Flow Matching

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1 Notations

We start by defining a probability density path $p : [0,1] \times \mathbb{R}^d \to \mathbb{R}^d$ meaning that for each time t, p_t is density function i.e. $\int p_t(x)dx = 1$.

A simple example of such a path is a path p interpolating two density p_0 and p_1 with $p_t = tp_1 + (1-t)p_0$

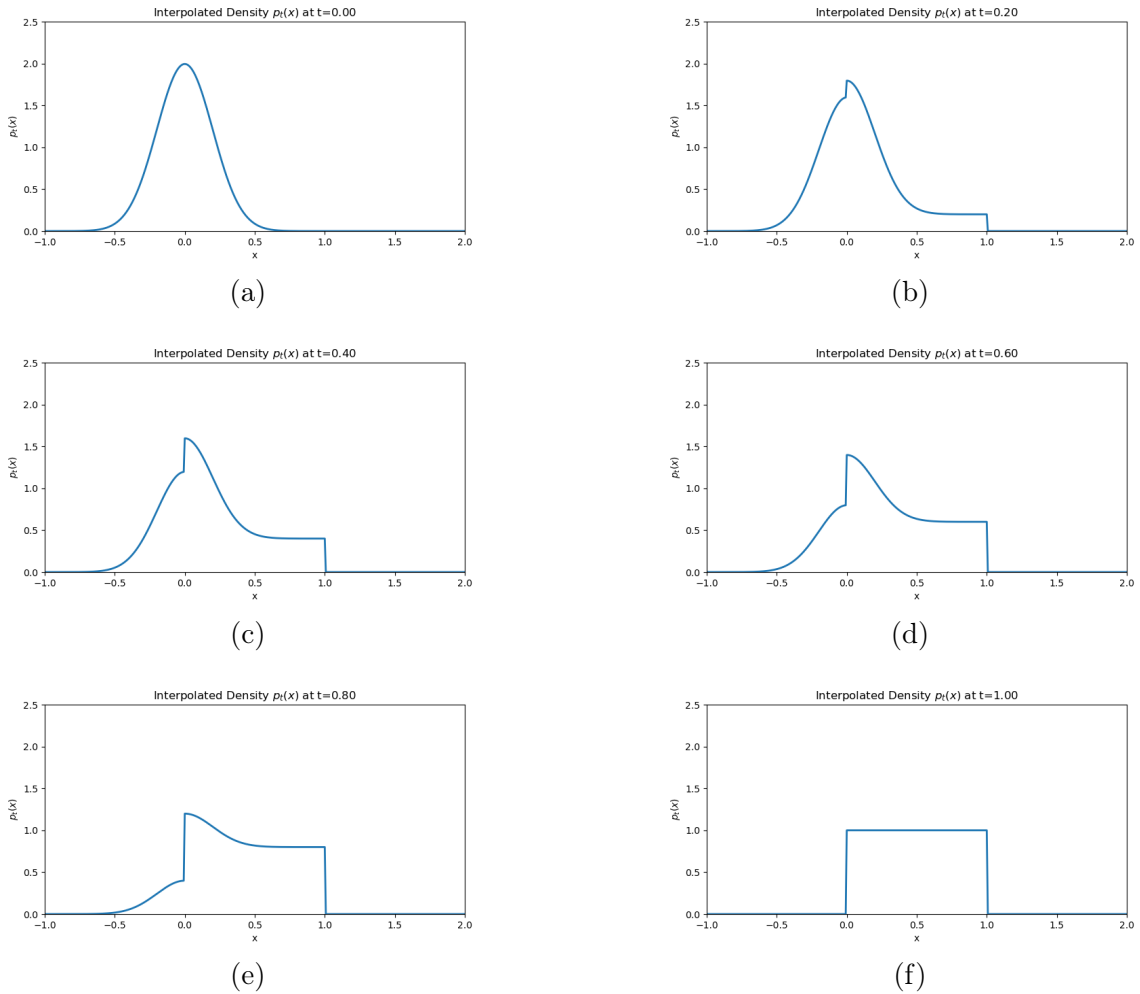Figure 1: A probability path interpolating $\mathcal{N}(0, 0.2)$ and $\mathcal{U}([0,1])$
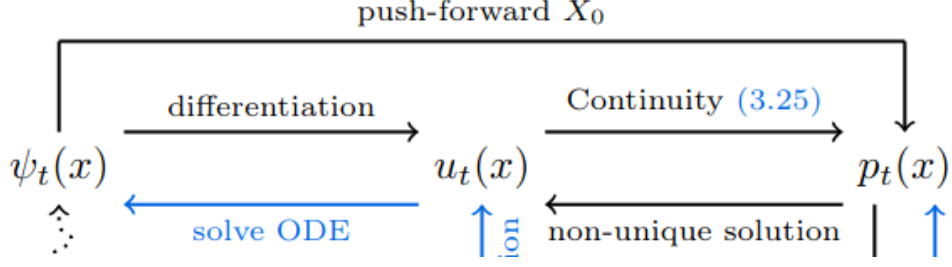
Figure 2: How the notions are linked together, from [1]

Next we introduce a core object, a time dependant vector field $v : [0, 1] \times \mathbb{R}^d \to \mathbb{R}^d$ which can be used to construct a map $\phi : [0, 1] \times \mathbb{R}^d \to \mathbb{R}^d$, called a flow, by the following ODE

$$\frac{d}{dt}\phi_t(x) = v_t(\phi_t(x)) \tag{1}$$
$$\phi_0(x) = x$$

The link between the flow and the probability path is given by the change of variables formula

$$p_t(x) = q(\phi_t^{-1}(x)) \det\left[\frac{\partial \phi_t^{-1}}{\partial x}(x)\right] \tag{2}$$

This coincides with the normalizing framework.

The link between the vector field and the probability path is given by the continuity equation

$$\frac{d}{dt}p_t(x) + \operatorname{div}(p_t(x)v_t(x)) = 0 \tag{3}$$

It said that the vector field v_t generates the probability path p_t if the continuity equation holds.

2   Objective

Given a target probability path p_t and a corresponding v_t vector field, the naïve flow matching loss is

$$\mathcal{L}_{\text{FM}}(\theta) = \mathbb{E}_{t,p_t(x)}\left[\|v_t^\theta(x) - v_t(x)\|^2\right] \tag{4}$$

But we don't have acces to v_t and p_t. To adress this problem and given a particular data sample x_1, we introduce conditional probability path $p_t(x|x_1)$ such that $p_0(x|x_1) = q(x)$ at time $t = 0$ and by marginalizing over x_1 we can recover the marginal probability path

$$p_t(x) = \int p_t(x|x_1)q(x_1)dx_1 \tag{5}$$

So instead of defining a path between two entire distributions, we take a samples from our distributions and we just define how to go from one to the other.

In the same vein, we can define a conditional vector field, assuming $p_t(x)$ for all t and x

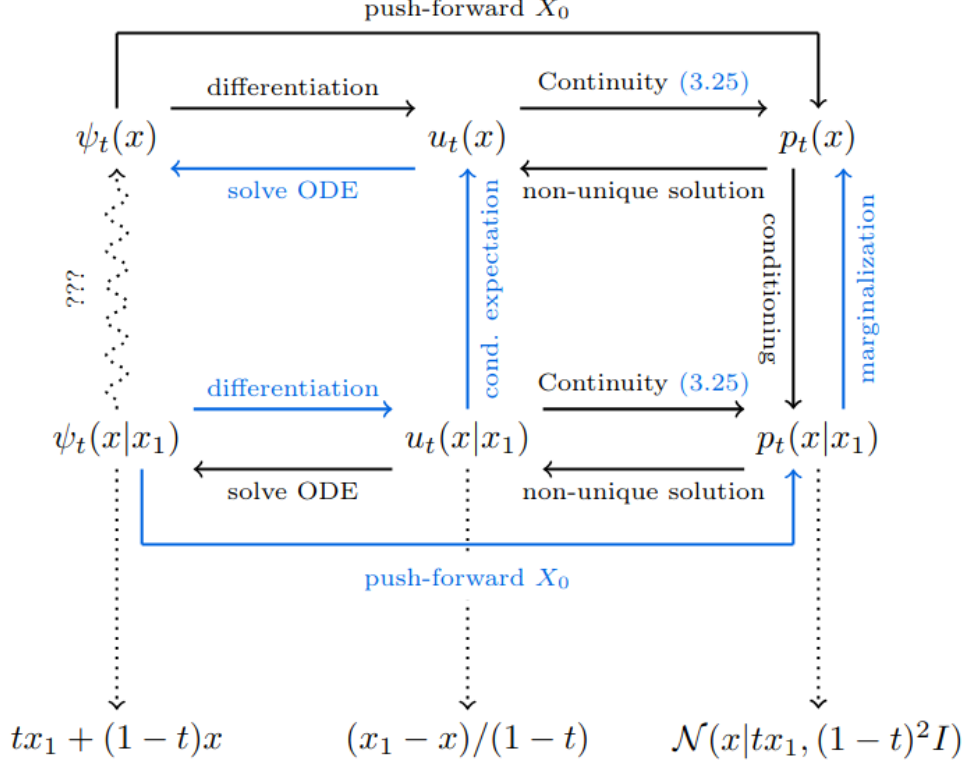$$v_t(x) = \int v_t(x|x_1) \frac{p_t(x|x_1)q(x_1)}{p_t(x)} dx_1 \tag{6}$$

Figure 3: A visual in [1] that illustates well the full framework

Then the author introduces a new loss function called the conditional flow matching loss

$$\mathcal{L}_{\text{CFM}}(\theta) = \mathbb{E}_{t,q(x_1),p_t(x|x_1)} \left[\|v_t^\theta(x|x_1) - v_t(x|x_1)\|^2 \right] \tag{7}$$

with a strong property : $\mathcal{L}_{\text{FM}}(\theta) = \mathcal{L}_{\text{CFM}}(\theta)$ up to a constant independent of θ.

So the focus is now on designing a conditional probability path and vector field and it turns out "the conditional flow matching objective works with any choice of conditional probability path and conditional vector fields". Futhermore, there is an infinite number of vector fields that generate any particular probability path.

3   Example

References

[1] Yaron Lipman, Marton Havasi, Peter Holderrieth, Neta Shaul, Matt Le, Brian Karrer, Ricky T. Q. Chen, David Lopez-Paz, Heli Ben-Hamu, and Itai Gat. Flow matching guide and code, 2024.