abstract definition of an SDE so far, then don't worry about it. A more intuitive way of thinking about SDEs is given by answering the question: How might we simulate an SDE? The simplest such scheme is known as the **Euler-Maruyama method**, and is essentially to SDEs what the Euler method is to ODEs. Using the Euler-Maruyama method, we initialize $X_0 = x_0$ and update iteratively via

$$X_{t+h} = X_t + h u_t(X_t) + \sqrt{h} \sigma_t \epsilon_t, \quad \epsilon_t \sim \mathcal{N}(0, I_d) \quad (9)$$

where $h = n^{-1} > 0$ is a step size hyper-parameter with $n \in \mathbb{N}$. In other words, to simulate using the Euler-Maruyama method, we take a small step in the direction of $u_t(X_t)$ as well as add a little bit of Gaussian noise scaled by $\sqrt{h} \sigma_t$. When simulating SDEs in this class (such as in labs), we will usually stick to the Euler-Maruyama method.

Diffusion Models. We can now construct a generative model via an SDE in the same way as we did for ODEs. Remember that our goal was to convert a simple distribution p_{init} into a complex distribution p_{data} . Like for ODEs, the simulation of an SDE randomly initialized with $X_0 \sim p_{\text{init}}$ is a natural choice for this transformation. To parameterize this SDE, we can simply make its central ingredient - the vector field u_t - a neural network u_t^θ . A

Algorithm 2 Sampling from a Diffusion Model (Euler-Maruyama method)

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

- 1: Set $t = 0$
- 2: Set step size $h = \frac{1}{n}$
- 3: Draw a sample $X_0 \sim p_{\text{init}}$
- 4: **for** $i = 1, \dots, n - 1$ **do**
- 5: Draw a sample $\epsilon \sim \mathcal{N}(0, I_d)$
- 6: $X_{t+h} = X_t + h u_t^\theta(X_t) + \sigma_t \sqrt{h} \epsilon$
- 7: Update $t \leftarrow t + h$
- 8: **end for**
- 9: **return** X_1

diffusion model is given by

$$\begin{aligned} X_0 &\sim p_{\text{init}} && \text{(random initialization)} \\ dX_t &= u_t^\theta(X_t) dt + \sigma_t dW_t && \text{(SDE)} \end{aligned}$$

In algorithm 2, we describe the algorithm to sample from a diffusion model with the Euler-Maruyama method. We can summarize the results of this section as:

Summary 6 (SDE generative model)

Throughout this document, an **diffusion model** consists of a neural network u_t^θ with parameters θ that parameterize a vector field and a fixed diffusion coefficient σ_t :

$$\begin{aligned} \textbf{Neural Network: } &u^\theta : \mathbb{R}^d \times [0, 1] \rightarrow \mathbb{R}^d, (t, x) \mapsto u_t^\theta(x) \text{ with parameters } \theta \\ \textbf{Fixed: } &\sigma_t : [0, 1] \rightarrow [0, \infty), t \mapsto \sigma_t \end{aligned}$$

To obtain samples from our SDE model (i.e. generate objects), the procedure is as follows:

- | | |
|--|---|
| Initialization: $X_0 \sim p_{\text{init}}$ | ► Initialize with simple distribution, e.g. a Gaussian |
| Simulation: $dX_t = u_t^\theta(X_t) dt + \sigma_t dW_t$ | ► Simulate SDE from 0 to 1 |
| Goal: $X_1 \sim p_{\text{data}}$ | ► Goal is to make X_1 have distribution p_{data} |

A diffusion model with $\sigma_t = 0$ is a **flow model**.

3 Constructing the Training Target

In the previous section, we constructed flow and diffusion models where we obtain trajectories $(X_t)_{0 \leq t \leq 1}$ by simulating the ODE/SDE

$$X_0 \sim p_{\text{init}}, \quad dX_t = u_t^\theta(X_t)dt \quad (\text{Flow model}) \quad (10)$$

$$X_0 \sim p_{\text{init}}, \quad dX_t = u_t^\theta(X_t)dt + \sigma_t dW_t \quad (\text{Diffusion model}) \quad (11)$$

where u_t^θ is a neural network and σ_t is a fixed diffusion coefficient. Naturally, if we just randomly initialize the parameters θ of our neural network u_t^θ , simulating the ODE/SDE will just produce nonsense. As always in machine learning, we need to *train* the neural network. We accomplish this by minimizing a loss function $\mathcal{L}(\theta)$, such as the *mean squared error*

$$\mathcal{L}(\theta) = \|u_t^\theta(x) - \underbrace{u_t^{\text{target}}(x)}_{\text{training target}}\|^2,$$

where $u_t^{\text{target}}(x)$ is the **training target** that we would like to approximate. To derive a training algorithm, we proceed in two steps: **In this chapter, our goal is to characterize the training target u_t^{target} . In the next chapter, we will describe a training algorithm that approximates the training target u_t^{target} .** Naturally, like the neural network u_t^θ , the training target should itself be a vector field $u_t^{\text{target}} : \mathbb{R}^d \times [0, 1] \rightarrow \mathbb{R}^d$. Further, u_t^{target} should do what we want u_t^θ to do: convert noise into data. **Therefore, the goal of this chapter is to derive a formula for the training target u_t^{ref} such that the corresponding ODE/SDE converts p_{init} into p_{data} .** Along the way we will encounter two fundamental results from physics and stochastic calculus: *the continuity equation* and *the Fokker-Planck equation*. As before, we will first describe the key ideas for ODEs before generalizing to SDEs.

Remark 7

There are a number of different approaches to deriving a training target for flow and diffusion models. The approach we present carefully balances generality and simplicity and is in line with recent state-of-the-art models. However, it might well differ from other, older presentations of diffusion models you have seen. Later, we will discuss alternative formulations.

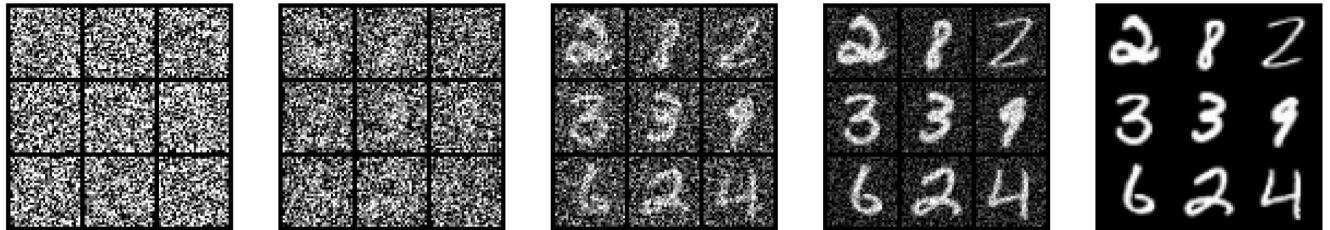


Figure 4: Gradual interpolation from noise to data via a Gaussian conditional probability path for a collection of images.

3.1 Conditional and Marginal Probability Path

The first step of constructing the training target u_t^{target} is by specifying a **probability path**. Intuitively, a probability path specifies a gradual interpolation between noise p_{init} and data p_{data} (see fig. 4). We explain the construction in this section. In the following, for a data point $z \in \mathbb{R}^d$, we denote with δ_z the **Dirac delta** “distribution”. This is the simplest distribution that one can imagine: sampling from δ_z always returns z (i.e. it is deterministic). A **conditional (interpolating) probability path** is a set of distribution $p_t(x|z)$ over \mathbb{R}^d such that:

$$p_0(\cdot|z) = p_{\text{init}}, \quad p_1(\cdot|z) = \delta_z \quad \text{for all } z \in \mathbb{R}^d. \quad (12)$$

In other words, a conditional probability path gradually converts a *single* data point into the distribution p_{init} (see e.g. fig. 4). You can think of a probability path as a trajectory in the space of distributions. Every conditional probability path $p_t(x|z)$ induces a **marginal probability path** $p_t(x)$ defined as the distribution that we obtain by first sampling a data point $z \sim p_{\text{data}}$ from the data distribution and then sampling from $p_t(\cdot|z)$:

$$z \sim p_{\text{data}}, \quad x \sim p_t(\cdot|z) \Rightarrow x \sim p_t \quad (\text{Sampling from marginal path}) \quad (13)$$

$$p_t(x) = \int p_t(x|z)p_{\text{data}}(z)dz \quad (\text{Density of marginal path}) \quad (14)$$

Note that we know how to sample from p_t but we don't know the density values $p_t(x)$ as the integral is intractable. Check for yourself that because of the conditions on $p_t(\cdot|z)$ in eq. (12), the marginal probability path p_t interpolates between p_{init} and p_{data} :

$$p_0 = p_{\text{init}} \quad \text{and} \quad p_1 = p_{\text{data}}. \quad (\text{Noise data interpolation}) \quad (15)$$

Example 8 (Gaussian Conditional Probability Path)

One particularly popular probability path is the **Gaussian probability path**. This is the **probability path used by e.g., denoising diffusion models**. Let α_t, β_t be **noise schedulers**: two continuously differentiable, monotonic functions with $\alpha_0 = \beta_1 = 0$ and $\alpha_1 = \beta_0 = 1$. We then define the conditional probability path

$$p_t(\cdot|z) = \mathcal{N}(\alpha_t z, \beta_t^2 I_d) \quad \blacktriangleright \text{ Gaussian conditional path} \quad (16)$$

which, by the conditions we imposed on α_t and β_t , fulfills

$$p_0(\cdot|z) = \mathcal{N}(\alpha_0 z, \beta_0^2 I_d) = \mathcal{N}(0, I_d), \quad \text{and} \quad p_1(\cdot|z) = \mathcal{N}(\alpha_1 z, \beta_1^2 I_d) = \delta_z,$$

where we have used the fact that a normal distribution with zero variance and mean z is just δ_z . Therefore, this choice of $p_t(x|z)$ fulfills eq. (12) for $p_{\text{init}} = \mathcal{N}(0, I_d)$ and is therefore a valid conditional interpolating path. The Gaussian conditional probability path has several useful properties which makes it especially amenable to our goals, and because of this we will use it as our prototypical example of a conditional probability path for the rest of the section. In fig. 4, we illustrate its application to an image. We can express sampling from the

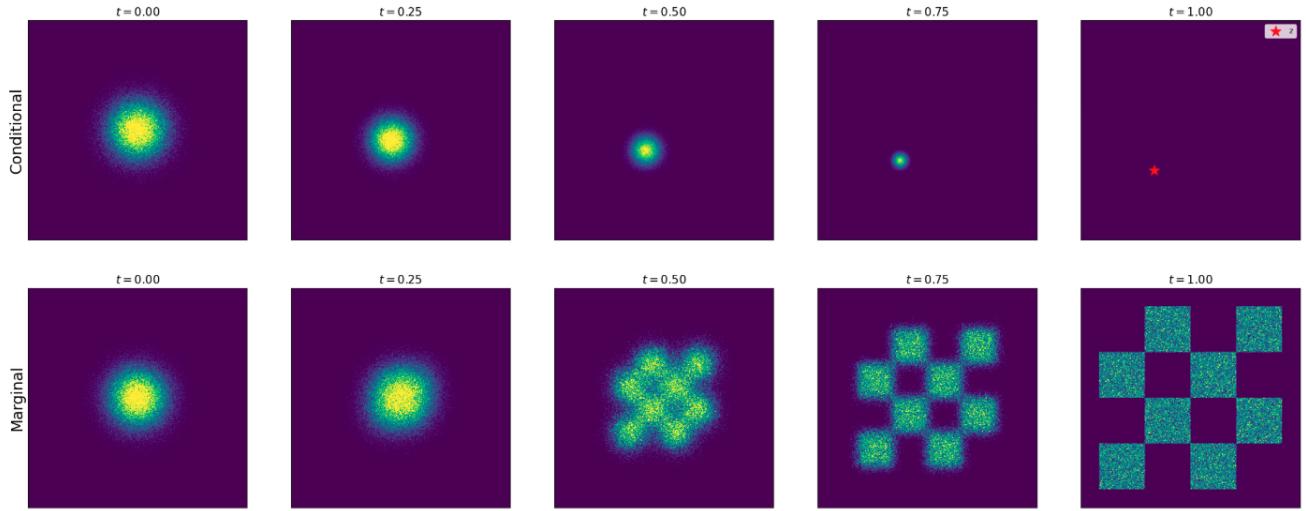


Figure 5: Illustration of a conditional (top) and marginal (bottom) probability path. Here, we plot a Gaussian probability path with $\alpha_t = t, \beta_t = 1 - t$. The conditional probability path interpolates a Gaussian $p_{\text{init}} = \mathcal{N}(0, I_d)$ and $p_{\text{data}} = \delta_z$ for single data point z . The marginal probability path interpolates a Gaussian and a data distribution p_{data} (Here, p_{data} is a toy distribution in dimension $d = 2$ represented by a chess board pattern.)

marginal path p_t as:

$$z \sim p_{\text{data}}, \epsilon \sim p_{\text{init}} = \mathcal{N}(0, I_d) \Rightarrow x = \alpha_t z + \beta_t \epsilon \sim p_t \quad \blacktriangleright \text{Sampling from marginal Gaussian path} \quad (17)$$

Intuitively, the above procedure adds more noise for lower t until time $t = 0$, at which point there is only noise. In fig. 5, we plot an example of such an interpolating path between Gaussian noise and a simple data distribution.

3.2 Conditional and Marginal Vector Fields

We proceed now by constructing a training target u_t^{target} for a flow model using the recently defined notion of a probability path p_t . The idea is to construct the target vector field from simple components that we can derive analytically by hand.

Theorem 9 (Marginalization trick)

For every data point $z \in \mathbb{R}^d$, let $u_t^{\text{target}}(\cdot|z)$ denote a **conditional vector field**, defined so that the corresponding ODE yields the conditional probability path $p_t(\cdot|z)$, viz.,

$$X_0 \sim p_{\text{init}}, \quad \frac{d}{dt} X_t = u_t^{\text{target}}(X_t|z) \quad \Rightarrow \quad X_t \sim p_t(\cdot|z) \quad (0 \leq t \leq 1). \quad (18)$$

Then the **marginal vector field** $u_t^{\text{target}}(x)$, defined by

$$u_t^{\text{target}}(x) = \int u_t^{\text{target}}(x|z) \frac{p_t(x|z)p_{\text{data}}(z)}{p_t(x)} dz, \quad (19)$$

follows the marginal probability path, i.e.

$$X_0 \sim p_{\text{init}}, \quad \frac{d}{dt} X_t = u_t^{\text{target}}(X_t) \quad \Rightarrow \quad X_t \sim p_t \quad (0 \leq t \leq 1). \quad (20)$$

In particular, $X_1 \sim p_{\text{data}}$ for this ODE, so that we might say " u_t^{target} converts noise p_{init} into data p_{data} ".

In fig. 6, we illustrate theorem 9. Before we prove theorem 9, let us first illustrate why it is useful: while the marginal vector field $u_t^{\text{target}}(\cdot)$ is generally intractable, we can often find a conditional vector field $u_t^{\text{target}}(\cdot|z)$ satisfying eq. (18) analytically by hand (i.e. by just doing some algebra ourselves). The marginalization trick from theorem 9 then allows us to relate the conditional and marginal vector fields. As it turns out, one may therefore substitute the conditional vector field $u_t^{\text{target}}(\cdot|z)$ in place of the marginal vector field $u_t^{\text{target}}(\cdot)$. We will make this intuition precise in the next section, when we discuss **flow matching**. Let us illustrate how to derive a conditional vector field $u_t(x|z)$ for our running example of a Gaussian probability path.

Example 10 (Target ODE for Gaussian probability paths)

As before, let $p_t(\cdot|z) = \mathcal{N}(\alpha_t z, \beta_t^2 I_d)$ for noise schedulers α_t, β_t (see eq. (16)). Let $\dot{\alpha}_t = \partial_t \alpha_t$ and $\dot{\beta}_t = \partial_t \beta_t$ denote respective time derivatives of α_t and β_t . Here, we want to show that the **conditional Gaussian vector field** given by

$$u_t^{\text{target}}(x|z) = \left(\dot{\alpha}_t - \frac{\dot{\beta}_t}{\beta_t} \alpha_t \right) z + \frac{\dot{\beta}_t}{\beta_t} x \quad (21)$$

is a valid conditional vector field model in the sense of theorem 9: its ODE trajectories X_t satisfy $X_t \sim p_t(\cdot|z) = \mathcal{N}(\alpha_t z, \beta_t^2 I_d)$ if $X_0 \sim \mathcal{N}(0, I_d)$. In fig. 6, we confirm this visually by comparing samples from the conditional probability path (ground truth) to samples from simulated ODE trajectories of this flow. As you can see, the distribution match. We will now prove this.

Proof. Let us construct a conditional flow model $\psi_t^{\text{target}}(x|z)$ first by defining

$$\psi_t^{\text{target}}(x|z) = \alpha_t z + \beta_t x. \quad (22)$$

If X_t is the ODE trajectory of $\psi_t^{\text{target}}(\cdot|z)$ with $X_0 \sim p_{\text{init}} = \mathcal{N}(0, I_d)$, then by definition

$$X_t = \psi_t^{\text{target}}(X_0|z) = \alpha_t z + \beta_t X_0 \sim \mathcal{N}(\alpha_t z, \beta_t^2 I_d) = p_t(\cdot|z).$$

We conclude that the trajectories are distributed like the conditional probability path (i.e, eq. (18) is fulfilled). It remains to extract the vector field $u_t^{\text{target}}(x|z)$ from $\psi_t^{\text{target}}(x|z)$. By the definition of a flow (eq. (2b)), it

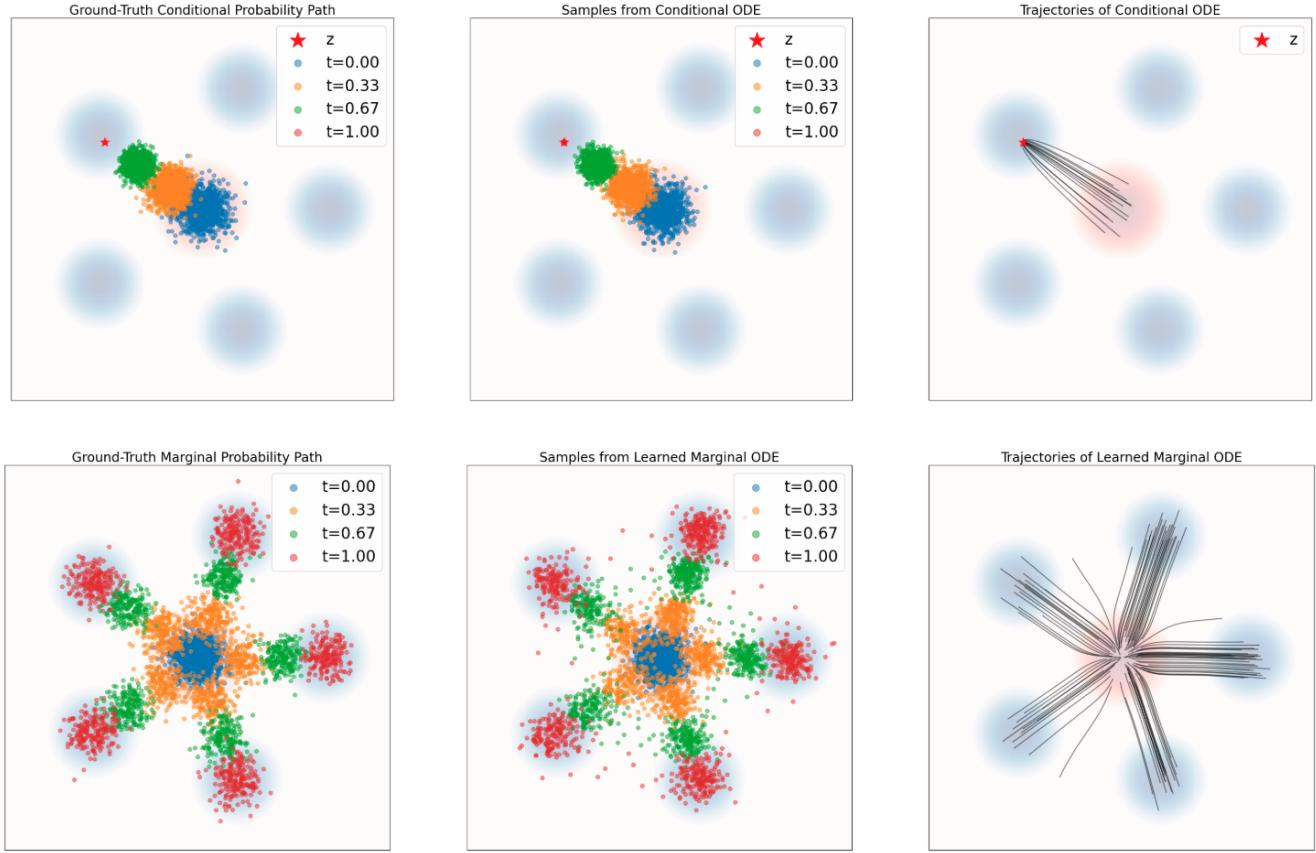


Figure 6: Illustration of theorem 9. Simulating a probability path with ODEs. Data distribution p_{data} in blue background. Gaussian p_{init} in red background. Top row: Conditional probability path. Left: Ground truth samples from conditional path $p_t(\cdot|z)$. Middle: ODE samples over time. Right: Trajectories by simulating ODE with $u_t^{\text{target}}(x|z)$ in eq. (21). Bottom row: Simulating a marginal probability path. Left: Ground truth samples from p_t . Middle: ODE samples over time. Right: Trajectories by simulating ODE with marginal vector field $u_t^{\text{flow}}(x)$. As one can see, the conditional vector field follows the conditional probability path and the marginal vector field follows the marginal probability path.

holds

$$\begin{aligned}
 & \frac{d}{dt} \psi_t^{\text{target}}(x|z) = u_t^{\text{target}}(\psi_t^{\text{target}}(x|z)|z) \quad \text{for all } x, z \in \mathbb{R}^d \\
 \stackrel{(i)}{\Leftrightarrow} & \dot{\alpha}_t z + \dot{\beta}_t x = u_t^{\text{target}}(\alpha_t z + \beta_t x|z) \quad \text{for all } x, z \in \mathbb{R}^d \\
 \stackrel{(ii)}{\Leftrightarrow} & \dot{\alpha}_t z + \dot{\beta}_t \left(\frac{x - \alpha_t z}{\beta_t} \right) = u_t^{\text{target}}(x|z) \quad \text{for all } x, z \in \mathbb{R}^d \\
 \stackrel{(iii)}{\Leftrightarrow} & \left(\dot{\alpha}_t - \frac{\dot{\beta}_t}{\beta_t} \alpha_t \right) z + \frac{\dot{\beta}_t}{\beta_t} x = u_t^{\text{target}}(x|z) \quad \text{for all } x, z \in \mathbb{R}^d
 \end{aligned}$$

where in (i) we used the definition of $\psi_t^{\text{target}}(x|z)$ (eq. (22)), in (ii) we reparameterized $x \rightarrow (x - \alpha_t z)/\beta_t$, and

in (iii) we just did some algebra. Note that the last equation is the conditional Gaussian vector field as we defined in eq. (21). This proves the statement. ^a □

^aOne can also double check this by plugging it into the continuity equation introduced later in this section.

The remainder of this section will now prove theorem 9 via the **continuity equation**, a fundamental result in mathematics and physics. To explain it, we will require the use of the **divergence** operator div , which we define as

$$\text{div}(v_t)(x) = \sum_{i=1}^d \frac{\partial}{\partial x_i} v_t(x) \quad (23)$$

Theorem 11 (Continuity Equation)

Let us consider an flow model with vector field u_t^{target} with $X_0 \sim p_{\text{init}}$. Then $X_t \sim p_t$ for all $0 \leq t \leq 1$ if and only if

$$\partial_t p_t(x) = -\text{div}(p_t u_t^{\text{target}})(x) \quad \text{for all } x \in \mathbb{R}^d, 0 \leq t \leq 1, \quad (24)$$

where $\partial_t p_t(x) = \frac{d}{dt} p_t(x)$ denotes the time-derivative of $p_t(x)$. Equation 24 is known as the **continuity equation**.

For the mathematically-inclined reader, we present a self-contained proof of the Continuity Equation in appendix B. Before we move on, let us try and understand intuitively the continuity equation. The left-hand side $\partial_t p_t(x)$ describes how much the probability $p_t(x)$ at x changes over time. Intuitively, the change should correspond to the net inflow of probability mass. For a flow model, a particle X_t follows along the vector field u_t^{target} . As you might recall from physics, the divergence measures a sort of net outflow from the vector field. Therefore, the negative divergence measures the net inflow. Scaling this by the total probability mass currently residing at x , we get that the net $-\text{div}(p_t u_t)$ measures the total inflow of probability mass. Since probability mass is conserved, the left-hand and right-hand side of the equation should be the same! We now proceed with a proof of the marginalization trick from theorem 9.

Proof. By theorem 11, we have to show that the marginal vector field u_t^{target} , as defined as in eq. (19), satisfies the continuity equation. We can do this by direct calculation:

$$\begin{aligned} \partial_t p_t(x) &\stackrel{(i)}{=} \partial_t \int p_t(x|z)p_{\text{data}}(z)dz \\ &= \int \partial_t p_t(x|z)p_{\text{data}}(z)dz \\ &\stackrel{(ii)}{=} \int -\text{div}(p_t(\cdot|z)u_t^{\text{target}}(\cdot|z))(x)p_{\text{data}}(z)dz \\ &\stackrel{(iii)}{=} -\text{div} \left(\int p_t(x|z)u_t^{\text{target}}(x|z)p_{\text{data}}(z)dz \right) \\ &\stackrel{(iv)}{=} -\text{div} \left(p_t(x) \int u_t^{\text{target}}(x|z) \frac{p_t(x|z)p_{\text{data}}(z)}{p_t(x)} dz \right)(x) \\ &\stackrel{(v)}{=} -\text{div}(p_t u_t^{\text{target}})(x), \end{aligned}$$

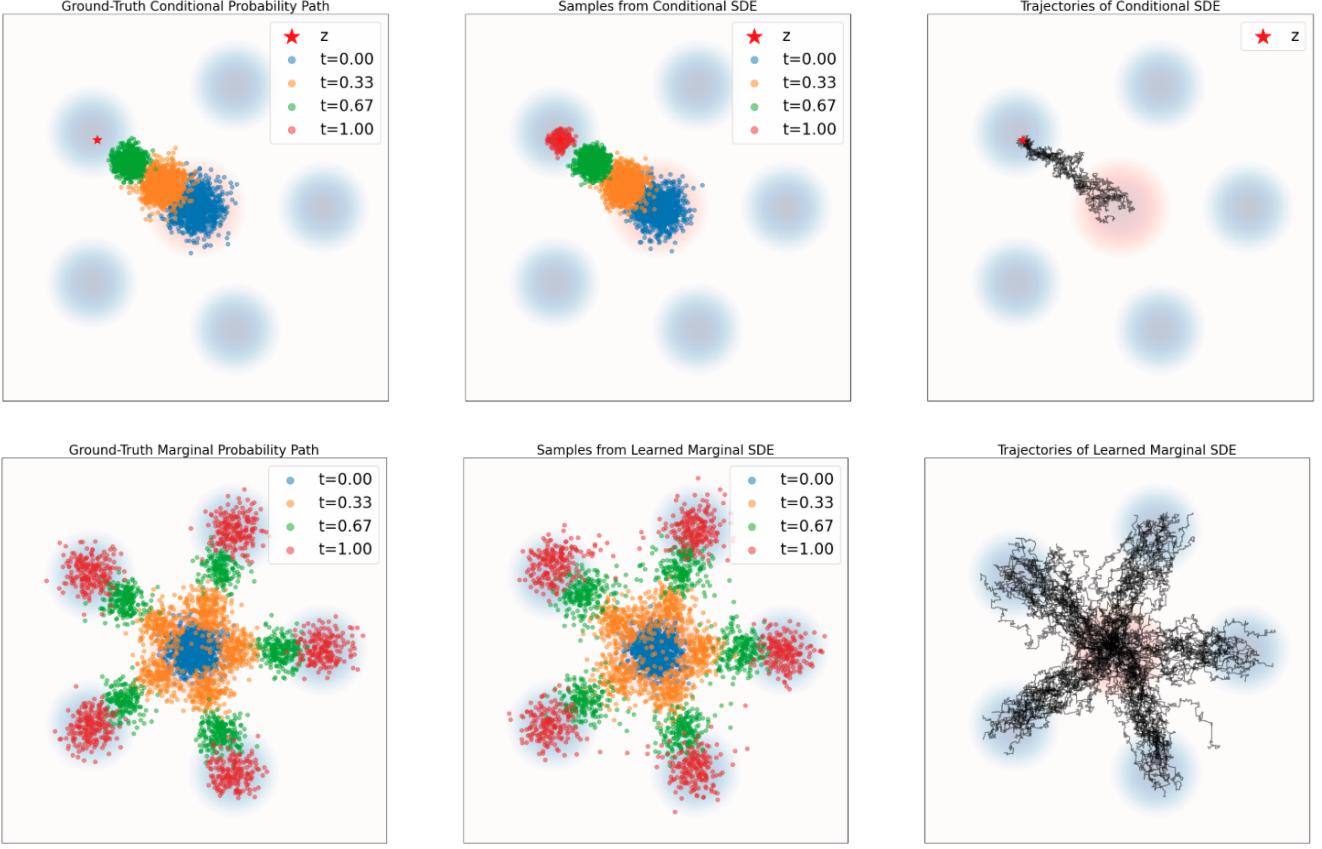


Figure 7: Illustration of theorem 12. Simulating a probability path with SDEs. This repeats the plots from fig. 6 with SDE sampling using eq. (25). Data distribution p_{data} in blue background. Gaussian p_{init} in red background. Top row: Conditional path. Bottom row: Marginal probability path. As one can see, the SDE transports samples from p_{init} into samples from δ_z (for the conditional path) and to p_{data} (for the marginal path).

where in (i) we used the definition of $p_t(x)$ in eq. (13), in (ii) we used the continuity equation for the conditional probability path $p_t(\cdot|z)$, in (iii) we swapped the integral and divergence operator using eq. (23), in (iv) we multiplied and divided by $p_t(x)$, and in (v) we used eq. (19). The beginning and end of the above chain of equations show that the continuity equation is fulfilled for u_t^{target} . By theorem 11, this is enough to imply eq. (20), and we are done. \square

3.3 Conditional and Marginal Score Functions

We just successfully constructed a training target for a flow model. We now extend this reasoning to SDEs. To do so, let us define the **marginal score function** of p_t as $\nabla \log p_t(x)$. We can use this to extend the ODE from the previous section to an SDE, as the following result demonstrates.

Theorem 12 (SDE extension trick)

Define the conditional and marginal vector fields $u_t^{\text{target}}(x|z)$ and $u_t^{\text{target}}(x)$ as before. Then, for diffusion coefficient $\sigma_t \geq 0$, we may construct an SDE which follows the same probability path, viz.,

$$X_0 \sim p_{\text{init}}, \quad dX_t = \left[u_t^{\text{target}}(X_t) + \frac{\sigma_t^2}{2} \nabla \log p_t(X_t) \right] dt + \sigma_t dW_t \quad (25)$$

$$\Rightarrow X_t \sim p_t \quad (0 \leq t \leq 1) \quad (26)$$

In particular, $X_1 \sim p_{\text{data}}$ for this SDE. The same identity holds if we replace the marginal probability $p_t(x)$ and vector field $u_t^{\text{target}}(x)$ with the conditional probability path $p_t(x|z)$ and vector field $u_t^{\text{target}}(x|z)$.

We illustrate the theorem in fig. 7. The formula in theorem 12 is useful because, similar to before, we can express the marginal score function via the **conditional score function** $\nabla \log p_t(x|z)$

$$\nabla \log p_t(x) = \frac{\nabla p_t(x)}{p_t(x)} = \frac{\nabla \int p_t(x|z)p_{\text{data}}(z)dz}{p_t(x)} = \int \frac{\nabla p_t(x|z)p_{\text{data}}(z)dz}{p_t(x)} = \int \nabla \log p_t(x|z) \frac{p_t(x|z)p_{\text{data}}(z)}{p_t(x)} dz \quad (27)$$

and the conditional score function $\nabla \log p_t(x|z)$ is something we usually know analytically, as illustrated by the following example.

Example 13 (Score Function for Gaussian Probability Paths.)

For the Gaussian path $p_t(x|z) = \mathcal{N}(x; \alpha_t z, \beta_t^2 I_d)$, we can use the form of the Gaussian probability density (see eq. (62)) to get

$$\nabla \log p_t(x|z) = \nabla \log \mathcal{N}(x; \alpha_t z, \beta_t^2 I_d) = -\frac{x - \alpha_t z}{\beta_t^2}. \quad (28)$$

Note that the score is a linear function of x . This is a unique feature of Gaussian distributions.

In the remainder of this section, we will prove theorem 12 via the *Fokker-Planck equation*, which extends the continuity equation from ODEs to SDEs. To do so, let us first define the **Laplacian** operator Δ via

$$\Delta w_t(x) = \sum_{i=1}^d \frac{\partial^2}{\partial^2 x_i} w_t(x) = \text{div}(\nabla w_t)(x). \quad (29)$$

Theorem 14 (Fokker-Planck Equation)

Let p_t be a probability path and let us consider the SDE

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

Then X_t has distribution p_t for all $0 \leq t \leq 1$ if and only if the **Fokker-Planck equation** holds:

$$\partial_t p_t(x) = -\text{div}(p_t u_t)(x) + \frac{\sigma_t^2}{2} \Delta p_t(x) \quad \text{for all } x \in \mathbb{R}^d, 0 \leq t \leq 1. \quad (30)$$

A self-contained proof of the Fokker-Planck equation can be found in appendix B. Note that the continuity equation is recovered from the Fokker-Planck equation when $\sigma_t = 0$. The additional Laplacian term Δp_t is unintuitive at first. Those familiar with physics will note that the same term also appears in the heat equation (which is in fact a special case of the Fokker-Planck equation). Let us now use the Fokker-Planck equation to help us prove theorem 12.

Proof of Theorem 12. By theorem 14, we need to show that the SDE defined in eq. (25) satisfies the Fokker-Planck equation for p_t . We can do this by direct calculation:

$$\begin{aligned} \partial_t p_t(x) &\stackrel{(i)}{=} -\text{div}(p_t u_t^{\text{target}})(x) \\ &\stackrel{(ii)}{=} -\text{div}(p_t u_t^{\text{target}})(x) - \frac{\sigma_t^2}{2} \Delta p_t(x) + \frac{\sigma_t^2}{2} \Delta p_t(x) \\ &\stackrel{(iii)}{=} -\text{div}(p_t u_t^{\text{target}})(x) - \text{div}\left(\frac{\sigma_t^2}{2} \nabla p_t\right)(x) + \frac{\sigma_t^2}{2} \Delta p_t(x) \\ &\stackrel{(iv)}{=} -\text{div}(p_t u_t^{\text{target}})(x) - \text{div}\left(p_t \left[\frac{\sigma_t^2}{2} \nabla \log p_t\right]\right)(x) + \frac{\sigma_t^2}{2} \Delta p_t(x) \\ &\stackrel{(v)}{=} -\text{div}\left(p_t \left[u_t^{\text{target}} + \frac{\sigma_t^2}{2} \nabla \log p_t\right]\right)(x) + \frac{\sigma_t^2}{2} \Delta p_t(x), \end{aligned}$$

where in (i) we used the Continuity Equation, in (ii) we added and subtracted the same term, in (iii) we used the definition of the Laplacian (eq. (29)), in (iv) we used that $\nabla \log p_t = \frac{\nabla p_t}{p_t}$, and in (v) we used the linearity of the divergence operator. The above derivation shows that the SDE defined in eq. (25) satisfies the Fokker-Planck equation for p_t . By theorem 14, this implies $X_t \sim p_t$ for $0 \leq t \leq 1$, as desired. \square

Remark 15 (Langevin dynamics.)

The above construction has a famous special case when the probability path is static, i.e. $p_t = p$ for a fixed distribution p . In this case, we set $u_t^{\text{target}} = 0$ and obtain the SDE

$$dX_t = \frac{\sigma_t^2}{2} \nabla \log p(X_t) dt + \sigma_t dW_t, \quad (31)$$

which is commonly known as **Langevin dynamics**. The fact that p_t is static implies that $\partial_t p_t(x) = 0$. It follows immediately from theorem 12 that these dynamics satisfy the Fokker-Planck equation for the static path $p_t = p$ in theorem 12. Therefore, we may conclude that p is a stationary distribution of Langevin dynamics, so that

$$X_0 \sim p \Rightarrow X_t \sim p \quad (t \geq 0)$$

As with many Markov chains, these dynamics converge to the stationary distribution p under rather general conditions (see section 3.3). That is, if we instead we take $X_0 \sim p' \neq p$, so that $X_t \sim p'_t$, then under mild conditions $p_t \rightarrow p$. This fact makes Langevin dynamics extremely useful, and it accordingly serves as the basis

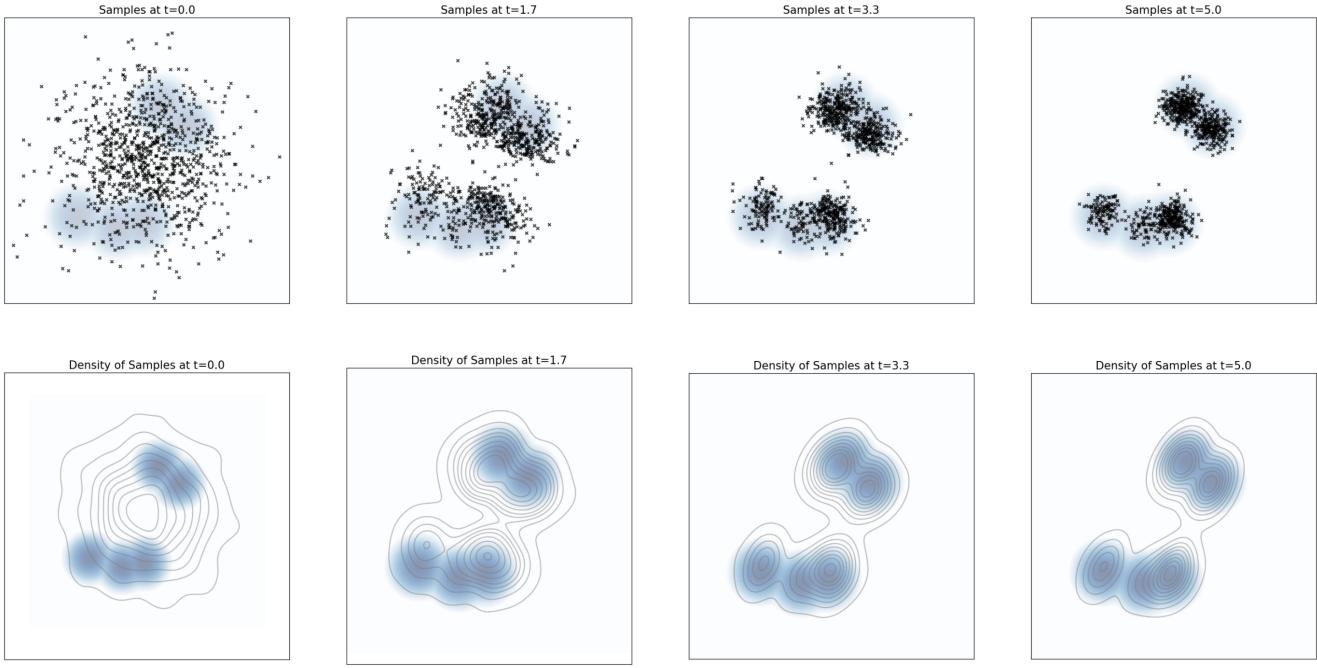


Figure 8: Top row: Particles evolving under the Langevin dynamics given by eq. (31), with $p(x)$ taken to be a Gaussian mixture with 5 modes. Bottom row: A kernel density estimate of the same samples shown in the top row. As one can see, the distribution of samples converges to the equilibrium distribution p (blue background colour).

for e.g., **molecular dynamics** simulations, and many other Markov chain Monte Carlo (MCMC) methods across Bayesian statistics and the natural sciences.

Let us summarize the results of this section.

Summary 16 (Derivation of the Training Target)

The flow training target is the marginal vector field. To construct a training target u_t^{target} for a flow model, we choose a **conditional probability path** $p_t(x|z)$ that fulfils $p_0(\cdot|z) = p_{\text{init}}$, $p_1(\cdot|z) = \delta_z$. Next, we find a **conditional vector field** $u_t^{\text{flow}}(x|z)$ such that its corresponding flow $\psi_t^{\text{target}}(x|z)$ fulfills

$$X_0 \sim p_{\text{init}} \quad \Rightarrow \quad X_t = \psi_t^{\text{target}}(X_0|z) \sim p_t(\cdot|z),$$

or, equivalently, that u_t^{target} satisfies the continuity equation. Then the **marginal vector field** defined by

$$u_t^{\text{target}}(x) = \int u_t^{\text{target}}(x|z) \frac{p_t(x|z)p_{\text{data}}(z)}{p_t(x)} dz, \quad (32)$$

follows the marginal probability path, i.e.,

$$X_0 \sim p_{\text{init}}, \quad dX_t = u_t^{\text{target}}(X_t)dt \Rightarrow X_t \sim p_t \quad (0 \leq t \leq 1). \quad (33)$$

In particular, $X_1 \sim p_{\text{data}}$ for this ODE, so that u_t^{target} "converts noise into data", as desired.

Extending to SDEs. For time-dependent diffusion coefficient $\sigma_t \geq 0$, we can extend the above ODE to an SDE with the same marginal probability path:

$$X_0 \sim p_{\text{init}}, \quad dX_t = \left[u_t^{\text{target}}(X_t) + \frac{\sigma_t^2}{2} \nabla \log p_t(X_t) \right] dt + \sigma_t dW_t \quad (34)$$

$$\Rightarrow X_t \sim p_t \quad (0 \leq t \leq 1), \quad (35)$$

where $\nabla \log p_t(x)$ is the **marginal score function**

$$\nabla \log p_t(x) = \int \nabla \log p_t(x|z) \frac{p_t(x|z)p_{\text{data}}(z)}{p_t(x)} dz. \quad (36)$$

In particular, for the trajectories X_t of the above SDE, it holds that $X_1 \sim p_{\text{data}}$, so that the SDE "converts noise into data", as desired. An important example is the **Gaussian probability path**, yielding the formulae:

$$p_t(x|z) = \mathcal{N}(x; \alpha_t z, \beta_t^2 I_d) \quad (37)$$

$$u_t^{\text{flow}}(x|z) = \left(\dot{\alpha}_t - \frac{\dot{\beta}_t}{\beta_t} \alpha_t \right) z + \frac{\dot{\beta}_t}{\beta_t} x \quad (38)$$

$$\nabla \log p_t(x|z) = - \frac{x - \alpha_t z}{\beta_t^2}, \quad (39)$$

for **noise schedulers** $\alpha_t, \beta_t \in \mathbb{R}$: continuously differentiable, monotonic functions such that $\alpha_0 = \beta_1 = 0$ $\alpha_1 = \beta_0 = 1$.

4 Training the Generative Model

In the last two sections, we showed how to construct a generative model with a vector field u_t^θ given by a neural network, and we derived a formula for the training target u_t^{target} against which we might regress u_t^θ . In this section, we will describe how to train the neural network u_t^θ to approximate the training target u_t^{target} . First, we restrict ourselves to ODEs again, in doing so recovering **flow matching**. Second, we explain how to extend the approach to SDEs via **score matching**. Finally, we consider the special case of Gaussian probability paths, in doing so recovering **denoising diffusion models**. With these tools, we will at last have an end-to-end procedure to train and sample from a generative model with ODEs and SDEs.

4.1 Flow Matching

As before, let us consider a flow model given by

$$X_0 \sim p_{\text{init}}, \quad dX_t = u_t^\theta(X_t) dt. \quad (\text{flow model}) \quad (40)$$

As we learned, we want the neural network u_t^θ to equal the marginal vector field u_t^{target} . In other words, we would like to find parameters θ so that $u_t^\theta \approx u_t^{\text{target}}$. In the following, we denote by $\text{Unif} = \text{Unif}_{[0,1]}$ the uniform distribution on the interval $[0, 1]$, and by \mathbb{E} , the expected value operator. Perhaps the most direct way of obtaining $u_t^\theta \approx u_t^{\text{target}}$ is to regress directly with the **flow matching loss**, defined as,

$$\mathcal{L}_{\text{fm}}(\theta) = \mathbb{E}_{t \sim \text{Unif}, x \sim p_t} [\|u_t^\theta(x) - u_t^{\text{target}}(x)\|^2] \quad (41)$$

$$\stackrel{(i)}{=} \mathbb{E}_{t \sim \text{Unif}, z \sim p_{\text{data}}, x \sim p_t(\cdot|z)} [\|u_t^\theta(x) - u_t^{\text{target}}(x)\|^2], \quad (42)$$

where $p_t(x) = \int p_t(x|z)p_{\text{data}}(z)dz$ is the marginal probability path and in (i) we used the sampling procedure given by eq. (13). Intuitively, this loss says: First, draw a random time $t \in [0, 1]$. Second, draw a random point z from our data set, sample from $p_t(\cdot|z)$ (e.g. by adding some noise), and compute $u_t^\theta(x)$. Finally, compute the mean squared error between the output of our neural network and the marginal vector field $u_t^{\text{target}}(x)$. Unfortunately, we are *not* done here. While we do know the formula for u_t^{target} by theorem 9

$$u_t^{\text{target}}(x) = \int u_t^{\text{target}}(x|z) \frac{p_t(x|z)p_{\text{data}}(z)}{p_t(x)} dz, \quad (43)$$

we cannot compute it efficiently because the above integral is intractable. Instead, we will exploit the fact that the *conditional* velocity field $u_t^{\text{target}}(x|z)$ is tractable. To do so, let us define the **conditional flow matching loss**

$$\mathcal{L}_{\text{cfm}}(\theta) = \mathbb{E}_{z \sim p_{\text{data}}, x \sim p_t(\cdot|z)} [\|u_t^\theta(x) - u_t^{\text{target}}(x|z)\|^2]. \quad (44)$$

Note the difference to eq. (41): we use the conditional vector field $u_t^{\text{target}}(x|z)$ instead of the marginal vector $u_t^{\text{target}}(x)$. As we have an analytical formula for $u_t^{\text{target}}(x|z)$, we can minimize the above loss easily. But wait, what sense does it make to regress against the conditional vector field if it's the marginal vector field we care about? As it turns out, by *explicitly* regressing against the tractable, conditional vector field, we are *implicitly* regressing against the intractable, marginal vector field. The next result makes this intuition precise.

Theorem 17

The marginal flow matching loss equals the conditional flow matching loss up to a constant. That is,

$$\mathcal{L}_{\text{fm}}(\theta) = \mathcal{L}_{\text{cfm}}(\theta) + C,$$

where C is independent of θ . Therefore, their gradients coincide:

$$\nabla_{\theta} \mathcal{L}_{\text{fm}}(\theta) = \nabla_{\theta} \mathcal{L}_{\text{cfm}}(\theta).$$

Hence, minimizing $\mathcal{L}_{\text{cfm}}(\theta)$ with e.g., stochastic gradient descent (SGD) is equivalent to minimizing $\mathcal{L}_{\text{fm}}(\theta)$ with in the same fashion. In particular, for the minimizer θ^* of $\mathcal{L}_{\text{cfm}}(\theta)$, it will hold that $u_t^{\theta^*} = u_t^{\text{target}}$ (assuming an infinitely expressive parameterization).

Proof. The proof works by expanding the mean squared error into 3 components and removing constants:

$$\begin{aligned} \mathcal{L}_{\text{fm}}(\theta) &\stackrel{(i)}{=} \mathbb{E}_{t \sim \text{Unif}, x \sim p_t} [\|u_t^{\theta}(x) - u_t^{\text{target}}(x)\|^2] \\ &\stackrel{(ii)}{=} \mathbb{E}_{t \sim \text{Unif}, x \sim p_t} [\|u_t^{\theta}(x)\|^2 - 2u_t^{\theta}(x)^T u_t^{\text{target}}(x) + \|u_t^{\text{target}}(x)\|^2] \\ &\stackrel{(iii)}{=} \mathbb{E}_{t \sim \text{Unif}, x \sim p_t} [\|u_t^{\theta}(x)\|^2] - 2\mathbb{E}_{t \sim \text{Unif}, x \sim p_t} [u_t^{\theta}(x)^T u_t^{\text{target}}(x)] + \underbrace{\mathbb{E}_{t \sim \text{Unif}_{[0,1]}, x \sim p_t} [\|u_t^{\text{target}}(x)\|^2]}_{=:C_1} \\ &\stackrel{(iv)}{=} \mathbb{E}_{t \sim \text{Unif}, z \sim p_{\text{data}}, x \sim p_t(\cdot|z)} [\|u_t^{\theta}(x)\|^2] - 2\mathbb{E}_{t \sim \text{Unif}, x \sim p_t} [u_t^{\theta}(x)^T u_t^{\text{target}}(x)] + C_1 \end{aligned}$$

where (i) holds by definition, in (ii) we used the formula $\|a - b\|^2 = \|a\|^2 - 2a^b + \|b\|^2$, in (iii) we define a constant C_1 and in (iv) we used the sampling procedure of p_t given by eq. (13). Let us re-express the second summand:

$$\begin{aligned} \mathbb{E}_{t \sim \text{Unif}, x \sim p_t} [u_t^{\theta}(x)^T u_t^{\text{target}}(x)] &\stackrel{(i)}{=} \int_0^1 \int p_t(x) u_t^{\theta}(x)^T u_t^{\text{target}}(x) dx dt \\ &\stackrel{(ii)}{=} \int_0^1 \int p_t(x) u_t^{\theta}(x)^T \left[\int u_t^{\text{target}}(x|z) \frac{p_t(x|z)p_{\text{data}}(z)}{p_t(x)} dz \right] dx dt \\ &\stackrel{(iii)}{=} \int_0^1 \int \int u_t^{\theta}(x)^T u_t^{\text{target}}(x|z) p_t(x|z) p_{\text{data}}(z) dz dx dt \\ &\stackrel{(iv)}{=} \mathbb{E}_{t \sim \text{Unif}, z \sim p_{\text{data}}, x \sim p_t(\cdot|z)} [u_t^{\theta}(x)^T u_t^{\text{target}}(x|z)] \end{aligned}$$

where in (i) we expressed the expected value as an integral, in (ii) we use eq. (43), in (iii) we use the fact that integrals are linear, in (iv) we express the integral as an expected value. Note that this was really the crucial step of the proof: The beginning of the equality used the marginal vector field $u_t^{\text{target}}(x)$, while the end uses the

conditional vector field $u_t^{\text{target}}(x|z)$. We plug this into the equation for \mathcal{L}_{fm} to get:

$$\begin{aligned}\mathcal{L}_{\text{fm}}(\theta) &\stackrel{(i)}{=} \mathbb{E}_{t \sim \text{Unif}, z \sim p_{\text{data}}, x \sim p_t(\cdot|z)} [\|u_t^\theta(x)\|^2] - 2\mathbb{E}_{t \sim \text{Unif}, z \sim p_{\text{data}}, x \sim p_t(\cdot|z)} [u_t^\theta(x)^T u_t^{\text{target}}(x|z)] + C_1 \\ &\stackrel{(ii)}{=} \mathbb{E}_{t \sim \text{Unif}, z \sim p_{\text{data}}, x \sim p_t(\cdot|z)} [\|u_t^\theta(x)\|^2 - 2u_t^\theta(x)^T u_t^{\text{target}}(x|z) + \|u_t^{\text{target}}(x|z)\|^2 - \|u_t^{\text{target}}(x|z)\|^2] + C_1 \\ &\stackrel{(iii)}{=} \mathbb{E}_{t \sim \text{Unif}, z \sim p_{\text{data}}, x \sim p_t(\cdot|z)} [\|u_t^\theta(x) - u_t^{\text{target}}(x|z)\|^2] + \underbrace{\mathbb{E}_{t \sim \text{Unif}, z \sim p_{\text{data}}, x \sim p_t(\cdot|z)} [-\|u_t^{\text{target}}(x|z)\|^2]}_{C_2} + C_1 \\ &\stackrel{(iv)}{=} \mathcal{L}_{\text{cfm}}(\theta) + \underbrace{C_2 + C_1}_{=:C}\end{aligned}$$

where in (i) we plugged in the derived equation, in (ii) we added and subtracted the same value, in (iii) we used the formula $\|a - b\|^2 = \|a\|^2 - 2a^T b + \|b\|^2$ again, and in (iv) we defined a constant in θ . This finishes the proof. \square

Once u_t^θ has been trained, we may simulate the ODE model

$$X_0 \sim p_{\text{init}}, \quad dX_t = u_t^\theta(X_t) dt \quad (45)$$

via e.g., algorithm 1 to obtain samples $X_1 \sim p_{\text{data}}$. This whole pipeline is called **flow matching** in the literature [8, 10]. The training procedure is summarized in algorithm 3 and visualized in fig. 9. Let us now instantiate the conditional flow matching loss for the choice of Gaussian probability paths:

Example 18 (Flow Matching for Gaussian Conditional Probability Paths)

Let us return to the example of Gaussian probability paths $p_t(\cdot|z) = \mathcal{N}(\alpha_t z; \beta_t^2 I_d)$, where we may sample from the conditional path via

$$\epsilon \sim \mathcal{N}(0, I_d) \quad \Rightarrow \quad x_t = \alpha_t z + \beta_t \epsilon \sim \mathcal{N}(\alpha_t z, \beta_t^2 I_d) = p_t(\cdot|z). \quad (46)$$

As we derived in eq. (21), the conditional vector field $u_t^{\text{target}}(x|z)$ is given by

$$u_t^{\text{target}}(x|z) = \left(\dot{\alpha}_t - \frac{\dot{\beta}_t}{\beta_t} \alpha_t \right) z + \frac{\dot{\beta}_t}{\beta_t} x, \quad (47)$$

where $\dot{\alpha}_t = \partial_t \alpha_t$ and $\dot{\beta}_t = \partial_t \beta_t$ are the respective time derivatives. Plugging in this formula, the conditional flow matching loss reads

$$\begin{aligned}\mathcal{L}_{\text{cfm}}(\theta) &= \mathbb{E}_{t \sim \text{Unif}, z \sim p_{\text{data}}, x \sim \mathcal{N}(\alpha_t z, \beta_t^2 I_d)} [\|u_t^\theta(x) - \left(\dot{\alpha}_t - \frac{\dot{\beta}_t}{\beta_t} \alpha_t \right) z - \frac{\dot{\beta}_t}{\beta_t} x\|^2] \\ &\stackrel{(i)}{=} \mathbb{E}_{t \sim \text{Unif}, z \sim p_{\text{data}}, \epsilon \sim \mathcal{N}(0, I_d)} [\|u_t^\theta(\alpha_t z + \beta_t \epsilon) - (\dot{\alpha}_t z + \dot{\beta}_t \epsilon)\|^2]\end{aligned}$$

where in (i) we plugged in eq. (46) and replaced x by $\alpha_t z + \beta_t \epsilon$. Note the simplicity of \mathcal{L}_{cfm} : We sample a data point z , sample some noise ϵ and then we take a mean squared error. Let us make this even more concrete for the special case of $\alpha_t = t$, and $\beta_t = 1 - t$. The corresponding probability $p_t(x|z) = \mathcal{N}(tz, (1-t)^2)$ is sometimes

referred to as the (Gaussian) **CondOT probability path**. Then we have $\dot{\alpha}_t = 1$, $\dot{\beta}_t = -1$, so that

$$\mathcal{L}_{\text{cfm}}(\theta) = \mathbb{E}_{t \sim \text{Unif}, z \sim p_{\text{data}}, \epsilon \sim \mathcal{N}(0, I_d)} [\|u_t^\theta(tz + (1-t)\epsilon) - (z - \epsilon)\|^2]$$

Many famous state-of-the-art models have been trained using this simple yet effective procedure, e.g. *Stable Diffusion 3*, *Meta’s MovieGen*, and probably many more proprietary models. In fig. 9, we visualize it in a simple example and in algorithm 3 we summarize the training procedure.

Algorithm 3 Flow Matching Training Procedure (here for Gaussian CondOT path $p_t(x|z) = \mathcal{N}(tz, (1-t)^2)$)

Require: A dataset of samples $z \sim p_{\text{data}}$, neural network u_t^θ

$$\mathcal{L}(\theta) = \|u_t^\theta(x) - (z - \epsilon)\|^2 \quad (\text{General case: } = \|u_t^\theta(x) - u_t^{\text{target}}(x|z)\|^2)$$

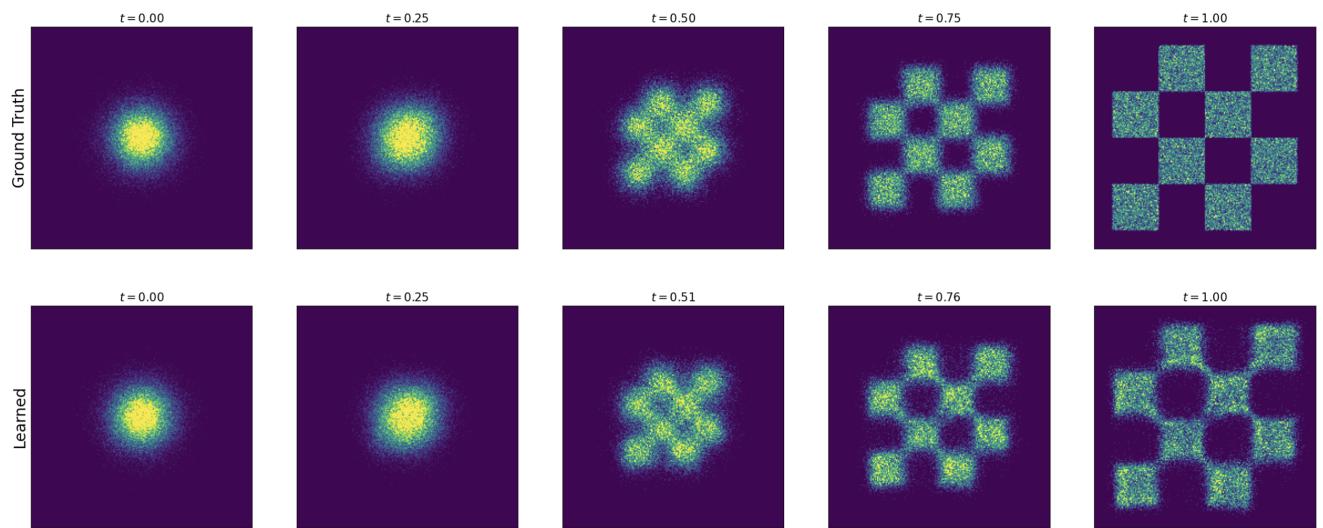


Figure 9: Illustration of theorem 17 with a Gaussian CondOT probability path: simulating an ODE from a trained flow matching model. The data distribution is the chess board pattern (top right). Top row: Histogram from ground truth marginal probability path $p_t(x)$. Bottom row: Histogram of samples from flow matching model. As one can see, the top row and bottom row match after training (up to training error). The model was trained using algorithm 3.

4.2 Score matching

Let us extend the algorithm we just found from ODEs to SDEs. Remember we can extend the target ODE to an SDE with the same marginal distribution given by

$$X_0 \sim p_{\text{init}}, \quad dX_t = \left[u_t^{\text{target}}(X_t) + \frac{\sigma_t^2}{2} \nabla \log p_t(X_t) \right] dt + \sigma_t dW_t \quad (48)$$

$$\Rightarrow X_t \sim p_t \quad (0 \leq t \leq 1) \quad (49)$$

where u_t^{target} is the marginal vector field and $\nabla \log p_t(x)$ is the **marginal score** function represented via the formula:

$$\nabla \log p_t(x) = \int \nabla \log p_t(x|z) \frac{p_t(x|z)p_{\text{data}}(z)}{p_t(x)} dz \quad (50)$$

To approximate the marginal score $\nabla \log p_t$, we can use a neural network that we call **score network** $s_t^\theta : \mathbb{R}^d \times [0, 1] \rightarrow \mathbb{R}^d$. In the same way as before, we can design a **score matching** loss and a conditional loss, commonly called the **denoising score matching** loss:

$$\begin{aligned} \mathcal{L}_{\text{sm}}(\theta) &= \mathbb{E}_{t \sim \text{Unif}, z \sim p_{\text{data}}, x \sim p_t(\cdot|z)} [\|s_t^\theta(x) - \nabla \log p_t(x)\|^2] && \text{(score matching loss)} \\ \mathcal{L}_{\text{dsm}}(\theta) &= \mathbb{E}_{t \sim \text{Unif}, z \sim p_{\text{data}}, x \sim p_t(\cdot|z)} [\|s_t^\theta(x) - \nabla \log p_t(x|z)\|^2] && \text{(denoising score matching loss)} \end{aligned}$$

where again the difference is using the marginal score $\nabla \log p_t(x)$ vs. using the conditional score $\nabla \log p_t(x|z)$. As before, we ideally would want to minimize the score matching loss but can't because we don't know $\nabla \log p_t(x)$. But similarly as before, the denoising score matching loss is a tractable alternative:

Theorem 19

The score matching loss equals the denoising score matching loss up to a constant:

$$\mathcal{L}_{\text{sm}}(\theta) = \mathcal{L}_{\text{dsm}}(\theta) + C$$

where C is independent of parameters θ . Therefore, their gradients coincide:

$$\nabla_\theta \mathcal{L}_{\text{sm}}(\theta) = \nabla_\theta \mathcal{L}_{\text{dsm}}(\theta)$$

In particular, for the minimizer θ^* , it will hold that $s_t^{\theta^*} = \nabla \log p_t$.

Proof. Note that the formula for $\nabla \log p_t$ (eq. (50)) looks the same as the formula for u_t^{target} (eq. (43)). Therefore, the proof is identical to the proof of theorem 17 replacing u_t^{target} with $\nabla \log p_t$. \square

The above procedure describes the vanilla procedure of training a diffusion model. After training, we can choose an arbitrary diffusion coefficient $\sigma_t \geq 0$ and then simulate the SDE

$$X_0 \sim p_{\text{init}}, \quad dX_t = \left[u_t^\theta(X_t) + \frac{\sigma_t^2}{2} s_t^\theta(X_t) \right] dt + \sigma_t dW_t \quad (51)$$

to generate samples $X_1 \sim p_{\text{data}}$. In theory, every σ_t should give samples $X_1 \sim p_{\text{data}}$ at perfect training. In practice, we encounter two types of errors: (1) simulation errors by simulating the SDE imperfectly and (2) training errors (by

not training perfectly). Therefore, there is an optimal unknown noise level σ_t - this can be determined empirically by just testing our different values of empirically (see e.g. [1, 7, 11]). At first sight, it might seem to be a disadvantage that we have to learn both s_t^θ, u_t^θ if we wanted to use diffusion model now as opposed to a flow model. However, note we can often express s_t^θ, u_t^θ in one single network with two outputs. So it is usual minimally more computational effort. Further, as we will see now, for the special case for the Gaussian probability path, we don't have to train them separately as they can be converted into one another.

Remark 20 (Denoising Diffusion Models)

If you are familiar with diffusion models, you have probably encountered the term **denoising diffusion model**. This model has become so popular that most people nowadays drop the word "denoising" and simply use the term "diffusion model" to describe it. While denoising diffusion models do not traditionally operate in unit time (i.e., noise at $t = 0$ and data at $t = 1$), they involve a nearly identical notion of probability path which, under appropriate time re-scaling, can be seen to correspond to the special case of Gaussian probability paths $p_t(\cdot|z) = \mathcal{N}(\alpha_t z; \beta_t^2 I_d)$ defined in these notes. As we will see next, in this case, we don't have to learn s_t^θ and u_t^θ separately.

Example 21 (Denoising Diffusion Models: Score Matching for Gaussian Probability Paths)

First, let us instantiate the denoising score matching loss for the case of $p_t(x|z) = \mathcal{N}(\alpha_t z; \beta_t^2 I_d)$. As we derived in eq. (28), the conditional score $\nabla \log p_t(x|z)$ has the formula

$$\nabla \log p_t(x|z) = -\frac{x - \alpha_t z}{\beta_t^2} \quad (52)$$

Plugging in this formula, the denoising score matching loss becomes:

$$\begin{aligned} \mathcal{L}_{\text{dsm}}(\theta) &= \mathbb{E}_{t \sim \text{Unif}, z \sim p_{\text{data}}, x \sim p_t(\cdot|z)} [\|s_t^\theta(x) + \frac{x - \alpha_t z}{\beta_t^2}\|^2] \\ &\stackrel{(i)}{=} \mathbb{E}_{t \sim \text{Unif}, z \sim p_{\text{data}}, \epsilon \sim \mathcal{N}(0, I_d)} [\|s_t^\theta(\alpha_t z + \beta_t \epsilon) + \frac{\epsilon}{\beta_t}\|^2] \\ &= \mathbb{E}_{t \sim \text{Unif}, z \sim p_{\text{data}}, \epsilon \sim \mathcal{N}(0, I_d)} [\frac{1}{\beta_t^2} \|\beta_t s_t^\theta(\alpha_t z + \beta_t \epsilon) + \epsilon\|^2] \end{aligned}$$

where in (i) we plugged in eq. (46) and replaced x by $\alpha_t z + \beta_t \epsilon$. It was soon realized that the above loss is numerically unstable for $\beta_t \approx 0$ close to zero (i.e. denoising score matching only works if you add a sufficient amount of noise). In some of the first works on denoising diffusion models (see *Denoising Diffusion Probabilistic Models*, [5]) it was therefore proposed to drop the constant $\frac{1}{\beta_t^2}$ in the loss and reparameterize s_t^θ into a **noise predictor** network $\epsilon_t^\theta : \mathbb{R}^d \times [0, 1] \rightarrow \mathbb{R}^d$ via:

$$-\beta_t s_t^\theta(x) = \epsilon_t^\theta(x) \quad \Rightarrow \quad \mathcal{L}_{\text{ddpm}}(\theta) = \mathbb{E}_{t \sim \text{Unif}, z \sim p_{\text{data}}, \epsilon \sim \mathcal{N}(0, I_d)} [\|\epsilon_t^\theta(\alpha_t z + \beta_t \epsilon) - \epsilon\|^2]$$

Note that the network ϵ_t^θ essentially learns to predict the noise that was used to corrupt a data sample z . With this, it also becomes apparent why it is called *denoising* score matching: because the network learns to predict the noise ϵ that corrupted a data point z . In algorithm 4, we summarize the training procedure.

Algorithm 4 Score Matching Training Procedure for Gaussian probability path

Require: A dataset of samples $z \sim p_{\text{data}}$, score network s_t^θ or noise predictor ϵ_t^θ

- 1: **for** each mini-batch of data **do**
- 2: Sample a data example z from the dataset.
- 3: Sample a random time $t \sim \text{Unif}_{[0,1]}$.
- 4: Sample noise $\epsilon \sim \mathcal{N}(0, I_d)$
- 5: Set $x_t = \alpha_t z + \beta_t \epsilon$ (General case: $x_t \sim p_t(\cdot|z)$)
- 6: Compute loss

$$\mathcal{L}(\theta) = \|s_t^\theta(x_t) + \frac{\epsilon}{\beta_t}\|^2 \quad (\text{General case: } = \|s_t^\theta(x_t) - \nabla \log p_t(x_t|z)\|^2)$$

Alternatively: $\mathcal{L}(\theta) = \|\epsilon_t^\theta(x_t) - \epsilon\|^2$

- 7: Update the model parameters θ via gradient descent on $\mathcal{L}(\theta)$.
- 8: **end for**

Beyond its simplicity, there is another useful property of the Gaussian probability path: By learning s_t^θ or ϵ_t^θ , we also learn u_t^θ automatically and the other way around:

Proposition 1 (Conversion formula for Gaussian probability path)

For the Gaussian probability path $p_t(x|z) = \mathcal{N}(\alpha_t z, \beta_t^2 I_d)$, it holds that that the conditional (resp. marginal) vector field can be converted into the conditional (resp. marginal) score:

$$\begin{aligned} u_t^{\text{target}}(x|z) &= \left(\beta_t^2 \frac{\dot{\alpha}_t}{\alpha_t} - \dot{\beta}_t \beta_t \right) \nabla \log p_t(x|z) + \frac{\dot{\alpha}_t}{\alpha_t} x \\ u_t^{\text{target}}(x) &= \left(\beta_t^2 \frac{\dot{\alpha}_t}{\alpha_t} - \dot{\beta}_t \beta_t \right) \nabla \log p_t(x) + \frac{\dot{\alpha}_t}{\alpha_t} x \end{aligned}$$

where the formula for the above marginal vector field u_t^{target} is called **probability flow ODE** in the literature (more correctly, the corresponding ODE).

Proof. For the conditional vector field and conditional score, we can derive:

$$u_t^{\text{target}}(x|z) = \left(\dot{\alpha}_t - \frac{\dot{\beta}_t}{\beta_t} \alpha_t \right) z + \frac{\dot{\beta}_t}{\beta_t} x \stackrel{(i)}{=} \left(\beta_t^2 \frac{\dot{\alpha}_t}{\alpha_t} - \dot{\beta}_t \beta_t \right) \left(\frac{\alpha_t z - x}{\beta_t^2} \right) + \frac{\dot{\alpha}_t}{\alpha_t} x = \left(\beta_t^2 \frac{\dot{\alpha}_t}{\alpha_t} - \dot{\beta}_t \beta_t \right) \nabla \log p_t(x|z) + \frac{\dot{\alpha}_t}{\alpha_t} x$$

where in (i) we just did some algebra. By taking integrals, the same identity holds for the marginal flow vector field and the marginal score function:

$$\begin{aligned} u^{\text{target}}(x) &= \int u_t^{\text{target}}(x|z) \frac{p_t(x|z)p_{\text{data}}(z)}{p_t(x)} dz = \int \left[\left(\beta_t^2 \frac{\dot{\alpha}_t}{\alpha_t} - \dot{\beta}_t \beta_t \right) \nabla \log p_t(x|z) + \frac{\dot{\alpha}_t}{\alpha_t} x \right] \frac{p_t(x|z)p_{\text{data}}(z)}{p_t(x)} dz \\ &\stackrel{(i)}{=} \left(\beta_t^2 \frac{\dot{\alpha}_t}{\alpha_t} - \dot{\beta}_t \beta_t \right) \nabla \log p_t(x) + \frac{\dot{\alpha}_t}{\alpha_t} x \end{aligned}$$

where in (i) we used eq. (50). \square

We can use the conversion formula to parameterize the score network s_t^θ and the vector field network u_t^θ into one

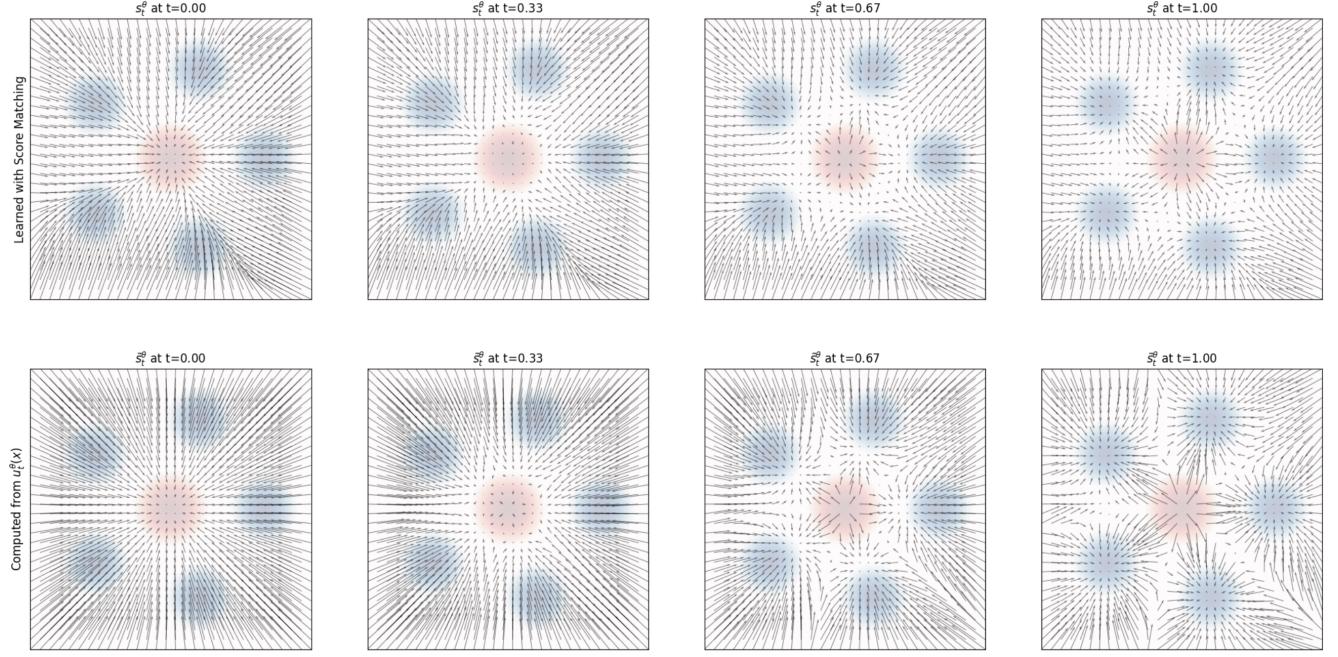


Figure 10: A comparison of the score, as parameterized in two different ways. Top: A visualization of the score field $s_t^\theta(x)$ learned independently with score matching (see algorithm 4). Bottom: A visualization of the score field $\tilde{s}_t^\theta(x)$ parameterized using $u_t^\theta(x)$ as in eq. (54).

another via

$$u_t^\theta = \left(\beta_t^2 \frac{\dot{\alpha}_t}{\alpha_t} - \dot{\beta}_t \beta_t \right) s_t^\theta(x) + \frac{\dot{\alpha}_t}{\alpha_t} x. \quad (53)$$

Similarly, so long as $\beta_t^2 \dot{\alpha}_t - \alpha_t \dot{\beta}_t \beta_t \neq 0$ (always true for $t \in [0, 1]$), it follows that

$$s_t^\theta(x) = \frac{\alpha_t u_t^\theta(x) - \dot{\alpha}_t x}{\beta_t^2 \dot{\alpha}_t - \alpha_t \dot{\beta}_t \beta_t}. \quad (54)$$

Using this parameterization, it can be shown that the denoising score matching and the conditional flow matching losses are the same up to a constant. We conclude that **for Gaussian probability paths there is no need to separately train both the marginal score and the marginal vector field, as knowledge of one is sufficient to compute the other. In particular, we can choose whether we want to use flow matching or score matching to train it.** In fig. 10, we compare visually the score as approximated using score matching and the parameterized score using eq. (54). If we have trained a score network s_t^θ , we know by eq. (51) that we can use arbitrary $\sigma_t \geq 0$ to sample from the SDE

$$X_0 \sim p_{\text{init}}, \quad dX_t = \left[\left(\beta_t^2 \frac{\dot{\alpha}_t}{\alpha_t} - \dot{\beta}_t \beta_t + \frac{\sigma_t^2}{2} \right) s_t^\theta(x) + \frac{\dot{\alpha}_t}{\alpha_t} x \right] dt + \sigma_t dW_t \quad (55)$$

to obtain samples $X_1 \sim p_{\text{data}}$ (up to training and simulation error). This corresponds to **stochastic sampling from a denoising diffusion model.**

4.3 Optional: A Guide to the Diffusion Model Literature

There is a whole family of models around diffusion models and flow matching in the literature. If you will read these papers, you will likely find a different way of presenting the material from this class. This makes it sometimes a little confusing to read these papers. For this reason, we want to give a brief overview over various frameworks and their differences and put them also in their historical context. **This is not necessary to understand the remainder of this document** but rather intended to be a support for you in case you read the literature.

Discrete time vs. continuous time. The first denoising diffusion model papers [15, 16, 5] did not use SDEs but constructed Markov chains in **discrete time**, i.e. with time steps $t = 0, 1, 2, 3, \dots$. To this date, you will find a lot of works in the literature working with this discrete-time formulation. While this construction is appealing due its simplicity, the disadvantage of the time-discrete approach was that it forces you to choose a time discretization before training. Further, the loss function needed to be approximated via an **evidence lower bound (ELBO)** - which is, as the name suggests, only a lower bound to the loss we actually want to minimize. Later, Song et al. [19] showed that these constructions were essentially approximation of a time-continuous SDEs. Further, the ELBO loss becomes tight (i.e. it is not a lower bound anymore) in the time-continuous case (e.g. note that theorem 17 and theorem 19 are equalities and not lower bounds - this would be different in the time discrete case). This made the SDE construction popular because this construction was considered mathematically "cleaner" and that one could control the simulation error via ODE/SDE samplers post training. It is important to note however that both models employ the same loss and are *not* fundamentally different.

"Forward process" vs probability paths. The first wave of denoising diffusion models [15, 16, 5, 19] did not use the term *probability path* but constructed a noising procedure of a data point $z \in \mathbb{R}^d$ via a so-called **forward process**. This is an SDE of the form

$$\bar{X}_0 = z, \quad d\bar{X}_t = u_t^{\text{forw}}(\bar{X}_t)dt + \sigma_t^{\text{forw}}d\bar{W}_t \quad (56)$$

The idea is that after drawing a data point $z \sim p_{\text{data}}$ one simulates the forward process and thereby corrupts or "noises" the data. The forward process is designed such that for $t \rightarrow \infty$ its distribution converges to a Gaussian $\mathcal{N}(0, I_d)$. In other words, for $T \gg 0$, $\bar{X}_T \sim \mathcal{N}(0, I_d)$ approximately. Note that this essentially corresponds to a probability path: the conditional distribution of \bar{X}_t given $\bar{X}_0 = z$ is a conditional probability path $\bar{p}_t(\cdot|z)$ and the distribution of \bar{X}_t marginalized over $z \sim p_{\text{data}}$ corresponds to a marginal probability path \bar{p}_t .² The term probability path was introduced by flow matching [8] to both simplify the construction and make it more general at the same time: First, the "forward process" of diffusion models is never actually simulated (only samples from $\bar{p}_t(\cdot|z)$ are drawn during training). Second, a forward process only converges for $t \rightarrow \infty$ (i.e. we will never arrive at p_{init} in finite time). Finally, with this construction, we need to know the distribution of $X_t | X_0 = z$ in closed form in order to train our models to avoid simulating the SDE. This essentially restricts the vector field u_t^{forw} to ones such that we know the distribution $\bar{X}_t | \bar{X}_0 = z$ in closed form. Therefore, throughout the diffusion model literature, vector fields in forward processes are always of the affine form, i.e. $u_t^{\text{forw}}(x) = a_t x$ for some continuous function a_t . For

²Note however that they use an **inverted time convention**: $\bar{p}_0(\cdot|z) = p_{\text{data}}$ here.

this choice, we can use known formulas of the conditional distribution [14, 18, 7]:

$$\bar{X}_t | \bar{X}_0 = z \sim \mathcal{N}(\alpha_t z, \beta_t^2 I), \quad \alpha_t = \exp\left(\int_0^t a_r dr\right), \quad \beta_t^2 = \alpha_t^2 \int_0^t \frac{(\sigma_r^{\text{forw}})^2}{\alpha_r^2} dr$$

Note that these are simply Gaussian probability paths. Therefore, one can say that **a forward process is a specific way of constructing a (Gaussian) probability path.**

Time-Reversals vs Solving the Fokker-Planck equation. The original description of diffusion models did not construct the training target u_t^{target} or $\nabla \log p_t$ via the Fokker-Planck equation (or Continuity equation) but via a **time-reversal** of the forward process [2]. A time-reversal $(X_t)_{0 \leq t \leq T}$ is an SDE with the same distribution over trajectories inverted in time, i.e.

$$\mathbb{P}[\bar{X}_{t_1} \in A_1, \dots, \bar{X}_{t_n} \in A_n] = \mathbb{P}[X_{T-t_1} \in A_1, \dots, X_{T-t_n} \in A_n] \quad (57)$$

$$\text{for all } 0 \leq t_1, \dots, t_n \leq T, \text{ and } A_1, \dots, A_n \subset S \quad (58)$$

As shown in Anderson [2], one can obtain a time-reversal satisfying the above condition by the SDE:

$$dX_t = [-u_t(X_t) + \sigma_t^2 \nabla \log p_t(X_t)] dt + \sigma_t dW_t, \quad u_t(x) = u_{T-t}^{\text{forw}}(x), \sigma_t = \bar{\sigma}_{T-t}$$

As $u_t(X_t) = a_t X_t$, the above corresponds to a specific instance of training target we derived in proposition 1 (this is not immediately trivial as different time conventions are used. See e.g. [9] for a derivation). However, for the purposes of generative modeling, we often only use the final point X_1 of the Markov process (e.g., as a generated image) and discard earlier time points. Therefore, whether a Markov process is a “true” time-reversal or follows along a probability path does not matter for many applications. Therefore, using a time-reversal is not necessary and often leads to suboptimal results, e.g. the probability flow ODE is often better [7, 11]. All ways of sampling from a diffusion models that are different from the time-reversal rely again on using the Fokker-Planck equation. We hope that this illustrates why nowadays many people construct the training targets directly via the Fokker-Planck equation - as pioneered by [8, 10, 1] and done in this class.

Flow Matching [8] and Stochastic Interpolants [1]. The framework that we present is most closely related to the frameworks of flow matching and **stochastic interpolants (SIs)**. As we learnt, flow matching restricts itself to flows. In fact, one of the key innovations of flow matching was to show that one does need a construction via a forward process and SDEs but flow models alone can be trained in a scalable manner. Due this restriction, you should keep in mind that sampling from a Flow Matching model will be deterministic (only the initial $X_0 \sim p_{\text{init}}$ will be random). Stochastic interpolants included both the pure flow and the SDE extension via “Langevin dynamics” that we use here (see theorem 12). Stochastic interpolants get their name from a **interpolant function** $I(t, x, z)$ intended to interpolate between two distributions. In the terminology we use here, this corresponds to a different yet (mainly) equivalent way of constructing a conditional and marginal probability path. The advantage of flow matching and stochastic interpolants is both their simplicity and their generality: their training framework is very simple but at the same time they allow you to go from an arbitrary distribution p_{init} to an arbitrary distribution p_{data} - while denoising diffusion models only work for Gaussian initial distributions and Gaussian probability path.

This opens up new possibilities for generative modeling that we will touch upon briefly later in this class.

Let us summarize the results of this section:

Summary 22 (Training the Generative Model)

Flow matching consists of training a neural network u_t^θ via minimizing the **conditional flow matching loss**

$$\mathcal{L}_{\text{cfm}}(\theta) = \mathbb{E}_{z \sim p_{\text{data}}, x \sim p_t(\cdot|z)} [\|u_t^\theta(x) - u_t^{\text{target}}(x|z)\|^2] \quad (\text{conditional flow matching loss}) \quad (59)$$

where $u_t^{\text{target}}(x|z)$ is the conditional vector field (see algorithm 3). After training, one generates samples by simulating the corresponding ODE (see algorithm 1). To extend this to a diffusion model, we can use a **score network** s_t^θ and train it via **denoising score matching**

$$\mathcal{L}_{\text{dsm}}(\theta) = \mathbb{E}_{z \sim p_{\text{data}}, x \sim p_t(\cdot|z)} [\|s_t^\theta(x) - \nabla \log p_t(x|z)\|^2] \quad (\text{denoising score matching loss})$$

For every diffusion coefficient $\sigma_t \geq 0$, simulating the SDE (e.g. via algorithm 2)

$$X_0 \sim p_{\text{init}}, \quad dX_t = \left[u_t^\theta(X_t) + \frac{\sigma_t^2}{2} s_t^\theta(X_t) \right] dt + \sigma_t dW_t \quad (60)$$

will result in generating approximate samples from p_{data} . One can empirically find the optimal $\sigma_t \geq 0$.

Gaussian probability paths: For the special case of a Gaussian probability path $p_t(x|z) = \mathcal{N}(x; \alpha_t z, \beta_t^2 I_d)$, the denoising score matching and conditional flow matching loss are given by:

$$\begin{aligned} \mathcal{L}_{\text{cfm}}(\theta) &= \mathbb{E}_{t \sim \text{Unif}, z \sim p_{\text{data}}, \epsilon \sim \mathcal{N}(0, I_d)} [\|u_t^\theta(\alpha_t z + \beta_t \epsilon) - (\dot{\alpha}_t z + \dot{\beta}_t \epsilon)\|^2] \\ \mathcal{L}_{\text{dsm}}(\theta) &= \mathbb{E}_{t \sim \text{Unif}, z \sim p_{\text{data}}, \epsilon \sim \mathcal{N}(0, I_d)} [\|s_t^\theta(\alpha_t z + \beta_t \epsilon) + \frac{\epsilon}{\beta_t}\|^2] \end{aligned}$$

In this case, there is no need to train s_t^θ and u_t^θ separately as we can convert them post training via the formula:

$$u_t^\theta = \left(\beta_t^2 \frac{\dot{\alpha}_t}{\alpha_t} - \dot{\beta}_t \beta_t + \frac{\sigma_t^2}{2} \right) s_t^\theta(x) + \frac{\dot{\alpha}_t}{\alpha_t} x$$

Also here, after training we can simulate the SDE in eq. (60) via algorithm 2 to obtain samples X_1 .

Denoising diffusion models: Denoising diffusion models are diffusion models with Gaussian probability paths. For this reason, it is sufficient for them to learn either u_t^θ or s_t^θ as they can be converted into one another. While flow matching only allows for a simulation procedure that is deterministic via ODE, they allow for a simulation that is deterministic (probability flow ODE) or stochastic (SDE sampling). However, unlike flow matching or stochastic interpolants that allow to convert arbitrary distributions p_{init} into arbitrary distributions p_{data} via arbitrary probability paths p_t , denoising diffusion models only works for Gaussian initial distributions $p_{\text{init}} = \mathcal{N}(0, I_d)$ and a Gaussian probability path.

Literature: Alternative formulations for diffusion models that are popular in the literature are:

1. **Discrete-time:** Approximations of SDEs via discrete-time Markov chains are often used.

2. **Inverted time convention:** It is popular to use an inverted time convention where $t = 0$ corresponds to p_{data} (as opposed to here where $t = 0$ corresponds to p_{init}).
3. **Forward process:** Forward processes (or noising processes) are ways of constructing (Gaussian) probability paths.
4. **Training target via time-reversal:** A training target can also be constructed via the time-reversal of SDEs. This is a specific instance of the construction presented here (with an inverted time convention).

5 References

- [1] Michael S Albergo, Nicholas M Boffi, and Eric Vanden-Eijnden. “Stochastic interpolants: A unifying framework for flows and diffusions”. In: *arXiv preprint arXiv:2303.08797* (2023).
- [2] Brian DO Anderson. “Reverse-time diffusion equation models”. In: *Stochastic Processes and their Applications* 12.3 (1982), pp. 313–326.
- [3] Earl A Coddington, Norman Levinson, and T Teichmann. *Theory of ordinary differential equations*. 1956.
- [4] Lawrence C Evans. *Partial differential equations*. Vol. 19. American Mathematical Society, 2022.
- [5] Jonathan Ho, Ajay Jain, and Pieter Abbeel. “Denoising diffusion probabilistic models”. In: *Advances in neural information processing systems* 33 (2020), pp. 6840–6851.
- [6] Arieh Iserles. *A first course in the numerical analysis of differential equations*. Cambridge university press, 2009.
- [7] Tero Karras et al. “Elucidating the design space of diffusion-based generative models”. In: *Advances in Neural Information Processing Systems* 35 (2022), pp. 26565–26577.
- [8] Yaron Lipman et al. “Flow matching for generative modeling”. In: *arXiv preprint arXiv:2210.02747* (2022).
- [9] Yaron Lipman et al. “Flow Matching Guide and Code”. In: *arXiv preprint arXiv:2412.06264* (2024).
- [10] Xingchao Liu, Chengyue Gong, and Qiang Liu. “Flow straight and fast: Learning to generate and transfer data with rectified flow”. In: *arXiv preprint arXiv:2209.03003* (2022).
- [11] Nanye Ma et al. “Sit: Exploring flow and diffusion-based generative models with scalable interpolant transformers”. In: *arXiv preprint arXiv:2401.08740* (2024).
- [12] Xuerong Mao. *Stochastic differential equations and applications*. Elsevier, 2007.
- [13] Lawrence Perko. *Differential equations and dynamical systems*. Vol. 7. Springer Science & Business Media, 2013.
- [14] Simo Särkkä and Arno Solin. *Applied stochastic differential equations*. Vol. 10. Cambridge University Press, 2019.
- [15] Jascha Sohl-Dickstein et al. “Deep unsupervised learning using nonequilibrium thermodynamics”. In: *International conference on machine learning*. PMLR. 2015, pp. 2256–2265.
- [16] Yang Song and Stefano Ermon. “Generative modeling by estimating gradients of the data distribution”. In: *Advances in neural information processing systems* 32 (2019).

-
- [17] Yang Song et al. *Score-Based Generative Modeling through Stochastic Differential Equations*. 2021. arXiv: 2011.13456 [cs.LG]. URL: <https://arxiv.org/abs/2011.13456>.
 - [18] Yang Song et al. “Score-Based Generative Modeling through Stochastic Differential Equations”. In: *International Conference on Learning Representations (ICLR)*. 2021.
 - [19] Yang Song et al. “Score-based generative modeling through stochastic differential equations”. In: *arXiv preprint arXiv:2011.13456* (2020).

A A Reminder on Probability Theory

We present a brief overview of basic concepts from probability theory. This section was partially taken from [9].

A.1 Random vectors

Consider data in the d -dimensional Euclidean space $x = (x^1, \dots, x^d) \in \mathbb{R}^d$ with the standard Euclidean inner product $\langle x, y \rangle = \sum_{i=1}^d x^i y^i$ and norm $\|x\| = \sqrt{\langle x, x \rangle}$. We will consider random variables (RVs) $X \in \mathbb{R}^d$ with continuous probability density function (PDF), defined as a *continuous* function $p_X : \mathbb{R}^d \rightarrow \mathbb{R}_{\geq 0}$ providing event A with probability

$$\mathbb{P}(X \in A) = \int_A p_X(x) dx, \quad (61)$$

where $\int p_X(x) dx = 1$. By convention, we omit the integration interval when integrating over the whole space ($\int \equiv \int_{\mathbb{R}^d}$). To keep notation concise, we will refer to the PDF p_{X_t} of RV X_t as simply p_t . We will use the notation $X \sim p$ or $X \sim p(X)$ to indicate that X is distributed according to p . One common PDF in generative modeling is the d -dimensional isotropic Gaussian:

$$\mathcal{N}(x; \mu, \sigma^2 I) = (2\pi\sigma^2)^{-\frac{d}{2}} \exp\left(-\frac{\|x - \mu\|_2^2}{2\sigma^2}\right), \quad (62)$$

where $\mu \in \mathbb{R}^d$ and $\sigma \in \mathbb{R}_{>0}$ stand for the mean and the standard deviation of the distribution, respectively.

The expectation of a RV is the constant vector closest to X in the least-squares sense:

$$\mathbb{E}[X] = \arg \min_{z \in \mathbb{R}^d} \int \|x - z\|^2 p_X(x) dx = \int x p_X(x) dx. \quad (63)$$

One useful tool to compute the expectation of *functions of RVs* is the *Law of the Unconscious Statistician*:

$$\mathbb{E}[f(X)] = \int f(x) p_X(x) dx. \quad (64)$$

When necessary, we will indicate the random variables under expectation as $\mathbb{E}_X f(X)$.

A.2 Conditional densities and expectations

Given two random variables $X, Y \in \mathbb{R}^d$, their joint PDF $p_{X,Y}(x, y)$ has marginals

$$\int p_{X,Y}(x, y) dy = p_X(x) \text{ and } \int p_{X,Y}(x, y) dx = p_Y(y). \quad (65)$$

See fig. 11 for an illustration of the joint PDF of two RVs in \mathbb{R} ($d = 1$). The *conditional* PDF $p_{X|Y}$ describes the PDF of the random variable X when conditioned on an event $Y = y$ with density $p_Y(y) > 0$:

$$p_{X|Y}(x|y) := \frac{p_{X,Y}(x, y)}{p_Y(y)}, \quad (66)$$

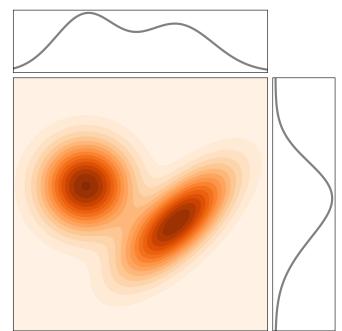


Figure 11: Joint PDF $p_{X,Y}$ (in shades) and its marginals p_X and p_Y (in black lines). Figure from [9]

and similarly for the conditional PDF $p_{Y|X}$. Bayes' rule expresses the conditional PDF $p_{Y|X}$ with $p_{X|Y}$ by

$$p_{Y|X}(y|x) = \frac{p_{X|Y}(x|y)p_Y(y)}{p_X(x)}, \quad (67)$$

for $p_X(x) > 0$.

The *conditional expectation* $\mathbb{E}[X|Y]$ is the best approximating function $g_*(Y)$ to X in the least-squares sense:

$$\begin{aligned} g_* &:= \arg \min_{g: \mathbb{R}^d \rightarrow \mathbb{R}^d} \mathbb{E} [\|X - g(Y)\|^2] = \arg \min_{g: \mathbb{R}^d \rightarrow \mathbb{R}^d} \int \|x - g(y)\|^2 p_{X,Y}(x,y) dx dy \\ &= \arg \min_{g: \mathbb{R}^d \rightarrow \mathbb{R}^d} \int \left[\int \|x - g(y)\|^2 p_{X|Y}(x|y) dx \right] p_Y(y) dy. \end{aligned} \quad (68)$$

For $y \in \mathbb{R}^d$ such that $p_Y(y) > 0$ the conditional expectation function is therefore

$$\mathbb{E}[X|Y = y] := g_*(y) = \int x p_{X|Y}(x|y) dx, \quad (69)$$

where the second equality follows from taking the minimizer of the inner brackets in eq. (68) for $Y = y$, similarly to eq. (63). Composing g_* with the random variable Y , we get

$$\mathbb{E}[X|Y] := g_*(Y), \quad (70)$$

which is a random variable in \mathbb{R}^d . Rather confusingly, both $\mathbb{E}[X|Y = y]$ and $\mathbb{E}[X|Y]$ are often called *conditional expectation*, but these are different objects. In particular, $\mathbb{E}[X|Y = y]$ is a function $\mathbb{R}^d \rightarrow \mathbb{R}^d$, while $\mathbb{E}[X|Y]$ is a random variable assuming values in \mathbb{R}^d . To disambiguate these two terms, our discussions will employ the notations introduced here.

The *tower property* is an useful property that helps simplify derivations involving conditional expectations of two RVs X and Y :

$$\mathbb{E}[\mathbb{E}[X|Y]] = \mathbb{E}[X] \quad (71)$$

Because $\mathbb{E}[X|Y]$ is a RV, itself a function of the RV Y , the outer expectation computes the expectation of $\mathbb{E}[X|Y]$. The tower property can be verified by using some of the definitions above:

$$\begin{aligned} \mathbb{E}[\mathbb{E}[X|Y]] &= \int \left(\int x p_{X|Y}(x|y) dx \right) p_Y(y) dy \\ &\stackrel{(66)}{=} \int \int x p_{X,Y}(x,y) dx dy \\ &\stackrel{(65)}{=} \int x p_X(x) dx \\ &= \mathbb{E}[X]. \end{aligned}$$

Finally, consider a helpful property involving two RVs $f(X, Y)$ and Y , where X and Y are two arbitrary RVs. Then, by using the Law of the Unconscious Statistician with (69), we obtain the identity

$$\mathbb{E}[f(X, Y)|Y = y] = \int f(x, y) p_{X|Y}(x|y) dx. \quad (72)$$

B A Proof of the Fokker-Planck equation

In this section, we give here a self-contained proof of the Fokker-Planck equation (theorem 14) which includes the continuity equation as a special case (theorem 11). We stress that **this section is not necessary to understand the remainder of this document** and is mathematically more advanced. If you desire to understand where the Fokker-Planck equation comes from, then this section is for you.

We start by showing that the Fokker-Planck is a necessary condition, i.e. if $X_t \sim p_t$, then the Fokker-Planck equation is fulfilled. The trick for the proof is to use **test functions** f , i.e. functions $f : \mathbb{R}^d \rightarrow \mathbb{R}$ that are infinitely differentiable ("smooth") and are only non-zero within a bounded domain (compact support). We use the fact that for arbitrary integrable functions $g_1, g_2 : \mathbb{R}^d \rightarrow \mathbb{R}$ it holds that

$$g_1(x) = g_2(x) \text{ for all } x \in \mathbb{R}^d \Leftrightarrow \int f(x)g_1(x)dx = \int f(x)g_2(x)dx \text{ for all test functions } f \quad (73)$$

In other words, we can express the pointwise equality as equality of taking integrals. The useful thing about test functions is that they are smooth, i.e. we can take gradients and higher-order derivatives. In particular, we can use **integration by parts** for arbitrary test functions f_1, f_2 :

$$\int f_1(x) \frac{\partial}{\partial x_i} f_2(x) dx = - \int f_2(x) \frac{\partial}{\partial x_i} f_1(x) dx \quad (74)$$

By using this together with the definition of the divergence and Laplacian (see eq. (23)), we get the identities:

$$\int \nabla f_1^T(x) f_2(x) dx = - \int f_1(x) \operatorname{div}(f_2)(x) dx \quad (f_1 : \mathbb{R}^d \rightarrow \mathbb{R}, f_2 : \mathbb{R}^d \rightarrow \mathbb{R}^d) \quad (75)$$

$$\int f_1(x) \Delta f_2(x) dx = \int f_2(x) \Delta f_1(x) dx \quad (f_1 : \mathbb{R}^d \rightarrow \mathbb{R}, f_2 : \mathbb{R}^d \rightarrow \mathbb{R}) \quad (76)$$

Now let's proceed to the proof. We use the stochastic update of SDE trajectories as in eq. (6):

$$X_{t+h} = X_t + h u_t(X_t) + \sigma_t(W_{t+h} - W_t) + h R_t(h) \quad (77)$$

$$\approx X_t + h u_t(X_t) + \sigma_t(W_{t+h} - W_t) \quad (78)$$

where for now we simply ignore the error term $R_t(h)$ for readability as we will take $h \rightarrow 0$ anyway. We can then make the following calculation:

$$\begin{aligned} & f(X_{t+h}) - f(X_t) \\ \stackrel{(78)}{=} & f(X_t + h u_t(X_t) + \sigma_t(W_{t+h} - W_t)) - f(X_t) \\ \stackrel{(i)}{=} & \nabla f(X_t)^T (h u_t(X_t) + \sigma_t(W_{t+h} - W_t)) \\ & + \frac{1}{2} (h u_t(X_t) + \sigma_t(W_{t+h} - W_t))^T \nabla^2 f(X_t) (h u_t(X_t) + \sigma_t(W_{t+h} - W_t)) \\ \stackrel{(ii)}{=} & h \nabla f(X_t)^T u_t(X_t) + \sigma_t \nabla f(X_t)^T (W_{t+h} - W_t) \\ & + \frac{1}{2} h^2 u_t(X_t)^T \nabla^2 f(X_t) u_t(X_t) + h \sigma_t u_t(X_t)^T \nabla^2 f(X_t) (W_{t+h} - W_t) + \frac{1}{2} \sigma_t^2 (W_{t+h} - W_t)^T \nabla^2 f(X_t) (W_{t+h} - W_t) \end{aligned}$$

where in (i) we used a 2nd Taylor approximation of f around X_t and in (ii) we used the fact that the Hessian $\nabla^2 f$ is a symmetric matrix. Note that $\mathbb{E}[W_{t+h} - W_t | X_t] = 0$ and $W_{t+h} - W_t | X_t \sim \mathcal{N}(0, hI_d)$. Therefore

$$\begin{aligned} & \mathbb{E}[f(X_{t+h}) - f(X_t) | X_t] \\ &= h \nabla f(X_t)^T u_t(X_t) + \frac{1}{2} h^2 u_t(X_t)^T \nabla^2 f(X_t) u_t(X_t) + \frac{h}{2} \sigma_t^2 \mathbb{E}_{\epsilon_t \sim \mathcal{N}(0, I_d)} [\epsilon_t^T \nabla^2 f(X_t) \epsilon_t] \\ &\stackrel{(i)}{=} h \nabla f(X_t)^T u_t(X_t) + \frac{1}{2} h^2 u_t(X_t)^T \nabla^2 f(X_t) u_t(X_t) + \frac{h}{2} \sigma_t^2 \text{trace}(\nabla^2 f(X_t)) \\ &\stackrel{(ii)}{=} h \nabla f(X_t)^T u_t(X_t) + \frac{1}{2} h^2 u_t(X_t)^T \nabla^2 f(X_t) u_t(X_t) + \frac{h}{2} \sigma_t^2 \Delta f(X_t) \end{aligned}$$

where in (i) we used the fact that $\mathbb{E}_{\epsilon_t \sim \mathcal{N}(0, I_d)} [\epsilon_t^T A \epsilon_t] = \text{trace}(A)$ and in (ii) we used the definition of the Laplacian and the Hessian matrix. With this, we get that

$$\begin{aligned} & \partial_t \mathbb{E}[f(X_t)] \\ &= \lim_{h \rightarrow 0} \frac{1}{h} \mathbb{E}[f(X_{t+h}) - f(X_t)] \\ &= \lim_{h \rightarrow 0} \frac{1}{h} \mathbb{E}[\mathbb{E}[f(X_{t+h}) - f(X_t) | X_t]] \\ &= \mathbb{E}[\lim_{h \rightarrow 0} \frac{1}{h} \left(h \nabla f(X_t)^T u_t(X_t) + \frac{1}{2} h^2 u_t(X_t)^T \nabla^2 f(X_t) u_t(X_t) + \frac{h}{2} \sigma_t^2 \Delta f(X_t) \right)] \\ &= \mathbb{E}[\nabla f(X_t)^T u_t(X_t) + \frac{1}{2} \sigma_t^2 \Delta f(X_t)] \\ &\stackrel{(i)}{=} \int \nabla f(x)^T u_t(x) p_t(x) dx + \int \frac{1}{2} \sigma_t^2 \Delta f(x) p_t(x) dx \\ &\stackrel{(ii)}{=} - \int f(x) \text{div}(u_t p_t)(x) dx + \int \frac{1}{2} \sigma_t^2 f(x) \Delta p_t(x) dx \\ &= \int f(x) \left(-\text{div}(u_t p_t)(x) + \frac{1}{2} \sigma_t^2 \Delta p_t(x) \right) dx \end{aligned}$$

where in (i) we used the assumption that p_t as the distribution of X_t and in (ii) we used eq. (75) and eq. (76). Therefore, it holds that

$$\partial_t \mathbb{E}[f(X_t)] = \int f(x) \left(-\text{div}(p_t u_t)(x) + \frac{\sigma_t^2}{2} \Delta p_t(x) \right) dx \quad (\text{for all } f \text{ and } 0 \leq t \leq 1) \quad (79)$$

$$\stackrel{(i)}{\Leftrightarrow} \partial_t \int f(x) p_t(x) dx = \int f(x) \left(-\text{div}(p_t u_t)(x) + \frac{\sigma_t^2}{2} \Delta p_t(x) \right) dx \quad (\text{for all } f \text{ and } 0 \leq t \leq 1) \quad (80)$$

$$\stackrel{(ii)}{\Leftrightarrow} \int f(x) \partial_t p_t(x) dx = \int f(x) \left(-\text{div}(p_t u_t)(x) + \frac{\sigma_t^2}{2} \Delta p_t(x) \right) dx \quad (\text{for all } f \text{ and } 0 \leq t \leq 1) \quad (81)$$

$$\stackrel{(iii)}{\Leftrightarrow} \partial_t p_t(x) = -\text{div}(p_t u_t)(x) + \frac{\sigma_t^2}{2} \Delta p_t(x) \quad (\text{for all } x \in \mathbb{R}^d, 0 \leq t \leq 1) \quad (82)$$

where in (i) we used the assumption that $X_t \sim p_t$, in (ii) we swapped the derivative with the integral and (iii) we used eq. (73). This completes the proof that the Fokker-Planck equation is a necessary condition.

Finally, we explain why it is also a sufficient condition. The Fokker-Planck equation is a partial differential equation (PDE). More specifically, it is a so-called *parabolic partial differential equation*. Similar to theorem 2,

such differential equations have a unique solution given fixed initial conditions (see e.g. [4, Chapter 7]). Now, if eq. (30) holds for p_t , we just shown above that it must also hold for true distribution q_t of X_t (i.e. $X_t \sim q_t$) - in other words, both p_t and q_t are solutions to the parabolic PDE. Further, we know that the initial conditions are the same, i.e. $p_0 = q_0 = p_{\text{init}}$ by construction of an interpolating probability path (see ??). Hence, by uniqueness of the solution of the differential equation, we know that $p_t = q_t$ for all $0 \leq t \leq 1$ - which means $X_t \sim q_t = p_t$ and which is what we wanted to show.