

Mathematics of Generative Models : Homework 2

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In this homework, we will work on flow matching models in 2D. Consider the ODE

$$\frac{dx}{dt} = v(x, t) \quad t \in [0, 1]. \quad (1)$$

The solution to the ODE above at time t starting with the initial condition $x \in \mathbb{R}^2$ is given by $\varphi^t(x) \in \mathbb{R}^2$. The function $(t, x) \rightarrow \varphi^t(x)$ is also called the flow of the vector field v . The flow, φ^t , is deterministic, but we will consider the initial conditions to be random variables taking values in \mathbb{R}^2 . Let X_0 be the random variable denoting the initial condition and having a distribution, μ , with probability density ρ_0 . Let $X_t = \varphi^t(X_0)$, with a probability density, ρ_t . We have already seen that ρ_t solves the continuity equation given by,

$$\frac{\partial \rho_t}{\partial t} = -\text{div}(\rho_t v(\cdot, t)). \quad (2)$$

At time 1, we want the random variable X_1 to have the desired distribution p_{data} , which may not have a density. Flow matching models learn a time dependent vector field v so that the density ρ_1 is an approximate density of p_{data} . But, they must learn v using only independent samples $\{x^{(1)}, \dots, x^{(m)}\}$ from p_{data} and no other information about p_{data} . Let $\hat{p}_{\text{data}, m} = \text{Unif}\{x^{(1)}, \dots, x^{(m)}\}$ be the empirical distribution over the given samples from the target distribution, p_{data} . Similarly, let $\hat{\mu}_m$ denote the empirical distribution over m independent samples from μ . For this homework, take $p_{\text{data}} = \frac{1}{4}\mathcal{N}(\mu_1, \Sigma_1) + \frac{3}{4}\mathcal{N}(\mu_2, \Sigma_2)$ with means $\mu_1 = (-2, 0)^\top$, $\mu_2 = (2, 0)^\top$ and covariances $\Sigma_1 = \begin{pmatrix} 2 & 0 \\ 0 & 0.5 \end{pmatrix}$, $\Sigma_2 = I_2$.

1. Let $Z = (X_0, X_1)$ be a random variable distributed according to $\hat{\mu}_m \times \hat{p}_{\text{data}}$. Given $Z = (x_0, x_1)$, suppose we choose an interpolation path $\varphi^t(x_0|Z = (x_0, x_1)) = \alpha_t x_0 + \beta_t x_1$. What is the conditional vector field, $u(\cdot, t)$? (1 point)
2. What is the solution of the continuity equation for $u(\cdot, t)$? (1 point)
3. Let v_θ be a neural network approximation of v . The flow matching loss is

$$l_{\text{FM}}(\theta) = \int \|v(t, x) - v_\theta(t, x)\|^2 \rho_t(x) dx dt,$$

where the integrals are approximated with uniform time discretization and Monte Carlo integration. Rewrite this loss in terms of the conditional vector field and the corresponding solutions to the continuity equation, and explain why it is equivalent to the flow matching loss above. (3 points)

4. Choose α_t, β_t , and an optimal coupling between X_0 and X_1 as the distribution of Z . Apply conditional flow matching for the specified target distribution. Attach a plot of the vector field v_θ at $t=0, 0.5$ and 1 and interpret your results. You are allowed to use rather than write your own implementation. (5 points)
5. Is the vector field you obtain close to the solution of the Benamou-Brenier formulation? Why or why not? (3 points)