Appendix A: Proof of Theorem 1

Proof:, By definition, $w(\boldsymbol{x}) = \rho(\boldsymbol{x})/p(\boldsymbol{x})$, $\nabla_{\boldsymbol{x}} w(\boldsymbol{x}) = w(\boldsymbol{x})\boldsymbol{s}_\rho(\boldsymbol{x}) - w(\boldsymbol{x})\boldsymbol{s}_p(\boldsymbol{x})$,

$$
\begin{aligned}
\mathcal{A}_p^\top(w(\boldsymbol{x})\boldsymbol{\phi}(\boldsymbol{x})) &= w(\boldsymbol{x})\boldsymbol{s}_p(\boldsymbol{x})^\top\boldsymbol{\phi}(\boldsymbol{x}) + \nabla_{\boldsymbol{x}}^\top(w(\boldsymbol{x})\boldsymbol{\phi}(\boldsymbol{x}))\\
&= w(\boldsymbol{x})\boldsymbol{s}_p(\boldsymbol{x})^\top\boldsymbol{\phi}(\boldsymbol{x}) + \nabla_{\boldsymbol{x}} w(\boldsymbol{x})^\top\boldsymbol{\phi}(\boldsymbol{x}) + w(\boldsymbol{x})\nabla_{\boldsymbol{x}}^\top\boldsymbol{\phi}(\boldsymbol{x})\\
&= w(\boldsymbol{x})\boldsymbol{s}_\rho(\boldsymbol{x})^\top\boldsymbol{\phi}(\boldsymbol{x}) + w(\boldsymbol{x})\nabla_{\boldsymbol{x}}^\top\boldsymbol{\phi}(\boldsymbol{x}) = w(\boldsymbol{x})\mathcal{A}_\rho^\top\boldsymbol{\phi}(\boldsymbol{x}).
\end{aligned}
$$

Therefore, we have

$$
\begin{aligned}
\mathbb{D}_{\mathcal{F},\rho}(q \,||\, p) &= \max_{\boldsymbol{\phi}\in\mathcal{F}}\left\{\mathbb{E}_{\boldsymbol{x}\sim q}[\mathcal{A}_p^\top\left(w(\boldsymbol{x})\boldsymbol{\phi}(\boldsymbol{x})\right)]\right\} && (27)\\
&= \max_{\boldsymbol{\phi}\in w\mathcal{F}}\left\{\mathbb{E}_{\boldsymbol{x}\sim q}[\mathcal{A}_p^\top\boldsymbol{\phi}(\boldsymbol{x})]\right\} && (28)\\
&= \mathbb{D}_{w\mathcal{F}}(q \,||\, p).
\end{aligned}
$$

Appendix B: Proof of Theorem 2

Proof: When $\mathcal{H}$ is an RKHS with kernel $k(\boldsymbol{x}, \boldsymbol{x}')$, then $w\mathcal{H}$ is also an RKHS, with an "importance weighted kernel"

$$
\tilde{k}(\boldsymbol{x}, \boldsymbol{x}') = w(\boldsymbol{x})w(\boldsymbol{x}')k(\boldsymbol{x}, \boldsymbol{x}'). \tag{29}
$$

Following Lemma 3.2 in Liu & Wang (2016), the optimal solution of the optimization problem (28) is,

$$
\begin{aligned}
w(\cdot)\boldsymbol{\phi}^*(\cdot) &= \mathbb{E}_{\boldsymbol{x}\sim q}[\boldsymbol{s}_p(\boldsymbol{x})w(\boldsymbol{x})k(\boldsymbol{x},\cdot)w(\cdot) + \nabla_{\boldsymbol{x}}(w(\boldsymbol{x})k(\boldsymbol{x},\cdot)w(\cdot))]\\
&= w(\cdot)\mathbb{E}_{\boldsymbol{x}\sim q}[w(\boldsymbol{x})\mathcal{A}_\rho k(\boldsymbol{x},\cdot)].
\end{aligned}
$$

This gives

$$
\boldsymbol{\phi}^*(\cdot) = \mathbb{E}_{\boldsymbol{x}\sim q}[w(\boldsymbol{x})\mathcal{A}_\rho k(\boldsymbol{x},\cdot)].
$$

Following Theorem 3.6 (Liu et al., 2016), we can show that

$$
\mathbb{D}_{\mathcal{F},\rho}(q \,||\, p) = (\mathbb{E}_{\boldsymbol{x},\boldsymbol{x}'\sim q}[\tilde{\kappa}_p(\boldsymbol{x}, \boldsymbol{x}')])^{\frac{1}{2}}, \tag{30}
$$

where

$$
\tilde{\kappa}_p(\boldsymbol{x}, \boldsymbol{x}') = (\mathcal{A}_p')^\top(\mathcal{A}_p\tilde{k}(\boldsymbol{x}, \boldsymbol{x}')).
$$

and $\mathcal{A}_p$ and $\mathcal{A}_p'$ denote the Stein operator applied on variable $\boldsymbol{x}$ and $\boldsymbol{x}'$, respectively. Applying Theorem 1, we have

$$
\begin{aligned}
\tilde{\kappa}_p(\boldsymbol{x}, \boldsymbol{x}') &= (\mathcal{A}_p')^\top\left(\mathcal{A}_p(w(\boldsymbol{x})w(\boldsymbol{x}')k(\boldsymbol{x}, \boldsymbol{x}'))\right)\\
&= (\mathcal{A}_p')^\top(w(\boldsymbol{x})\mathcal{A}_\rho\left(w(\boldsymbol{x}')k(\boldsymbol{x}, \boldsymbol{x}')\right))\\
&= (\mathcal{A}_p')^\top(w(\boldsymbol{x}')w(\boldsymbol{x})\mathcal{A}_\rho\left(k(\boldsymbol{x}, \boldsymbol{x}')\right))\\
&= w(\boldsymbol{x}')w(\boldsymbol{x})(\mathcal{A}_\rho')^\top(\mathcal{A}_\rho\left(k(\boldsymbol{x}, \boldsymbol{x}')\right))\\
&= w(\boldsymbol{x}')w(\boldsymbol{x})\kappa_\rho(\boldsymbol{x}, \boldsymbol{x}'),
\end{aligned}
$$

where we recall that $\kappa_\rho(\boldsymbol{x}, \boldsymbol{x}') = (\mathcal{A}_\rho')^\top\left(\mathcal{A}_\rho k(\boldsymbol{x}, \boldsymbol{x}')\right)$. Therefore, $\mathbb{D}_{\mathcal{F},\rho}(q, p)$ in (30) equals

$$
\mathbb{D}_{\mathcal{F},\rho}(q, p) = (\mathbb{E}_{\boldsymbol{x},\boldsymbol{x}'\sim q}[w(\boldsymbol{x})\kappa_\rho(\boldsymbol{x}, \boldsymbol{x}')w(\boldsymbol{x}')])^{\frac{1}{2}}.
$$

This completes the proof. □