Section - 4.1

Particle - Based Update Rule

(I) The optimization objective

$$D(q,p) = \max_{\substack{\phi \in H^d \\ \|\phi\|_{H^d} \leq 1}} E_{x \sim q} [\mathrm{trace}(A_p \phi(x))]$$

We have to find the optimal direcⁿ ϕ in RKHS that gives maximum descent of KL divergence.

(II) Use the Stein Operator

$$A_p \phi(x) = \nabla_x \log p(x) \cdot \phi(x)^T + \nabla_x \phi(x)$$

We have to find,

$$E_{x \sim q} [\mathrm{trace}(A_p \phi(x))]$$

We can rewrite this as -

$$E_{x \sim q} [\mathrm{trace}(A_p \phi(x))] =$$

$$E_{x \sim q} [\mathrm{trace}(\nabla_x \log p(x) \cdot \phi(x)^T + \nabla_x \phi(x))]$$

Use linearity property of trace,

$$= E_{x \sim q}[\nabla_x \log p(x)^T \phi(x) + \text{trace}(\nabla_x \phi(x))]$$

III) RKHS Ball Optimization

Maximize the inner product in RKHS,

$$\langle \phi, \phi^*_{q,p} \rangle_{H^d}$$

$$\phi^*_{q,p} = \underset{\|\phi\|_{H^d} \leq 1}{\arg\max} \; E_{x \sim q}[\text{trace}(A_p \phi(x))]$$

$$= \nabla_f KL[q[f] \| p]) \Big|_{f=0}$$

This means that optimal direction is basically the gradient of KL divergence in RKHS. We can also show it using the kernel trick.

IV) RKHS Form

In RKHS, represent any eqn $\phi(x) \in H^d$ as

$$\phi(x) = \sum_{i=1}^{n} a_i k(x_i, x)$$

Rewriting functional gradient of KL as,

$$\phi^*_{q,p}(x) = E_{x' \sim q}[A_p k(x', x)]$$

Here, we apply the stein operator to the kernel func^n, $k(x', x)$.

V) Apply Stein Operator to Kernel

Apply A_p to $k(x', x)$

$$A_p \cancel{k}(x', x) = \nabla_{x'} \log p(x') \cdot k(x', x) + \nabla_{x'} k(x', x)$$

Take expecta^n over $x' \sim q$,

$$\boxed{\phi^*_{q,p}(x) = E_{x' \sim q}[\nabla_{x'} \log p(x') \cdot k(x', x) + \nabla_{x'} k(x', x)]}$$

→ This is eq^n 6. It helps to update balances attrac^n to the posterior & diversity across particles.