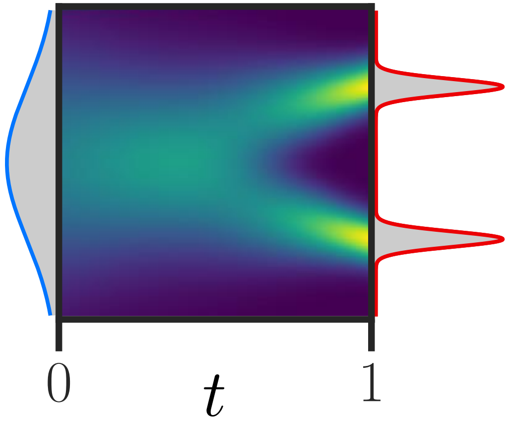
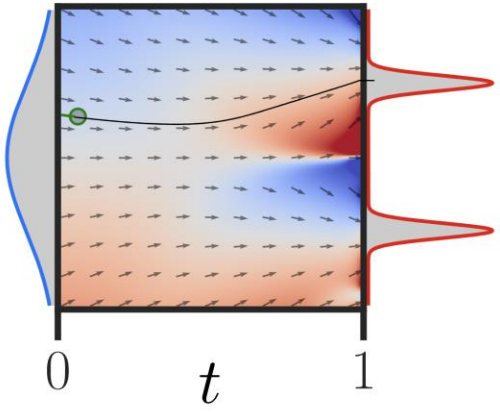
Flow Matching

Flow Matching

Learn the vector field to transport probability distribution





$$\partial_t p_t + \nabla \cdot u_t p_t = 0$$

$$x(0) = x^{(i)} + \int_1^0 u_\theta(x(t), t)\mathrm{d}t$$

Ref: https://dl.heeere.com/conditional-flow-matching/blog/conditional-flow-matching/

Flow Matching

Central Idea: Learn the final flow from conditioned flows

$$
\begin{tikzcd}[column sep=huge, row sep=huge]
\overbrace{\forall z \in Z}^{\textbf{choice 1}} \quad \overbrace{p(x|t,z)}^{\textbf{choice 2}} \arrow[r, leftrightarrow, "\substack{\text{determines}\\ \text{explicitly}}", "\text{(by continuity eq.)}"'] \arrow[d, "\substack{\text{determines}\\ \text{(by expectation over } z\text{)}}"'] & u^{\text{cond}}(x,t,z) \arrow[d, blue] \\
p(x|t) \arrow[r, leftrightarrow, "\substack{\text{determines}\\ \text{implicitly}}", "\text{(by continuity eq.)}"'] & u(x,t)
\end{tikzcd}
$$

Flow Matching

$$\forall x \;\; \mathbb{E}_z\left[p(x|z,t=0)\right] = p_0(x) \;\; ,$$
$$\forall x \;\; \mathbb{E}_z\left[p(x|z,t=1)\right] = p_{\text{data}}(x) \;\; .$$

$$\boldsymbol{\partial_t p_t + \nabla \cdot u_t p_t = 0}$$

$$\begin{tikzcd}[column sep=huge, row sep=huge]
\forall \overbrace{z \in Z}^{\textbf{choice 1}} \;\; \overbrace{p(x|t,z)}^{\textbf{choice 2}} \arrow[r, leftrightarrow, "\substack{\text{determines}\\ \text{explicitly}}", "\text{(by continuity eq.)}"'] \arrow[d, "\substack{\text{determines}\\ \text{(by expectation over } z\text{)}}"'] & u^{\text{cond}}(x,t,z) \arrow[d, blue] \\
p(x|t) \arrow[r, leftrightarrow, "\substack{\text{determines}\\ \text{implicitly}}", "\text{(by continuity eq.)}"'] & u(x,t)
\end{tikzcd}$$

$$\boldsymbol{p(x|t) = \mathbb{E}_z\left[p(x|t,z)\right]}$$

$$\boldsymbol{u(x,t) = \mathbb{E}_{z|x,t}\left[u^{\text{cond}}(x,t,z)\right]}$$

$$\boldsymbol{\partial_t p_t + \nabla \cdot u_t p_t = 0}$$

Flow Matching

Linear Paths

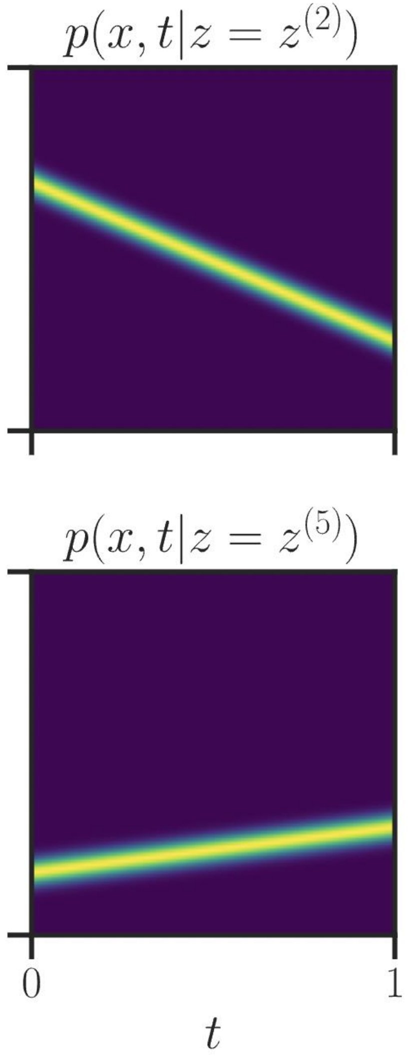
$$z \overset{\text{choice}}{=} (x_0, x_1) \sim p_0 \times p_{\text{data}}$$

$$p\big(x|t, z = (x_0, x_1)\big) \overset{\text{choice}}{=} \mathcal{N}((1-t)\cdot x_0 + t \cdot x_1, \sigma^2 \mathrm{Id})$$

$$p\big(x|t, z = (x_0, x_1)\big) \overset{\text{choice}}{=} \delta_{(1-t)\cdot x_0 + t\cdot x_1}(x)$$

$$\forall x \;\; \mathbb{E}_z\left[p(x|z, t=0)\right] = p_0(x) \;\; ,$$
$$\forall x \;\; \mathbb{E}_z\left[p(x|z, t=1)\right] = p_{\text{data}}(x) \;\; .$$

$$u^{\text{cond}}(x, t, z = (x_0, x_1)) = x_1 - x_0$$



Flow Matching

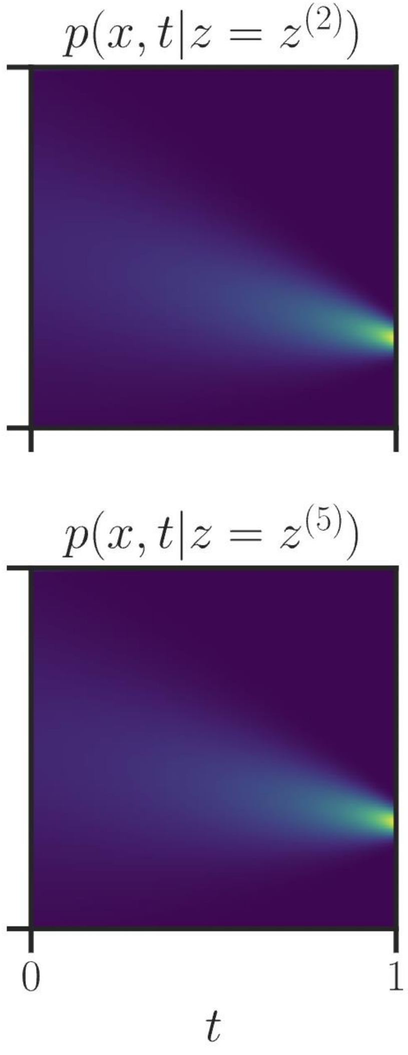
Gaussian Paths

$$z \overset{\text{choice}}{=} x_1 \sim p_{\text{data}}$$

$$p(x|t, z = x_1) \overset{\text{choice}}{=} \mathcal{N}(tx_1, (1-t)^2 \text{Id})$$

$$\forall x \;\; \mathbb{E}_z \left[p(x|z, t=0) \right] = p_0(x) \;\; ,$$
$$\forall x \;\; \mathbb{E}_z \left[p(x|z, t=1) \right] = p_{\text{data}}(x) \;\; .$$

$$u^{\text{cond}}(x, t, z = x_1) = \tfrac{x - x_1}{1 - t}$$



Flow Matching

Velocity flow from conditioned velocity flow

$$u(x,t) = \mathbb{E}_{z|x,t}\left[u^{\text{cond}}(x,t,z)\right]$$

To get the above result

$$\forall\, t,\ x,\ u(x,t) = \mathbb{E}_z\left[\frac{u^{\text{cond}}(x,t,z)p(x|t,z)}{p(x|t)}\right]$$

This gives us the loss function

$$\mathcal{L}^{\text{CFM}}(\theta) \overset{\text{def}}{=} \mathbb{E}_{\substack{t\sim\mathcal{U}([0,1])\\ z\sim p_z \\ x\sim p(\cdot|t,z)}} \|u_\theta^{\text{CFM}}(x,t) - \underbrace{u^{\text{cond}}(x,t,z)}_{\substack{\text{chosen to be}\\ \text{explictly defined,}\\ \text{cheap to compute,}\\ \text{e.g., } x_1 - x_0}}\|^2$$

Flow Matching

Proof:

$$
\begin{aligned}
\forall\, t,\, x,\, p(x|t) &= \int_z p(x, z|t)\mathrm{d}z \\
\forall\, t,\, x,\, \frac{\partial p(x|t)}{\partial t} &= \frac{\partial}{\partial t}\mathbb{E}_z\left[p(x|t, z)\right] \\
&= \mathbb{E}_z\left[\frac{\partial}{\partial t}p(x|t, z)\right] \quad \text{(under technical conditions)} \\
&= -\mathbb{E}_z\left[\nabla \cdot \left(u^{\text{cond}}(x, t, z)p(x|t, z)\right)\right] \quad \text{continuity equation for } p(x|t, z) \\
&= -\nabla \cdot \mathbb{E}_z\left[u^{\text{cond}}(x, t, z)p(x|t, z)\right] \quad \text{(under technical conditions)} \\
&= -\nabla \cdot \mathbb{E}_z\left[u^{\text{cond}}(x, t, z)p(x|t, z)\frac{p(x|t)}{p(x|t)}\right] \\
&= -\nabla \cdot \left(\mathbb{E}_z\left[\frac{u^{\text{cond}}(x, t, z)p(x|t, z)}{p(x|t)}\right]p(x|t)\right) \quad (p(x|t) \text{ is independent of } z)
\end{aligned}
$$

Hence $\forall\, t,\, x,\, u(x, t) = \mathbb{E}_z\left[\frac{u^{\text{cond}}(x,t,z)p(x|t,z)}{p(x|t)}\right]$

Flow Matching

Proof:

$$
\begin{aligned}
\forall\, t,\, x,\, u(x,t) &= \mathbb{E}_z\left[\frac{u^{\text{cond}}(x,t,z)p(x|t,z)}{p(x|t)}\right] \\
&= \int_z \frac{u^{\text{cond}}(x,t,z)p(x|t,z)}{p(x|t)} p(z)\mathrm{d}z \\
&= \int_z u^{\text{cond}}(x,t,z)\, \underbrace{p(x|t,z)}_{=\frac{p(z|x,t)\cdot p(x,t)}{p(t,z)}} \cdot p(z) \cdot \underbrace{\frac{1}{p(x|t)}}_{=\frac{p(t)}{p(x,t)}} \mathrm{d}z \\
&= \int_z u^{\text{cond}}(x,t,z) \frac{p(z|x,t)\cdot p(x,t)}{p(t,z)} \cdot p(z) \cdot \frac{p(t)}{p(x,t)} \mathrm{d}z \\
&= \int_z u^{\text{cond}}(x,t,z) p(z|x,t) \underbrace{\frac{p(z)\cdot p(t)}{p(t,z)}}_{=1} \mathrm{d}z \\
&= \int_z u^{\text{cond}}(x,t,z) p(z|x,t)\mathrm{d}z \\
&= \mathbb{E}_{z|x,t}\left[u^{\text{cond}}(x,t,z)\right]
\end{aligned}
$$

Flow Matching

Flow Matching In Practice	**Linear Interpolation**	**Conical Gaussian Paths**
1. Define a variable z with some known distribution $p(z)$	$p(z = (x_0, x_1)) = p_0 \times p_{\text{data}}$	$p(z = x_1) = p_{\text{data}}$
2. Define a simple conditional distribution $p(x \mid t, z)$	$\mathcal{N}((1-t) \cdot x_0 + t \cdot x_1, \sigma^2 \cdot \text{Id})$	$\mathcal{N}(t \cdot x_1, (1-t)^2 \cdot \text{Id})$
3. Compute an associated velocity field $u^{\text{cond}}(x, t, z)$	$x_1 - x_0$	$\frac{x_1 - x}{1-t}$
4. Train model using the conditional loss $\mathcal{L}^{\text{CFM}}$ Sample $t \sim \mathcal{U}_{[0,1]}$, $z \sim p_z$, $x \sim p(x \mid t, z)$	Use data points $x^{(1)}, \dots, x^{(n)}$	
5. Sample from $p_1 \approx p_{\text{data}}$ Sample $x_0 \sim p_0$, Integration scheme on $t \in [0, 1]$	Numerical integration, e.g, Euler scheme: $x_{k+1} = x_k + \frac{1}{N} u_\theta(x_k, t)$	

Flow Matching

References:

1. Flow Matching for Generative Modeling, Lipman et. al.
2. Flow Matching Guide and Code, Lipman et. al.
3. A Visual Dive into Conditional Flow Matching, Gagneux et. al.