

## A Proofs for Section 2

### A.1 Proof of Proposition 1

For  $p = 1$ , the result follows immediately from the Kantorovich dual representation of  $W_1(\cdot, \cdot)$  [21]:

$$W_1(Q, Q') = \sup \left\{ |\mathbf{E}_Q F - \mathbf{E}_{Q'} F| : \sup_{\substack{z, z' \in \mathcal{Z} \\ z \neq z'}} \frac{|F(z) - F(z')|}{d_{\mathcal{Z}}(z, z')} \leq 1 \right\}$$

and from the fact that, for  $Q, Q' \in B_{\varrho, 1}^W(P)$ ,  $W_1(Q, Q') \leq 2\varrho$  by the triangle inequality. For  $p > 1$ , the result follows from the fact that  $W_1(Q, Q') \leq W_p(Q, Q')$  for all  $Q, Q' \in \mathcal{P}_p(\mathcal{Z})$ .

### A.2 Proof of Proposition 2

Fix some  $Q, Q' \in B_{\varrho, p}^W(P)$  and let  $M \in \mathcal{P}(\mathcal{Z} \times \mathcal{Z})$  achieve the infimum in (4) for  $W_p(Q, Q')$ . Then for  $(Z, Z') \sim M$  we have

$$\begin{aligned} f(Z') - f(Z) &\leq \int_0^1 G_f(\gamma(t)) dt \cdot d_{\mathcal{Z}}(Z, Z') \\ &\leq \frac{1}{2} (G_f(Z) + G_f(Z')) d_{\mathcal{Z}}(Z, Z'), \end{aligned}$$

where the first inequality is from (5) and the second one is by the assumed geodesic convexity of  $G_f$ . Taking expectations of both sides with respect to  $M$  and using Hölder's inequality, we obtain

$$\begin{aligned} R(Q', f) - R(Q, f) &\leq \frac{1}{2} (\mathbf{E}_M |G_f(Z) + G_f(Z')|^q)^{1/q} (\mathbf{E}_M d_{\mathcal{Z}}^p(Z, Z'))^{1/p} \\ &= \frac{1}{2} \|G_f(Z) + G_f(Z')\|_{L^q(M)} W_p(Q, Q'), \end{aligned}$$

where we have used the  $p$ -Wasserstein optimality of  $M$  for  $Q$  and  $Q'$ . By the triangle inequality, and since  $Z \sim Q$  and  $Z' \sim Q'$ ,

$$\begin{aligned} \|G_f(Z) + G_f(Z')\|_{L^q(M)} &\leq \|G_f(Z)\|_{L^q(Q)} + \|G_f(Z')\|_{L^q(Q')} \\ &\leq 2 \sup_{Q \in B_{\varrho, p}^W(P)} \|G_f(Z)\|_{L^q(Q)}. \end{aligned}$$

Interchanging the roles of  $Q$  and  $Q'$  and proceeding with the same argument, we obtain the estimate

$$\sup_{Q, Q' \in B_{\varrho, p}^W(P)} |R(Q, f) - R(Q', f)| \leq 2\varrho \sup_{Q \in B_{\varrho, p}^W(P)} \|G_f(Z)\|_{L^q(Q)},$$

from which it follows that

$$\begin{aligned} R(Q, f) &\leq R_{\varrho, p}(P, f) \\ &= \sup_{Q' \in B_{\varrho, p}^W(P)} [R(Q', f) - R(Q, f) + R(Q, f)] \\ &\leq R(Q, f) + 2\varrho \sup_{Q \in B_{\varrho, p}^W(P)} \|G_f(Z)\|_{L^q(Q)}. \end{aligned}$$

### A.3 Proof of Proposition 3

As a subset of  $\mathbb{R}^{d+1}$ ,  $\mathcal{Z}$  is a geodesic space: for any pair  $z, z' \in \mathcal{Z}$  there is a unique constant-speed geodesic  $\gamma(t) = (1-t)z + tz'$ . We claim that  $G_f(z) = G_f(x, y) = 2(B+M)(1+L\|\nabla h(x)\|_2)$  is a geodesically convex upper gradient for  $f(z) = f(x, y) = (y - h(x))^2$ . In this flat Euclidean setting, geodesic convexity coincides with the usual definition of convexity, and the map  $z \mapsto G_f(z)$  is evidently convex:

$$G_f((1-t)z + tz') \leq (1-t)G_f(z) + tG_f(z').$$

Next, by the mean-value theorem,

$$\begin{aligned}
f(z') - f(z) &= \int_0^1 \langle z' - z, \nabla f((1-t)z + tz') \rangle dt \\
&\leq \int_0^1 \|\nabla f((1-t)z + tz')\|_2 dt \cdot \|z - z'\|_2 \\
&= \int_0^1 \|\nabla f((1-t)z + tz')\|_2 dt \cdot d_Z(z, z'),
\end{aligned}$$

and a simple calculation shows that

$$\begin{aligned}
\|\nabla f(z)\|_2^2 &= \|\nabla f(x, y)\|_2^2 \\
&= 4f(z) (1 + \|\nabla h(z)\|_2^2) \\
&\leq 4(B + M)^2(1 + L^2\|x\|_2^2).
\end{aligned}$$

Therefore,  $\|\nabla f(z)\|_2 \leq G_f(z)$  for  $z = (x, y)$ , as claimed. Thus, by Proposition (2),

$$\begin{aligned}
R(Q, f) &\leq R_{\varrho, 2}(P, f) \\
&\leq R(Q, f) + 2 \sup_{Q \in B_{\varrho, 2}^W(P)} \|G_f(Z)\|_{L^2(Q)} \varrho \\
&= R(Q, f) + 4(B + M) \left(1 + L \sup_{Q \in B_{\varrho, 2}^W(P)} \mathbf{E}_Q \|X\|_2\right) \varrho \\
&= R(Q, f) + 4(B + M) \left(1 + L \sup_{Q \in B_{\varrho, 2}^W(P)} \sigma_{Q, X}\right) \varrho.
\end{aligned}$$

## B The illustrative example of Section 2.2

Consider  $Z \sim \text{Unif}[0, 1] =: P$  on data space  $\mathcal{Z} = [0, 2]$ , along with the hypothesis class  $\mathcal{F}$  with only two hypotheses

$$f_0(z) = 1, \quad f_1(z) = \begin{cases} 0, & z \in [0, 1) \\ \alpha, & z \in [1, 2] \end{cases},$$

for some constant  $\alpha \gg 1$ . Also, let  $d_Z(z, z') = |z - z'|$ .

Now we calculate the local minimax risk of the hypothesis class for both empirical and population measure. The local worst-case risk of  $f_0$  for both measures is 1, by definition. For  $f_1$ , it is easy to see that the worst-case distribution for both  $P$  and  $P_n$  can be specified explicitly: For  $P$ , it is optimal to transport the mass to the point  $z = 1$  from the interval  $[\beta, 1)$ , with  $\beta \in [0, 1)$  specified according to the ambiguity radius  $\varrho > 0$ . For  $P$ , the optimal  $\beta$  can be calculated as a solution to

$$\left( \int_{\beta}^1 (1-z)^p dz \right)^{1/p} = \varrho,$$

which gives  $\beta = 1 - (p+1)^{\frac{1}{p+1}} \varrho^{\frac{p}{p+1}}$ , leading to the local worst-case risk  $R_{\varrho, p}(P, f_1) = \alpha \cdot (p+1)^{\frac{1}{p+1}} \varrho^{\frac{p}{p+1}}$ . For  $P_n$ , it is optimal to transport mass from the largest value among the training data  $\{Z_i\}_{i=1}^n$  to  $z = 1$ , where the amount of mass  $\gamma$  to be transported is given as a solution to

$$\left( \gamma \cdot (1 - \max_{i \in [n]} Z_i)^p \right)^{1/p} = \varrho,$$

which gives  $\gamma = \frac{\varrho^p}{(1 - \max_{i \in [n]} Z_i)^p}$  leading to the local worst-case risk of  $R_{\varrho, p}(P_n, f_1) = \frac{\alpha \varrho^p}{(1 - \max_{i \in [n]} Z_i)^p}$  2

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<sup>2</sup>Note that we are assuming that  $\varrho \leq (1 - \max_{i \in [n]} Z_i) \cdot n^{-1/p}$ ; otherwise, the local minimax risk of  $f_1$  can be smaller, which leads to even higher probability of choosing nonrobust hypothesis by local minimax ERM

The outcome of the local minimax ERM procedure is the hypothesis minimizing the local worst-case risk. In other words, the local minimax hypothesis is  $f_0$  whenever  $1 \leq \frac{\alpha \varrho^p}{(1 - \max Z_i)^p}$  holds, which is true whenever  $1 - \alpha^{1/p} \varrho < \max Z_i$ . Thus, the local minimax ERM procedure gives

$$\hat{f} = \begin{cases} f_1, & \text{with probability } \left(1 - \varrho \alpha^{\frac{1}{p}}\right)^n, \\ f_0 & \text{otherwise} \end{cases}$$

for any  $\varrho \leq \alpha^{-1/p}$ . On the other hand, the minimizer of the local minimax risk with respect to  $P$  is given by

$$f^* = \begin{cases} f_1, & \varrho \leq (p+1)^{-\frac{1}{p}} \alpha^{-\frac{p+1}{p}} \\ f_0, & \varrho \geq (p+1)^{-\frac{1}{p}} \alpha^{-\frac{p+1}{p}} \end{cases}$$

Now if we calculate the excess risk of the local minimax ERM hypothesis, we get

$$R_{\varrho,p}(\hat{f}, P) - R_{\varrho,p}(f^*, P) = \begin{cases} \alpha(p+1)^{\frac{1}{p+1}} \varrho^{\frac{p}{p+1}} - 1 & \text{w.p. } \left(1 - \varrho \alpha^{\frac{1}{p}}\right)^n, \\ 0, & \text{otherwise} \end{cases}$$

for any  $\varrho \in [(p+1)^{-1/p} \alpha^{-1-1/p}, \alpha^{-1/p}]$ , which is a nonempty interval as  $\alpha > 1$ . Now, if we look at the quantity

$$\varepsilon_\delta^*(\varrho) := \inf \left\{ \varrho \geq 0 : P \left[ R_{\varrho,p}(\hat{f}, P) - R_{\varrho,p}(f^*, P) > \varepsilon \right] < \delta \right\}$$

for some fixed  $\delta > 0$ , then we get

$$\varepsilon_\delta^*(\varrho) = \begin{cases} \alpha(p+1)^{\frac{1}{p+1}} \varrho^{\frac{p}{p+1}} - 1, & (p+1)^{-\frac{1}{p}} \alpha^{-\frac{p+1}{p}} \leq \varrho \leq (1 - \delta^{\frac{1}{n}}) \alpha^{-\frac{1}{p}}. \\ 0, & \text{otherwise.} \end{cases}$$

Now observe that for some fixed  $\varrho$  and  $\delta$ , we can select  $\alpha = (1 - \delta^{1/n})^p \varrho^{-p}$  to incur a nontrivial excess risk of order  $\varrho^{-\frac{p^2}{p+1}}$ . Moreover, this ‘selection of worst  $\alpha$ ’ can be done without changing the value of the Rademacher average of  $\mathcal{F}$ , as  $f_1$  does not change on the support of  $P$ .

## C Proofs for Section 3

### C.1 Proof of Theorem 1

The proof uses a modification of the techniques of Koltchinskii and Panchenko [14]. From the definition of the local minimax risk, we have, for any  $f \in \mathcal{F}$

$$\begin{aligned} R_{\varrho,p}(P, f) &= \min_{\lambda \geq 0} \{ \lambda \varrho^p + \mathbf{E}_P[\varphi_{\lambda,f}] \} \\ &\leq \min_{\lambda \geq 0} \left\{ \lambda \varrho^p + \mathbf{E}_{P_n}[\varphi_{\lambda,f}] + \sup_{f \in \mathcal{F}} (\mathbf{E}_P[\varphi_{\lambda,f}] - \mathbf{E}_{P_n}[\varphi_{\lambda,f}]) \right\}, \end{aligned}$$

where

$$X_\lambda := \sup_{f \in \mathcal{F}} (\mathbf{E}_P[\varphi_{\lambda,f}] - \mathbf{E}_{P_n}[\varphi_{\lambda,f}]) = \frac{1}{n} \sup_{f \in \mathcal{F}} \left[ \sum_{i=1}^n (\mathbf{E} \varphi_{\lambda,f}(Z) - \varphi_{\lambda,f}(Z_i)) \right]$$

is a data-dependent random variable for each  $\lambda \geq 0$ . Since  $\varphi_{\lambda,f}(Z_i) \in [0, M]$ , we know from McDiarmid’s inequality that, for any fixed  $\lambda \geq 0$ ,

$$\mathbf{P} \left( X_\lambda > \mathbf{E} X_\lambda + \frac{Mt}{\sqrt{n}} \right) \leq \exp(-2t^2).$$

Furthermore, using a standard symmetrization argument, we have

$$\mathbf{E} X_\lambda \leq 2 \cdot \mathbf{E} \sup_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^n \varepsilon_i \varphi_{\lambda,f}(Z_i)$$

where  $\varepsilon_1, \dots, \varepsilon_n$  are i.i.d. Rademacher random variables independent of  $Z_1, \dots, Z_n$ . The  $\mathcal{F}$ -indexed process  $Y = (Y_f)_{f \in \mathcal{F}}$  defined via

$$Y_f = \frac{1}{\sqrt{n}} \varepsilon_i \varphi_{\lambda, f}(Z_i)$$

is clearly zero-mean and subgaussian with respect to the metric  $\|f - f'\|_\infty$ , as

$$\begin{aligned} \mathbf{E}[\exp(t(Y_f - Y_{f'}))] &= \mathbf{E} \left[ \exp \left( \frac{t}{\sqrt{n}} \sum_{i=1}^n \varepsilon_i (\varphi_{\lambda, f}(Z_i) - \varphi_{\lambda, f'}(Z_i)) \right) \right] \\ &= \left( \mathbf{E} \left[ \exp \left( \frac{t}{\sqrt{n}} \varepsilon_1 \cdot \sup_{z'} \inf_{z''} \{f(z') - \lambda d_{\mathcal{Z}}^p(Z_1, z') - f'(z'') + \lambda d_{\mathcal{Z}}^p(Z_1, z'')\} \right) \right] \right)^n \\ &\leq \left( \mathbf{E} \left[ \exp \left( \frac{t}{\sqrt{n}} \varepsilon_1 \cdot \sup_{z'} \{f(z') - f'(z')\} \right) \right] \right)^n \\ &\leq \exp \left( \frac{t^2 \|f - f'\|_\infty^2}{2} \right), \end{aligned}$$

where the second line is by independence and last line is by Hoeffding's lemma. Invoking Dudley's entropy integral [19], we get

$$\mathbf{E} X_\lambda \leq \frac{24}{\sqrt{n}} \mathfrak{C}(\mathcal{F})$$

for any  $\lambda \geq 0$ . Summing up, we have, for any fixed  $\lambda \geq 0$ ,

$$\mathbf{P} \left( \exists f \in \mathcal{F} : R_{\varrho, p}(P, f) > \lambda \varrho^p + \mathbf{E}_{P_n}[\varphi_{\lambda, f}] + \frac{24}{\sqrt{n}} \mathfrak{C}(\mathcal{F}) + \frac{Mt}{\sqrt{n}} \right) \leq \exp(-2t^2).$$

Now, pick the sequences  $\lambda_k = k$  and  $t_k = t + \sqrt{\log k}$  for  $k = 1, 2, 3, \dots$ . Then, by the union bound,

$$\begin{aligned} \mathbf{P} \left( \exists f \in \mathcal{F} : R_{\varrho, p}(P, f) > \min_{k=1,2,\dots} \left\{ \lambda_k \varrho^p + \mathbf{E}_{P_n}[\varphi_{\lambda_k, f}] + \frac{24}{\sqrt{n}} \mathfrak{C}(\mathcal{F}) + \frac{Mt_k}{\sqrt{n}} \right\} \right) \\ \leq \sum_{k=1}^{\infty} \exp(-2t_k^2) \\ \leq \exp(-2t^2) \sum_{k=1}^{\infty} \exp(-2 \log k) \\ \leq 2 \exp(-2t^2). \end{aligned}$$

On the other hand,

$$\begin{aligned} \min_{k=1,2,\dots} \left\{ \lambda_k \varrho^p + \mathbf{E}_{P_n}[\varphi_{\lambda_k, f}] + \frac{24}{\sqrt{n}} \mathfrak{C}(\mathcal{F}) + \frac{Mt_k}{\sqrt{n}} \right\} \\ = \min_{k=1,2,\dots} \left\{ k \varrho^p + \mathbf{E}_{P_n}[\varphi_{k, f}] + \frac{24}{\sqrt{n}} \mathfrak{C}(\mathcal{F}) + \frac{Mt}{\sqrt{n}} + \frac{M\sqrt{\log k}}{\sqrt{n}} \right\} \\ \leq \min_{\lambda \geq 0} \left\{ (\lambda + 1) \varrho^p + \mathbf{E}_{P_n}[\varphi_{\lambda, f}] + \frac{24}{\sqrt{n}} \mathfrak{C}(\mathcal{F}) + \frac{Mt}{\sqrt{n}} + \frac{M\sqrt{\log(\lambda + 1)}}{\sqrt{n}} \right\}, \end{aligned}$$

where the last line holds since, for any  $\lambda \geq 0$ , there exists  $k \in \{1, 2, \dots\}$  such that  $\lambda \leq k \leq \lambda + 1$ , and  $\varphi_{\lambda_1, f} \leq \varphi_{\lambda_2, f}$  holds whenever  $\lambda_1 \geq \lambda_2$  (from the definition of  $\varphi_{\lambda, f}$ ).

For the other direction, notice that

$$R_{\varrho, p}(P_n, f) \leq \min_{\lambda \geq 0} \left\{ \lambda \varrho^p + \mathbf{E}_P[\varphi_{\lambda, f}] + \sup_{f \in \mathcal{F}} (\mathbf{E}_{P_n}[\varphi_{\lambda, f}] - \mathbf{E}_P[\varphi_{\lambda, f}]) \right\},$$

where the random variable  $\sup_{f \in \mathcal{F}} (\mathbf{E}_{P^n} [\varphi_{\lambda, f}] - \mathbf{E}_P [\varphi_{\lambda, f}])$  can be analyzed in the same way as above. This leads to

$$\mathbf{P} \left( \exists f \in \mathcal{F} : R_{\varrho, p}(P_n, f) > \min_{\lambda \geq 0} \left\{ (\lambda + 1) \varrho^p + \mathbf{E}_P [\varphi_{\lambda, f}(Z)] + \frac{M \sqrt{\log(\lambda + 1)}}{\sqrt{n}} \right\} + \frac{24 \mathfrak{C}(\mathcal{F})}{\sqrt{n}} + \frac{Mt}{\sqrt{n}} \right) \leq 2 \exp(-2t^2),$$

for any  $t > 0$ .

## C.2 Proof of Lemma 1

First note that we have

$$\tilde{\lambda} \cdot \varrho^p \leq \tilde{\lambda} \cdot \varrho^p + \mathbf{E}_Q \left[ \sup_{z' \in \mathcal{Z}} \{ \tilde{f}(z') - \tilde{f}(Z) - \tilde{\lambda} \cdot d_{\mathcal{Z}}^p(Z, z') \} \right],$$

as the left-hand side corresponds to the choice  $z' = Z$ . Now, by the optimality of  $\tilde{\lambda}$  with respect to  $\tilde{f}$ , the right-hand side can be further upper-bounded as follows for any  $\lambda \geq 0$ :

$$\begin{aligned} &\leq \lambda \cdot \varrho^p + \mathbf{E}_Q \left[ \sup_{z' \in \mathcal{Z}} \{ \tilde{f}(z') - \tilde{f}(Z) - \lambda \cdot d_{\mathcal{Z}}^p(Z, z') \} \right] \\ &\leq \lambda \cdot \varrho^p + \mathbf{E}_Q \left[ \sup_{z' \in \mathcal{Z}} \{ L \cdot d_{\mathcal{Z}}(Z, z') - \lambda \cdot d_{\mathcal{Z}}^p(Z, z') \} \right] \\ &\leq \lambda \cdot \varrho^p + \sup_{t \geq 0} \{ L \cdot t - \lambda \cdot t^p \}, \end{aligned}$$

where for the second line we used the Lipschitz property (Assumption 3) and the third line holds by parametrizing  $t = d_{\mathcal{Z}}(Z, z')$ . If  $p = 1$ , we can simply take  $\lambda = L$  to get the inequality

$$\tilde{\lambda} \cdot \varrho \leq L \cdot \varrho + \sup_{t \geq 0} \{ L \cdot t - L \cdot t \} = L \cdot \varrho,$$

which gives  $\tilde{\lambda} \leq L$ . If  $p > 1$ , we can use the optimal value of  $t = (L/p\lambda)^{1/(p-1)}$  to get

$$\leq \lambda \cdot \varrho^p + L^{\frac{p}{p-1}} p^{-\frac{p}{p-1}} (p-1) \lambda^{-\frac{1}{p-1}}.$$

Minimizing the right-hand side over  $\lambda \geq 0$  with the choice of  $\lambda = L/p\varrho^{p-1}$ , we get

$$\tilde{\lambda} \cdot \varrho^p \leq L\varrho,$$

which yields the stated bound on  $\tilde{\lambda}$ .

## C.3 Proof of Theorem 2

The proof is same as the proof of Theorem 3 given below, except that we use Lemma 1 instead of Lemma 2. Then, the expected Rademacher complexity of the function class satisfies

$$\mathfrak{R}_n(\Phi) \leq \frac{24}{\sqrt{n}} \mathfrak{C}(\mathcal{F}) + \frac{24L \cdot C_0 \cdot \text{diam}(\mathcal{Z})^p}{\sqrt{n} \varrho^{p-1}}$$

(see Section D), and the result follows.

## C.4 Proof of Lemma 2

Since  $\varphi_{\lambda, f} \geq 0$  for all  $\lambda, f$ , we arrive at

$$\tilde{\lambda} \leq \frac{R_{\varrho, p}^*(Q, \mathcal{F})}{\varrho^p}. \quad (\text{C.1})$$

We proceed to upper-bound the local minimax risk  $R_{\varrho,p}^*(Q, \mathcal{F})$ :

$$\begin{aligned} R_{\varrho,p}^*(Q, \mathcal{F}) &= \inf_{f \in \mathcal{F}} \min_{\lambda \geq 0} \left\{ \lambda \varrho^p + \int_{\mathcal{Z}} \sup_{z' \in \mathcal{Z}} [f(z') - \lambda d_{\mathcal{Z}}^p(z, z')] Q(dz') \right\} \\ &\leq \min_{\lambda \geq 0} \left\{ \lambda \varrho^p + \int_{\mathcal{Z}} \sup_{z' \in \mathcal{Z}} [f_0(z') - \lambda d_{\mathcal{Z}}^p(z, z')] Q(dz') \right\} \\ &\leq \min_{\lambda \geq 0} \left\{ \lambda \varrho^p + \int_{\mathcal{Z}} \sup_{z' \in \mathcal{Z}} [C_0 d_{\mathcal{Z}}^p(z', z_0) - \lambda d_{\mathcal{Z}}^p(z, z')] Q(dz') \right\}. \end{aligned}$$

For  $\lambda \geq C_0 2^{p-1}$ , the integrand can be upper-bounded as follows:

$$\begin{aligned} \sup_{z' \in \mathcal{Z}} [C_0 d_{\mathcal{Z}}^p(z', z_0) - \lambda d_{\mathcal{Z}}^p(z, z')] &\leq \sup_{z' \in \mathcal{Z}} [C_0 2^{p-1} d_{\mathcal{Z}}^p(z, z_0) + (C_0 2^{p-1} - \lambda) d_{\mathcal{Z}}^p(z, z')] \\ &\leq C_0 2^{p-1} d_{\mathcal{Z}}^p(z, z_0). \end{aligned}$$

Therefore,

$$\begin{aligned} R_{\varrho,p}^*(Q, \mathcal{F}) &\leq \min_{\lambda \geq C_0 2^{p-1}} \left\{ \lambda \varrho^p + C_0 2^{p-1} \int_{\mathcal{Z}} d_{\mathcal{Z}}^p(z, z_0) Q(dz) \right\} \\ &\leq C_0 2^{p-1} (\varrho^p + (\text{diam}(\mathcal{Z}))^p). \end{aligned}$$

Substituting this estimate into (C.1), we obtain what we want.

### C.5 Proof of Theorem 3

Let  $f^* \in \mathcal{F}$  be any achiever of the local minimax risk  $R_{\varrho,p}^*(P, \mathcal{F})$ . We start by decomposing the excess risk:

$$\begin{aligned} R_{\varrho,p}(P, \hat{f}) - R_{\varrho,p}^*(P, \mathcal{F}) &= R_{\varrho,p}(P, \hat{f}) - R_{\varrho,p}(P, f^*) \\ &\leq R_{\varrho,p}(P, \hat{f}) - R_{\varrho,p}(P_n, \hat{f}) + R_{\varrho,p}(P_n, f^*) - R_{\varrho,p}(P, f^*), \end{aligned}$$

where the last step follows from the definition of  $\hat{f}$ . Define

$$\hat{\lambda} := \arg \min_{\lambda \geq 0} \left\{ \lambda \varrho^p + \mathbf{E}_{P_n}[\varphi_{\lambda, \hat{f}}(Z)] \right\}, \quad \lambda^* := \arg \min_{\lambda \geq 0} \left\{ \lambda \varrho^p + \mathbf{E}_P[\varphi_{\lambda, f^*}(Z)] \right\}.$$

Then, using Proposition 4, we can write

$$\begin{aligned} R_{\varrho,p}(P, \hat{f}) - R_{\varrho,p}(P_n, \hat{f}) &= \min_{\lambda \geq 0} \left\{ \lambda \varrho^p + \int_{\mathcal{Z}} \varphi_{\lambda, \hat{f}}(z) P(dz) \right\} - \left( \hat{\lambda} \varrho^p + \int_{\mathcal{Z}} \varphi_{\hat{\lambda}, \hat{f}}(z) P_n(dz) \right) \\ &\leq \int_{\mathcal{Z}} \varphi_{\hat{\lambda}, \hat{f}}(z) (P - P_n)(dz) \end{aligned}$$

and, following similar logic,

$$R_{\varrho,p}(P_n, f^*) - R_{\varrho,p}(P, f^*) \leq \int_{\mathcal{Z}} \varphi_{\lambda^*, f^*}(z) (P_n - P)(dz). \quad (\text{C.2})$$

By Lemma 2,  $\hat{\lambda} \in \Lambda := [0, C_0 2^{p-1} (1 + (\text{diam}(\mathcal{Z})/\varrho)^p)]$ . Hence, defining the function class  $\Phi := \{\varphi_{\lambda, f} : \lambda \in \Lambda, f \in \mathcal{F}\}$ , we have

$$R_{\varrho,p}(P, \hat{f}) - R_{\varrho,p}(P_n, \hat{f}) \leq \sup_{\varphi \in \Phi} \left[ \int_{\mathcal{Z}} \varphi d(P - P_n) \right]. \quad (\text{C.3})$$

Since all  $f \in \mathcal{F}$  take values in  $[0, M]$ , the same holds for all  $\varphi \in \Phi$ . Therefore, by a standard symmetrization argument,

$$R_{\varrho,p}(P, \hat{f}) - R_{\varrho,p}(P_n, \hat{f}) \leq 2 \mathfrak{R}_n(\Phi) + M \sqrt{\frac{2 \log(2/\delta)}{n}} \quad (\text{C.4})$$

with probability at least  $1 - \delta/2$ , where

$$\mathfrak{R}_n(\Phi) := \mathbf{E} \left[ \sup_{\varphi \in \Phi} \frac{1}{n} \sum_{i=1}^n \varepsilon_i \varphi(Z_i) \right]$$

is the expected Rademacher average of  $\Phi$ , with i.i.d. Rademacher random variables  $\varepsilon_1, \dots, \varepsilon_n$  independent of  $Z_1, \dots, Z_n$ . Moreover, from (C.2) and from Hoeffding's inequality it follows that

$$R_{\ell,p}(P_n, f^*) - R_{\ell,p}(P, f^*) \leq M \sqrt{\frac{\log(2/\delta)}{2n}} \quad (\text{C.5})$$

with probability at least  $1 - \delta/2$ . Combining (C.4) and (C.5), and applying Lemma 5 from Appendix D, we obtain the theorem.

## C.6 Proof of Corollary 1

We first verify the regularity assumptions. Assumption 1 is evidently satisfied since  $\text{diam}(\mathcal{Z}) = \sqrt{\text{diam}(\mathcal{X})^2 + \text{diam}(\mathcal{Y})^2} \leq 2\sqrt{r_0^2 + B^2}$ . Each  $f \in \mathcal{F}$  is continuous, and Assumption 2 holds with  $M = (\|s\|_\infty + B)^2$ . To verify Assumption 3, we proceed as

$$\begin{aligned} |f(x, y) - f(x', y')| &= |(y - s(f_0^T x))^2 - (y' - s(f_0^T x'))^2| \\ &\leq |y + y' - s(f_0^T x) - s(f_0^T x')| \cdot |y - y' + s(f_0^T x') - s(f_0^T x)| \\ &\leq (2B + 2\|s\|_\infty) \cdot (|y - y'| + |s(f_0^T x') - s(f_0^T x)|) \\ &\leq (2B + 2\|s\|_\infty) \cdot (1 + \|s'\|_\infty) (|y - y'| + \|x' - x\|) \\ &\leq 2\sqrt{2}(B + \|s\|_\infty) \cdot (1 + \|s'\|_\infty) \sqrt{|y - y'|^2 + \|x - x'\|^2}, \end{aligned}$$

where the last line follows from Jensen's inequality. Hence, Assumption 3 holds with  $L = 2\sqrt{2}(B + \|s\|_\infty)(1 + \|s'\|_\infty)$ .

To evaluate the Dudley entropy integral in (3), we need to estimate the covering numbers  $\mathcal{N}(\mathcal{F}, \|\cdot\|_\infty, \cdot)$ . First observe that, for any two  $f, g \in \mathcal{F}$  corresponding to  $f_0, g_0 \in \mathbb{R}^d$ , we have

$$\begin{aligned} \sup_{x \in \mathcal{X}} \sup_{y \in \mathcal{Y}} |f(x, y) - g(x, y)| &= \sup_{x \in \mathcal{X}} \sup_{y \in \mathcal{Y}} |(y - s(f_0^T x))^2 - (y - s(g_0^T x))^2| \\ &\leq 2B \sup_{x \in \mathcal{X}} |s(f_0^T x) - s(g_0^T x)| + \sup_{x \in \mathcal{X}} |s^2(f_0^T x) - s^2(g_0^T x)| \\ &\leq \underbrace{2r_0 (B + \|s\|_\infty) \|s'\|_\infty}_{:=D} \|f_0 - g_0\|_2. \end{aligned}$$

Since  $f_0, g_0$  belong to the unit ball in  $\mathbb{R}^d$ ,

$$\mathcal{N}(\mathcal{F}, \|\cdot\|_\infty, u) \leq \left( \frac{3D}{u} \right)^d$$

for  $0 < u < D$ , and  $\mathcal{N}(\mathcal{F}, \|\cdot\|_\infty, u/2) = 1$  for  $u \geq 2D$ , which gives

$$\begin{aligned} \int_0^\infty \sqrt{\log \mathcal{N}(\mathcal{F}, \|\cdot\|_\infty, u)} du &\leq \int_0^D \sqrt{d \log(3D/u)} du \\ &= 3D\sqrt{d} \int_0^{1/3} \sqrt{\log(1/u)} du \\ &\leq 3D\sqrt{d}/2. \end{aligned}$$

Substituting this into the bound (10), we get the desired estimate.

## C.7 Proof of Corollary 2

We will denote by  $\langle \cdot, \cdot \rangle_K$  the inner product in  $\mathcal{H}_K$ , and by  $\|\cdot\|_K$  the induced norm.

For completeness, we state the covering number estimates by Cucker and Zhou [7, Thm 5.1].

**Proposition 6.** For compact  $\mathcal{X} \subset \mathbb{R}^d$ , the following holds for all  $u \in (0, r/2]$ .

$$\log \mathcal{N}(I_K(\mathcal{B}_r), \|\cdot\|_{\mathcal{X}}, u) \leq d \left( 32 + \frac{640d(\text{diam}(\mathcal{X}))^2}{\sigma^2} \right)^{d+1} \left( \log \frac{r}{u} \right)^{d+1}.$$

We would also need the following technical lemma.

**Lemma 4.** For any  $f, g \in \mathcal{F}$  induced by  $f_0, g_0 \in I_K(\mathcal{B}_r)$  (respectively), we have:

$$\begin{aligned} \|f\|_{\infty} &\leq 2(r^2 + B^2) \\ \|f - g\|_{\infty} &\leq 2(r + B)\|f_0 - g_0\|_{\mathcal{X}}. \end{aligned}$$

*Proof.* First note that  $\sqrt{K(x, x)} = 1$  holds for any  $x \in \mathcal{X}$  by the definition of Gaussian kernel. This leads immediately to the first claim: for any  $x \in \mathcal{X}, y \in [-B, B]$ ,

$$(f_0(x) - y)^2 \leq 2f_0^2(x) + 2y^2 \leq 2(\langle f_0, K_x \rangle_K)^2 + 2B^2 \leq 2(\langle f_0, f_0 \rangle_K) + 2B^2,$$

where the first inequality is by Jensen's inequality, the second is due to the reproducing kernel property of  $K$ , and the third is Cauchy-Schwarz inequality in  $\mathcal{H}_K$  ( $K_x$  denotes the kernel centered at  $x$ , i.e.  $x' \mapsto K(x, x')$ ). The second claim can be established similarly: for any  $x \in \mathcal{X}, y \in [-B, B]$ ,

$$\begin{aligned} |(f_0(x) - y)^2 - (g_0(x) - y)^2| &= |f_0(x) + g_0(x) - 2y| |f_0(x) - g_0(x)| \\ &\leq \left( 2 \sup_{h_0 \in I_K(\mathcal{B}_r)} |h_0(x)| + 2|y| \right) |f_0(x) - g_0(x)| \\ &\leq 2(r + B)\|f_0 - g_0\|_{\mathcal{X}}, \end{aligned}$$

where the last inequality is due to Cauchy-Schwarz inequality again.  $\square$

Before proceeding, we first observe that the Gaussian kernel is  $(\sqrt{2}/\sigma)$ -Lipschitz, i.e.  $\|K_x - K_{x'}\|_K \leq \sqrt{2}/\sigma \cdot \|x - x'\|_2$ . Indeed, we can proceed as

$$\begin{aligned} \|K_x - K_{x'}\|_K^2 &= \langle K_x - K_{x'}, K_x - K_{x'} \rangle_K \\ &= 2 - 2K(x, x') \\ &= 2 - 2 \exp \left( -\frac{\|x - x'\|_2^2}{\sigma^2} \right) \\ &\leq \frac{2}{\sigma^2} \|x - x'\|_2^2, \end{aligned}$$

where we used the fact that the function  $u \mapsto 2u/\sigma^2 - 2 + 2e^{-u/\sigma^2}$  is nonnegative for  $u \geq 0$ .

We now check the validity of Assumptions [1](#)-[3](#). Assumption [1](#) holds as  $\text{diam}(\mathcal{Z}) = \sqrt{\text{diam}(\mathcal{X})^2 + \text{diam}(\mathcal{Y})^2} \leq 2\sqrt{r_0^2 + B^2}$ . The functions in  $\mathcal{F}$  are continuous, and Assumption [2](#) holds with  $M = 2(r^2 + B^2)$  by virtue of the first estimate of Lemma [4](#). To verify Assumption [3](#), we proceed as

$$\begin{aligned} |f(x, y) - f(x', y')| &= |(y - f_0(x))^2 - (y' - f_0(x'))^2| \\ &\leq |y + y' - f_0(x) - f_0(x')| \cdot |y - y' + f_0(x') - f_0(x)| \\ &\leq 2(r + B) \cdot (|y - y'| + |\langle f_0, K_{x'} - K_x \rangle_K|) \\ &\leq 2(r + B) \cdot (|y - y'| + r \cdot \|K_{x'} - K_x\|_K) \\ &\leq 2(r + B) \cdot \left( |y - y'| + \frac{r\sqrt{2}}{\sigma} \|x - x'\|_2 \right) \\ &\leq 2(r + B) \cdot \left( 1 + r\sqrt{2}/\sigma \right) (|y - y'| + \|x - x'\|_2) \\ &\leq 2\sqrt{2}(r + B) \cdot \left( 1 + r\sqrt{2}/\sigma \right) \sqrt{|y - y'|^2 + \|x - x'\|_2^2}, \end{aligned}$$

where the fourth inequality holds by the Lipschitz continuity of the Gaussian reproducing kernel, and the last inequality is Jensen's inequality. Hence, Assumption [3](#) holds with  $L = 2\sqrt{2}(r + B) \cdot (1 + r\sqrt{2}/\sigma)$ .



Now we proceed to upper-bound the Dudley entropy integral for  $\mathcal{F}$ :

$$\begin{aligned} \int_0^\infty \sqrt{\log \mathcal{N}(\mathcal{F}, \|\cdot\|_\infty, u)} du &\leq \int_0^{2(r^2+Br)} \sqrt{\log \mathcal{N}\left(I_K(\mathcal{B}_r), \|\cdot\|_x, \frac{u}{2(r+B)}\right)} du \\ &\leq \underbrace{\int_0^{r^2+Br} \sqrt{\log \mathcal{N}\left(I_K(\mathcal{B}_r), \|\cdot\|_x, \frac{u}{2(r+B)}\right)} du}_{:=T_1} \\ &\quad + \underbrace{\int_{r^2+Br}^{2(r^2+Br)} \sqrt{\log \mathcal{N}\left(I_K(\mathcal{B}_r), \|\cdot\|_x, \frac{r}{2}\right)} du}_{:=T_2} \end{aligned}$$

where we used the second claim of Lemma 4 for the first inequality and the monotonicity of covering numbers for the second inequality. Plugging in the estimate from Proposition 6, we get

$$\begin{aligned} T_1 &\leq 2\sqrt{d} \left(32 + \frac{2560dr_0^2}{\sigma^2}\right)^{\frac{d+1}{2}} (r^2 + Br) \Gamma\left(\frac{d+3}{2}, \log 2\right) \\ T_2 &\leq \sqrt{d} \left(32 + \frac{2560dr_0^2}{\sigma^2}\right)^{\frac{d+1}{2}} (r^2 + Br) (\log 2)^{\frac{d+1}{2}}, \end{aligned}$$

and hence  $T_1 + T_2 \leq \frac{C_1}{48}(r^2 + Br)$ , where the constant  $C_1$  is

$$C_1 = 48\sqrt{d} \left(2\Gamma\left(\frac{d+3}{2}, \log 2\right) + (\log 2)^{\frac{d+1}{2}}\right) \left(32 + \frac{2560dr_0^2}{\sigma^2}\right)^{\frac{d+1}{2}},$$

## D Rademacher complexity of $\Phi$

**Lemma 5.** *The expected Rademacher complexity of the function class  $\Phi$  satisfies*

$$\mathfrak{R}_n(\Phi) \leq \frac{24}{\sqrt{n}} \mathfrak{C}(\mathcal{F}) + \frac{12C_0(2 \operatorname{diam}(\mathcal{Z}))^p}{\sqrt{n}} \left(1 + \left(\frac{\operatorname{diam}(\mathcal{Z})}{\varrho}\right)^p\right).$$

*Proof of Lemma 5* Define the  $\Phi$ -indexed process  $X = (X_\varphi)_{\varphi \in \Phi}$  via

$$X_\varphi := \frac{1}{\sqrt{n}} \sum_{i=1}^n \varepsilon_i \varphi(Z_i),$$

which is clearly zero-mean:  $\mathbf{E}[X_\varphi] = 0$  for all  $\varphi \in \Phi$ . To upper-bound the Rademacher average  $\mathfrak{R}_n(\Phi)$ , we first show that  $X$  is a subgaussian process with respect to a suitable pseudometric. For  $\varphi = \varphi_{\lambda, f}$  and  $\varphi' = \varphi_{\lambda', f'}$ , define

$$d_\Phi(\varphi, \varphi') := \|f - f'\|_\infty + (\operatorname{diam}(\mathcal{Z}))^p |\lambda - \lambda'|,$$

and it is not hard to show that  $\|\varphi - \varphi'\|_\infty \leq d_\Phi(\varphi, \varphi')$ . Then, for any  $t \in \mathbb{R}$ , using Hoeffding's lemma and the fact that  $(\varepsilon_i, Z_i)$  are i.i.d., we arrive at

$$\begin{aligned} \mathbf{E}[\exp(t(X_\varphi - X_{\varphi'}))] &= \mathbf{E}\left[\exp\left(\frac{t}{\sqrt{n}} \sum_{i=1}^n \varepsilon_i(\varphi(Z_i) - \varphi'(Z_i))\right)\right] \\ &= \left(\mathbf{E}\left[\exp\left(\frac{t}{\sqrt{n}} \varepsilon_1(\varphi(Z_1) - \varphi'(Z_1))\right)\right]\right)^n \\ &\leq \exp\left(\frac{t^2 d_\Phi^2(\varphi, \varphi')}{2}\right). \end{aligned}$$

Hence,  $X$  is subgaussian with respect to  $d_\Phi$ , and therefore the Rademacher average  $\mathfrak{R}_n(\Phi)$  can be upper-bounded by the Dudley entropy integral [19]:

$$\mathfrak{R}_n(\Phi) \leq \frac{12}{\sqrt{n}} \int_0^\infty \sqrt{\log \mathcal{N}(\Phi, d_\Phi, u)} du,$$

where  $\mathcal{N}(\Phi, d_\Phi, \cdot)$  are the covering numbers of  $(\Phi, d_\Phi)$ . From the definition of  $d_\Phi$ , it follows that

$$\mathcal{N}(\Phi, d_\Phi, u) \leq \mathcal{N}(\mathcal{F}, \|\cdot\|_\infty, u/2) \cdot \mathcal{N}(\Lambda, |\cdot|, u/2(\text{diam}(\mathcal{Z}))^p),$$

and therefore

$$\mathfrak{R}_n(\Phi) \leq \frac{12}{\sqrt{n}} \left( \int_0^\infty \sqrt{\log \mathcal{N}(\mathcal{F}, \|\cdot\|_\infty, u/2)} du + \int_0^\infty \sqrt{\log \mathcal{N}(\Lambda, |\cdot|, u/2(\text{diam}(\mathcal{Z}))^p)} du \right).$$

Since  $\Lambda$  is a compact interval, it is straightforward to upper-bound the second integral:

$$\begin{aligned} \int_0^\infty \sqrt{\log \mathcal{N}(\Lambda, |\cdot|, u/2(\text{diam}(\mathcal{Z}))^p)} du &\leq 2|\Lambda|(\text{diam}(\mathcal{Z}))^p \int_0^{1/2} \sqrt{\log(1/u)} du \\ &= 2c|\Lambda|(\text{diam}(\mathcal{Z}))^p, \end{aligned}$$

where  $|\Lambda| = C_0 2^{p-1} (1 + (\text{diam}(\mathcal{Z})/\varrho)^p)$  is the length of the interval  $\Lambda$  and the constant  $c = \frac{1}{2} (\sqrt{\log 2} + \sqrt{\pi} \cdot \text{erfc}(\sqrt{\log 2})) < 1$ . Consequently,

$$\begin{aligned} \mathfrak{R}_n(\Phi) &\leq \frac{12}{\sqrt{n}} \left( \int_0^\infty \sqrt{\log \mathcal{N}(\mathcal{F}, \|\cdot\|_\infty, u/2)} du + 2|\Lambda|(\text{diam}(\mathcal{Z}))^p \right) \\ &\leq \frac{24}{\sqrt{n}} \mathfrak{C}(\mathcal{F}) + \frac{12C_0(2 \text{diam}(\mathcal{Z}))^p}{\sqrt{n}} \left( 1 + \left( \frac{\text{diam}(\mathcal{Z})}{\varrho} \right)^p \right). \end{aligned}$$

□

## E Proofs for Section 4

### E.1 Proof of Lemma 3

First we prove that  $W_p(P, Q) \leq W_p(\mu, \nu)$ . Define the mapping  $\tilde{T} : \mathcal{Z} \rightarrow \mathcal{Z}$  by  $\tilde{T} := T \otimes \text{id}_Y$ , i.e.,  $\tilde{T}(z) = \tilde{T}(x, y) = (T(x), y)$ , and let  $\tilde{Q} = \tilde{T}_\# P$ , the pushforward of  $P$  by  $\tilde{T}$ . We claim that  $\tilde{Q} \equiv Q$ . Indeed, for any measurable sets  $A \subseteq \mathcal{X}$  and  $B \subseteq \mathcal{Y}$ ,

$$\begin{aligned} \tilde{Q}(A \times B) &= \tilde{T}_\# P(A \times B) \\ &= P(T^{-1}(A) \times B) \\ &= \int_{T^{-1}(A)} \mu(dx) P_{Y|X}(B|x) \\ &= \int_A T_\# \mu(dx) P_{Y|X}(B|T(x)) \\ &= \int_A \nu(dx) Q_{Y|X}(B|x), \end{aligned}$$

where we have used the relation (13) and the invertibility of  $T$ . Thus,

$$W_p^p(P, Q) \leq \mathbf{E}_P[d_{\mathcal{Z}}^p(Z, \tilde{T}(Z))] = \mathbf{E}_P[d_{\mathcal{X}}^p(X, T(X))] = W_p^p(\mu, \nu).$$

For the reverse inequality, let  $M \in \mathcal{P}(\mathcal{Z} \times \mathcal{Z})$  be the optimal coupling of  $P$  and  $Q$ . Then, for  $Z = (X, Y)$  and  $Z' = (X', Y')$  with  $(Z, Z') \sim M$ , the marginal  $M_{XX'}$  is evidently a coupling of the marginals  $\mu$  and  $\nu$ , and therefore

$$\begin{aligned} W_p^p(P, Q) &= \mathbf{E}_M[d_{\mathcal{Z}}^p(Z, Z')] \\ &= \mathbf{E}_M[d_{\mathcal{X}}^p(X, X')] + \mathbf{E}_M[d_{\mathcal{Y}}^p(Y, Y')] \\ &\geq \mathbf{E}_M[d_{\mathcal{X}}^p(X, X')] \\ &\geq W_p^p(\mu, \nu). \end{aligned}$$

## E.2 Proof of Theorem 4

For simplicity, we assume that there exists a hypothesis  $f^* \in \mathcal{F}$  that achieves  $R^*(Q, \mathcal{F})$ . Then, for any  $\varrho > 0$  such that  $W_p(P, Q) \leq \varrho$ , Proposition 1 implies that

$$\begin{aligned} R(Q, \hat{f}) - R(Q, f^*) &\leq R_{\varrho,p}(P, \hat{f}) - R_{\varrho,p}(P, f^*) + 2L\varrho \\ &\leq R_{\varrho,p}(P, \hat{f}) - R_{\varrho,p}^*(P, \mathcal{F}) + 2L\varrho. \end{aligned}$$

From Theorem 2, we know that

$$R_{\varrho,p}(P, \hat{f}) - R_{\varrho,p}^*(P, \mathcal{F}) \leq \frac{48\mathfrak{C}(\mathcal{F})}{\sqrt{n}} + \frac{48L\text{diam}^p(\mathcal{Z})}{\sqrt{n}\varrho^{p-1}} + \frac{3M\sqrt{\log(4/\delta)}}{\sqrt{2n}}$$

holds with probability at least  $1 - \delta/2$ . Thus, it remains to find the right  $\varrho$ , such that that  $W_p(P, Q) \leq \varrho$  holds with high probability. From Proposition 5, we see that each of the following two statements holds with probability at least  $1 - \delta/4$ :

$$W_p(\mu_n, \mu) \leq \left( \frac{\log(4C_a/\delta)}{C_b n} \right)^{p/d}, \quad W_p(\nu_m, \nu) \leq \left( \frac{\log(4C_a/\delta)}{C_b m} \right)^{p/d}.$$

Since  $W_p(P, Q) = W_p(\mu, \nu)$  by Lemma 3, we see that  $W_p(P, Q) \leq \widehat{\varrho}(\delta)$  with probability at least  $1 - \delta/2$ , where  $\widehat{\varrho}(\delta)$  is given by Eq. (17). The claim of the theorem follows from the union bound.