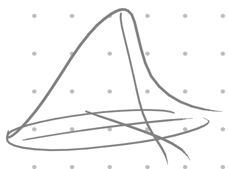
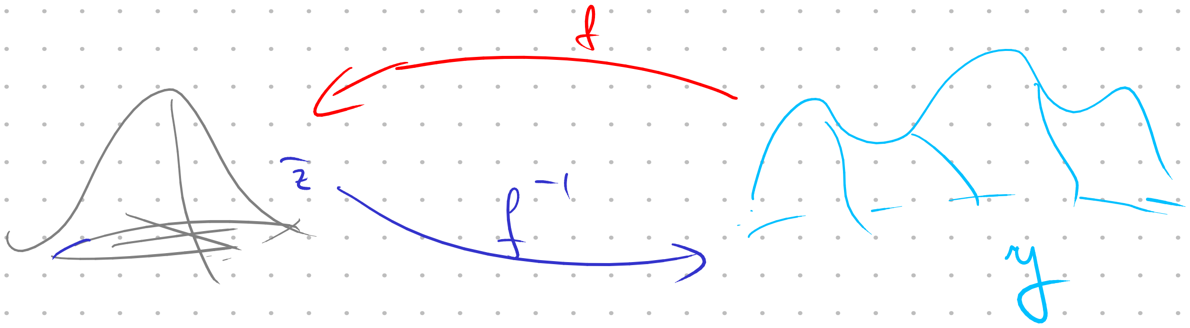
Flow-based models



$\bar z \sim q(\bar z)$ $\quad f \quad f^{-1}$

$y = f(\bar z)$

$$\boxed{p(f(\bar z)) = q(\bar z) \cdot \left| \det \frac{\partial f^{-1}}{\partial \bar z} \right|}$$



$$\bar z_K = f_K \circ f_{K-1} \dots \circ f_1(\bar z_0) \qquad \bar z_0 \sim q_0(\bar z_0)$$

$$\bar z_K \sim \underbrace{q_K(\bar z)}_{\text{update}(x)} = q_0(\bar z_0) \prod_{k=1}^{K} \left| \det \frac{\partial f_k}{\partial \bar z_{k-1}} \right|^{-1}$$

$$\log q_K = \log q_0 - \sum_k \log \left| \det \frac{\partial f_k}{\partial \bar z_{k-1}} \right|$$

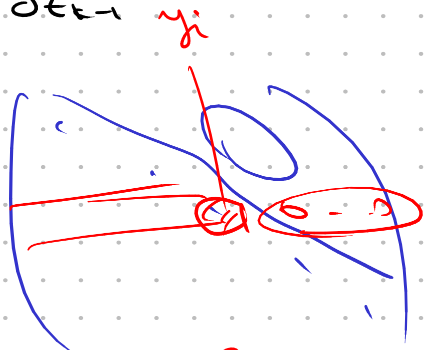
f: $\quad \det \frac{\partial f}{\partial \bar z}$

$$\bar y = f(\bar z)$$

$$(y_1, \dots, y_d) = f(z_1, \dots, z_d)$$

$$\boxed{\begin{aligned} y_i &= f(z_1, \dots, z_i) \\ \det \frac{\partial f}{\partial z} &= \prod_{i=1}^{d} \frac{\partial y_i}{\partial z_i} \end{aligned}}$$

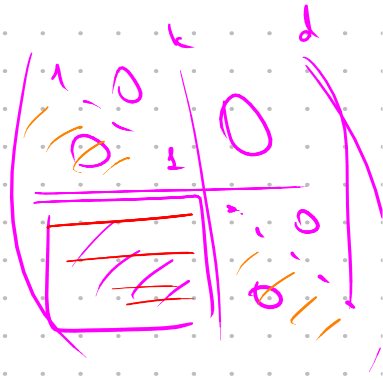
— autoregressive flows



R-NVP real non-volume-preserving flows

$$\bar y_{1..k} = \bar z_{1..k}$$

$$\bar y_{k+1..d} = \bar z_{k+1..d} \odot \bar\sigma(\bar z_{1..k}) + \bar\mu(\bar z_{1..k})$$



$$\det \frac{\partial \bar{y}}{\partial \bar{z}} = \prod_{i=k+1}^{d} \sigma_i(\bar{z}_{1..k})$$

$$\bar{y}_{k+1..d} = \bar{z}_{k+1..d} \odot \bar{\sigma}(\bar{z}_{1..k}) + \bar{\mu}(\bar{z}_{1..k})$$

$$\bar{z}_{k+1..d} = \left(\bar{y}_{k+1..d} - \bar{\mu}(\bar{z}_{1..k})\right) \odot \frac{1}{\bar{\sigma}(\bar{z}_{1..k})}$$

$$\bar{z}_{1..k} = \bar{y}_{1..k}$$

Masked Autoregressive Flows (MAF)

$$p(\bar{x}) = \prod_{i=1}^{D} p(x_i \mid \bar{x}_{1..i-1})$$

произв. функции

$$p(x_i \mid \bar{x}_{1..i-1}) = z_i \cdot \sigma_i(\bar{x}_{1..i-1}) + \mu_i(\bar{x}_{1..i-1})$$

$$\bar{z} \sim \pi(\bar{z}) \xrightarrow{f} \bar{x}$$

$$x_1 = z_1 \cdot \sigma_1 + \mu_1$$

$$x_2 = z_2 \cdot \sigma_2(x_1) + \mu_2(x_1)$$

$$\ldots$$

$$x_d = z_d \cdot \sigma_d(\bar{x}_{1..d-1}) + \mu_d(\bar{x}_{1..d-1})$$

$$\xleftarrow{f^{-1}}$$

$$z_i = \frac{x_i - \mu_i(\bar{x}_{1..i-1})}{\sigma_i(\bar{x}_{1..i-1})}$$

$$\bar{z} = \_\_\_(\bar{x})$$

Inverse Autoregressive Flows (IAF)

$$x_i \sim p(x_i \mid \bar{z}_{1..i}) = z_i \cdot \sigma_i(\bar{z}_{1..i-1}) + \mu_i(\bar{z}_{1..i-1})$$

$$z_i = \frac{x_i - \mu_i(\bar{z}_{1..i-1})}{\sigma_i(\bar{z}_{1..i-1})}$$

$$\bar{z} \sim \pi(\bar{z}) \xrightarrow{f} \bar{x} = \bar{z} \odot \bar{\sigma}(\bar{z}) + \bar{\mu}(\bar{z})$$

$$z_1 = \ldots$$

$$z_2 = \ldots(z_1)$$

$$z_d = \ldots(z_1 \ldots z_{d-1})$$

Diffusion-based models

$\bar{x}_0 \sim q(\bar{x})$

$\hookrightarrow \bar{x}_1 \to \bar{x}_2 \to \;\_\_\; \bar{x}_T$

α_t

$$q(\bar{x}_t | \bar{x}_{t-1}) = \mathcal{N}\left(\bar{x}_t \middle| \sqrt{1-\beta_t}\, \bar{x}_{t-1}, \beta_t I\right)$$

$$q(\bar{x}_1 \ldots \bar{x}_T | \bar{x}_0) = \prod_t q(\bar{x}_t | \bar{x}_{t-1})$$

Reparametrization trick

$$\bar{x}_t = \sqrt{1-\beta_t}\; \bar{x}_{t-1} + \sqrt{\beta_t} \cdot \bar{\varepsilon}_{t-1} = \qquad \bar{\varepsilon}_{t-1} \sim \mathcal{N}(\bar{0}, I)$$

$$= \sqrt{\alpha_t}\, \bar{x}_{t-1} + \sqrt{1-\alpha_t}\, \bar{\varepsilon}_{t-1} =$$

$$= \sqrt{\alpha_t \alpha_{t-1}}\; \bar{x}_{t-2} + \sqrt{1-\alpha_t}\, \bar{\varepsilon}_{t-1} + \sqrt{\alpha_t(1-\alpha_{t-1})}\, \bar{\varepsilon}_{t-2} =$$

$$\sim \mathcal{N}(\bar{0}, (1-\alpha_t) I) \quad + \quad \sim \mathcal{N}(\bar{0}, \alpha_t(1-\alpha_{t-1}) I)$$

$$= \sqrt{\alpha_t \alpha_{t-1}}\; \bar{x}_{t-2} + \sqrt{1-\alpha_t \alpha_{t-1}}\; \bar{\varepsilon}'_{t-2} = \ldots \qquad \mathcal{N}(\bar{0}, (1-\cancel{\alpha_t}+\cancel{\alpha_t}-\alpha_t\alpha_{t-1}) I)$$

$$\ldots = \sqrt{\alpha_t \alpha_{t-1} \ldots \alpha_1}\; \bar{x}_0 + \sqrt{1-\alpha_t\alpha_{t-1} \ldots \alpha_1}\; \bar{\varepsilon}$$

$$A_t = \alpha_1 \alpha_2 \ldots \alpha_t$$

$$q(\bar{x}_t | \bar{x}_0) = \mathcal{N}\left(\bar{x}_t \middle| \sqrt{A_t} \cdot \bar{x}_0, (1-A_t) I\right)$$

$$p_{\bar{\theta}}(\bar{x}_0, \bar{x}_1, \ldots \bar{x}_T) = p_{\bar{\theta}}(\bar{x}_T) \cdot \prod_{t=1}^{T} p_{\bar{\theta}}(\bar{x}_{t-1} | \bar{x}_t) \qquad \cancel{q(\bar{x}_{t-1} | \bar{x}_t)}$$

$$p_\theta(\bar{x}_{t-1} | \bar{x}_t) = \mathcal{N}\left(\bar{x}_{t-1} \middle| \bar{\mu}_\theta(\bar{x}_t, t), \Sigma_\theta(\bar{x}_t, t)\right)$$

$$q(\bar{x}_{t-1} | \bar{x}_t, \bar{x}_0) = q(\bar{x}_t | \bar{x}_{t-1}, \bar{x}_0) \cdot \frac{q(\bar{x}_{t-1} | \bar{x}_0)}{q(\bar{x}_t | \bar{x}_0)} =$$

$$= \mathrm{Const} \cdot e^{-\frac{1}{2}\left(\frac{(\bar{x}_t - \sqrt{\alpha_t}\,\bar{x}_{t-1})^2}{\beta_t} + \frac{(\bar{x}_{t-1} - \sqrt{A_{t-1}}\,\bar{x}_0)^2}{1-A_{t-1}} - \cancel{\frac{(\bar{x}_t - \sqrt{A_t}\,\bar{x}_0)^2}{1-A_t}}\right)}$$

$$= \mathrm{Const} \cdot e^{-\frac{1}{2}\left(\bar{x}_{t-1}^2 \cdot \left(\frac{\alpha_t}{\beta_t} + \frac{1}{1-A_{t-1}}\right) - 2\bar{x}_{t-1}\left(\frac{\sqrt{\alpha_t}\cdot \bar{x}_t}{\beta_t} + \frac{\sqrt{A_{t-1}}\cdot \bar{x}_0}{1-A_{t-1}}\right) + \_\_\right)}$$

$$q(\bar{x}_{t-1} \mid \bar{x}_t, \bar{x}_0) = \mathcal{N}\left(\bar{x}_{t-1} \mid \tilde{\mu}(\bar{x}_t, \bar{x}_0), \tilde{\beta}_t I\right)$$

где $\tilde{\beta}_t = \frac{1-A_{t-1}}{1-A_t}\beta_t$,

$$\bar{x}_t = \sqrt{A_t}\,\bar{x}_0 + \sqrt{1-A_t}\cdot\bar{\varepsilon}$$

$$\tilde{\mu}(\bar{x}_t, \bar{x}_0) = \frac{\sqrt{\alpha_t}(1-A_{t-1})}{1-A_t}\bar{x}_t + \frac{\sqrt{A_{t-1}}\cdot\beta_t}{1-A_t}\bar{x}_0 =$$

$\bar{x}_1 \ldots \bar{x}_T \sim q$

$$= \frac{1}{\sqrt{\alpha_t}}\left(\bar{x}_t - \frac{1-\alpha_t}{\sqrt{1-A_t}}\cdot\bar{\varepsilon}_t\right)$$

$$p_\theta(\bar{x}_0 \ldots \bar{x}_T) / p_\theta(\bar{x}_0)$$

$$\|$$

$$\log p_\theta(\bar{x}_0) \geq \log p_\theta(\bar{x}_0) - KL\left(q(\bar{x}_1 \ldots \bar{x}_T \mid \bar{x}_0) \,\|\, p_\theta(\bar{x}_1 \ldots \bar{x}_T \mid \bar{x}_0)\right) =$$

$$= \cancel{\log p_\theta(\bar{x}_0)} - \mathbb{E}_q\left[\log \frac{q(\bar{x}_1 \ldots \bar{x}_T \mid \bar{x}_0)}{p_\theta(\bar{x}_0 \ldots \bar{x}_T) / \cancel{p_\theta(\bar{x}_0)}}\right] =$$

$$= -\mathbb{E}_q\left[\log \frac{q(\bar{x}_1 \ldots \bar{x}_T \mid \bar{x}_0)}{p_\theta(\bar{x}_0 \ldots \bar{x}_T)}\right]$$

$$-\mathbb{E}_{q(\bar{x}_0)}\left[\log p_\theta(\bar{x}_0)\right] \leq \underbrace{\mathbb{E}_{q(\bar{x}_0, \bar{x}_1 \ldots \bar{x}_T)}\left[\log \frac{q(\bar{x}_1 \ldots \bar{x}_T \mid \bar{x}_0)}{p_\theta(\bar{x}_0 \ldots \bar{x}_T)}\right]}_{\xrightarrow{\theta} \min}$$

$$\mathbb{E}_q\left[\log \frac{\prod_{t=1}^{T} q(\bar{x}_t|\bar{x}_{t-1},\bar{x}_0)}{p_\theta(\bar{x}_T)\cdot\prod_{t=1}^{T} p_\theta(\bar{x}_{t-1}|\bar{x}_t)}\right] =$$

$$q(\bar{x}_{t-1}|\bar{x}_t,\bar{x}_0)\cdot\frac{q(\bar{x}_t|\bar{x}_0)}{q(\bar{x}_{t-1}|\bar{x}_0)}$$

$$= \mathbb{E}_q\left[-\log p_\theta(\bar{x}_T) + \sum_{t=2}^{T}\log\frac{q(\bar{x}_t|\bar{x}_{t-1},\bar{x}_0)}{p_\theta(\bar{x}_{t-1}|\bar{x}_t)} + \underbrace{\log\frac{q(\bar{x}_1|\bar{x}_0)}{p_\theta(\bar{x}_0|\bar{x}_1)}}_{\cancel{\log q(\bar{x}_1|\bar{x}_0)} - \log p_\theta(\bar{x}_0|\bar{x}_1)}\right]$$

$$= \mathbb{E}_q\left[-\log p_\theta(\bar{x}_T) + \sum_{t=2}^{T}\log\frac{q(\bar{x}_{t-1}|\bar{x}_t,\bar{x}_0)}{p_\theta(\bar{x}_{t-1}|\bar{x}_t)} + \underbrace{\sum_{t=2}^{T}\log\frac{q(\bar{x}_t|\bar{x}_0)}{q(\bar{x}_{t-1}|\bar{x}_0)}} + \right]$$

$$\log \ldots t - \log \ldots t{-}1 + \log \ldots t{-}1 - \log \ldots t{-}2$$

$$= \log q(\bar{x}_T|\bar{x}_0) - \cancel{\log q(\bar{x}_1|\bar{x}_0)}$$

$$= \mathbb{E}_q\left[\log\frac{q(\bar{x}_T|\bar{x}_0)}{p_\theta(\bar{x}_T)} + \sum_{t=2}^{T}\log\frac{q(\bar{x}_{t-1}|\bar{x}_t,\bar{x}_0)}{p_\theta(\bar{x}_{t-1}|\bar{x}_t)} - \log p_\theta(\bar{x}_0|\bar{x}_1)\right] \xrightarrow[\theta]{\min}$$

$$L_T + L_{T-1} + L_{T-2} + \ldots L_t + L_1 + L_0$$

$$L_T = KL(q(\bar{x}_T|\bar{x}_0)\,\|\,p_\theta(\bar{x}_T)) \qquad L_t = KL(q(\bar{x}_{t-1}|\bar{x}_t,\bar{x}_0)\,\|\,p_\theta(\bar{x}_{t-1}|\bar{x}_t))$$