Normalizing Flows

$p(x) \propto \tilde{p}(x)$

$$x = f_\phi(u) \quad \text{for} \quad u \sim q(u), \tag{1}$$

$$p = f_{\phi\#} q, \tag{2}$$

$$q_\phi(x) = q(f_\phi^{-1}(x)) \left| \det \nabla f_\phi(f_\phi^{-1}(x)) \right|^{-1}, \tag{3}$$

$f_K \circ \cdots \circ f_1$

$$\det \nabla (f_K \circ \cdots \circ f_1)(u) = \det \nabla f_K((f_{K-1} \circ \cdots \circ f_1)(u)) \cdots \det \nabla f_1(u). \tag{4}$$

Kullback-Leibler divergence

$$
\begin{aligned}
\mathrm{KL}(q_\phi(x)||p(x)) &= \int \log\left(\frac{q_\phi(x)}{p(x)}\right) q_\phi(x)dx \\
&= \int \log\left(\frac{q(u)\left|\det \nabla f_\phi\right|^{-1}}{p(f_\phi(u))}\right) q(u)du \\
&= \mathbb{E}_q\left[\log q(u) - \log\left|\det \nabla f_\phi\right| - \log p(f_\phi(u))\right] \\
&\propto -\mathbb{E}_q\left[\log\left|\det \nabla f_\phi\right| + \log \tilde{p}(f_\phi(u))\right], \qquad (5)
\end{aligned}
$$

$(\mathrm{KL}(p(x)||q_\phi(x)))$

Knothe-Rosenblatt re-arrangement (triangular)

$$x_i = f_{\phi,i}(u_1, \dots, u_i) \quad i = 1, \dots, d. \tag{6}$$

$|\det \nabla f_\phi(u)| = |\prod_{i=1}^{d} \nabla_i f_{\phi,i}(u)|$
if $\det \nabla f_\phi(u)$ same sign on all u then monotone.

$$\phi_i = NN(u_1, \dots, u_i) \quad i = 1, \dots, d. \tag{7}$$

Masked architecture

$H_0(u) = u$

$$H_i(u) = g_i(b_i + (W_i \odot M_i)H_{i-1}(u)) \quad i = 1, \ldots, h \tag{8}$$

$$\phi = g_{h+1}(b_{h+1} + (W_{h+1} \odot M_{h+1})H_h(u)) \tag{9}$$

Inverse Autoregressive Flow

$$x_i = \frac{u_i - \mu_i}{\sigma_i} \quad i = 1, \ldots, d, \tag{10}$$

$$\phi_i = (\mu_i, \log \sigma_i) \tag{11}$$

Coupling

$$p = f_{\#} q, \tag{12}$$

q with cdf F and p with quantile function G^{-1}, then

$$f = G^{-1} \circ F \tag{13}$$

Sum of Squares Polynomial Flow

$$x_i = \int_0^{u_i} \sum_{k=1}^{K} \left(\sum_{l=0}^{r} a_{l,r} u^l \right)^2 du + b \quad i = 1, \ldots, d, \tag{14}$$

$$\phi_i = (\boldsymbol{a}, b) \tag{15}$$