A Checklist

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes]
   (b) Did you describe the limitations of your work? [Yes] See Section 6 and Appendix H in the supplement.
   (c) Did you discuss any potential negative societal impacts of your work? [Yes] See Section 6 and Appendix I in the supplement.
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]
2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [Yes] See Section 4.3, Assumption 1 and 2.
   (b) Did you include complete proofs of all theoretical results? [Yes] See Appendix B and C in the supplement.
3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [Yes] See Section 5.1. We provide code and instructions to reproduce the main experimental results for our proposed method in the supplement.
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes] See Section 5.1 and Appendix E in the supplement.
   (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [Yes] See Figure 3 in the main text and Figure 5 in the supplement.
   (d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [Yes] See Section 5.1.
4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
   (a) If your work uses existing assets, did you cite the creators? [Yes] See Section 5.1.
   (b) Did you mention the license of the assets? [Yes] See Section 5.1 and Appendix D in the supplement.
   (c) Did you include any new assets either in the supplemental material or as a URL? [Yes] We provide code for our proposed method in the supplement.
   (d) Did you discuss whether and how consent was obtained from people whose data you're using/curating? [N/A]
   (e) Did you discuss whether the data you are using/curating contains personally identifiable information or offensive content? [N/A]
5. If you used crowdsourcing or conducted research with human subjects...
   (a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A]
   (b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? [N/A]
   (c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A]

B Proof of Theorem 1

Proof. The following lemma holds:

Lemma 3. *[10, 9] Let X, Z be random variables residing in metric spaces $\mathcal{X}$, $\mathcal{Z}$, respectively. Let also $\mathcal{F}, \mathcal{G}$ be the two separable RKHSs on $\mathcal{X}, \mathcal{Z}$ induced by k_X and k_Z, respectively. Then, the following inequality holds:*

$$\mathrm{HSIC}(X, Z) \geq \sup_{s \in \mathcal{F}, t \in \mathcal{G}} \mathrm{Cov}[s(X), t(Z)]. \tag{13}$$

Lemma 3 shows that HSIC bounds the supremum of the covariance between any pair of functions in the RKHS, $\mathcal{F},\mathcal{G}$. Assumption 2 states that functions in $\mathcal{F}$ and $\mathcal{G}$ are uniformly bounded by $M_\mathcal{F} > 0$ and $M_\mathcal{G} > 0$, respectively. Let $\tilde{\mathcal{F}}$ and $\tilde{\mathcal{G}}$ be the restriction of $\mathcal{F}$ and $\mathcal{G}$ to functions in the unit ball of the respective RKHSs through rescaling, i.e.:

$$\tilde{\mathcal{F}} = \left\{ \frac{h}{M_\mathcal{F}} : h \in \mathcal{F} \right\} \quad \text{and} \quad \tilde{\mathcal{G}} = \left\{ \frac{g}{M_\mathcal{G}} : g \in \mathcal{G} \right\}. \tag{14}$$

The following lemma links the covariance of the functions in the original RKHSs to their normalized version:

Lemma 4. *[9] Suppose $\mathcal{F}$ and $\mathcal{G}$ are RKHSs over $\mathcal{X}$ and $\mathcal{Z}$, s.t. $\|s\|_\infty \leq M_\mathcal{F}$ for all $s \in \mathcal{F}$ and $\|t\|_\infty \leq M_\mathcal{G}$ for all $t \in \mathcal{G}$. Then the following holds:*

$$\sup_{s\in\mathcal{F},t\in\mathcal{G}} \mathrm{Cov}[s(X),t(Z)] = M_\mathcal{F} M_\mathcal{G} \sup_{s\in\tilde{\mathcal{F}},t\in\tilde{\mathcal{G}}} \mathrm{Cov}[s(X),t(Z)]. \tag{15}$$

For simplicity in notation, we define the following sets containing functions that satisfy Assumption 1:

$$C_b(\mathcal{X}) = \{h \in C(\mathcal{X}) : ||h||_\infty \leq M_\mathcal{X}\} \quad \text{and} \quad C_b(\mathcal{Z}) = \{g \in C(\mathcal{Z}) : ||g||_\infty \leq M_\mathcal{Z}\}. \tag{16}$$

In Assumption 2, we mention that functions in $\mathcal{F}$ and $\mathcal{G}$ may require appropriate rescaling to keep the universality of corresponding kernels. To make the rescaling explicit, we define the following *rescaled* RKHSs:

$$\hat{\mathcal{F}} = \left\{ \frac{M_\mathcal{X}}{M_\mathcal{F}} \cdot h : h \in \mathcal{F} \right\} \quad \text{and} \quad \hat{\mathcal{G}} = \left\{ \frac{M_\mathcal{Z}}{M_\mathcal{G}} \cdot g : g \in \mathcal{G} \right\}. \tag{17}$$

This rescaling ensures that $||\hat{h}||_\infty \leq M_\mathcal{X}$ for every $\hat{h} \in \hat{\mathcal{F}}$. Similarly, $||\hat{g}||_\infty \leq M_\mathcal{Z}$ for every $\hat{g} \in \hat{\mathcal{G}}$.

We also want to prove $\mathcal{F}$ is convex. Given $f, g \in \mathcal{F}$, we need to show for all $0 \leq \alpha \leq 1$, the function $\alpha f + (1-\alpha)g \in \mathcal{F}$. As linear summation of RKHS functions is in the RKHS, we just need to check that $||\alpha f + (1-\alpha)g||_\infty \leq M_\mathcal{F}$; indeed:

$$||\alpha f + (1-\alpha)g||_\infty \leq \alpha||f||_\infty + (1-\alpha)||g||_\infty \leq \alpha M_\mathcal{F} + (1-\alpha)M_\mathcal{F} \tag{18}$$

We thus conclude that the bounded RKHS $\mathcal{F}$ is indeed convex. Hence any rescaling of the function, as long as it has a norm less than $M_\mathcal{F}$, remains inside $\mathcal{F}$.

Indeed, the following lemma holds:

Lemma 5. *If $\mathcal{F},\mathcal{G}$ are universal with respect to $C_b(\mathcal{X}), C_b(\mathcal{Z})$, then:*

$$\hat{\mathcal{F}} = C_b(\mathcal{X}) \quad \textit{and} \quad \hat{\mathcal{G}} = C_b(\mathcal{Z}). \tag{19}$$

Proof. We prove this by first showing $C_b(\mathcal{X}) \subseteq \hat{\mathcal{F}}$ and then $\hat{\mathcal{F}} \subseteq C_b(\mathcal{X})$, which leads to equality of the sets.

- $C_b(\mathcal{X}) \subseteq \hat{\mathcal{F}}$: For all $h \in C_b(\mathcal{X})$, we show $h \in \hat{\mathcal{F}}$. Based on the definition of $C_b(\mathcal{X})$ in (16), we know $\|h\|_\infty \leq M_\mathcal{X}$. From universality stated in Assumption 2, $h \in \mathcal{F}$. Let $g = \frac{M_\mathcal{F}}{M_\mathcal{X}} h$. Then $\|g\|_\infty = \|\frac{M_\mathcal{F}}{M_\mathcal{X}} h\|_\infty = \frac{M_\mathcal{F}}{M_\mathcal{X}} ||h||_\infty \leq M_\mathcal{F}$. Based on the convexity of $\mathcal{F}$, $g \in \mathcal{F}$. We rescale every function in $\mathcal{F}$ by $\frac{M_\mathcal{X}}{M_\mathcal{F}}$ to form $\hat{\mathcal{F}}$, so $\frac{M_\mathcal{X}}{M_\mathcal{F}} g = \frac{M_\mathcal{X}}{M_\mathcal{F}} \frac{M_\mathcal{F}}{M_\mathcal{X}} h = h \in \hat{\mathcal{F}}$.
- $\hat{\mathcal{F}} \subseteq C_b(\mathcal{X})$: On the other hand, for all $h \in \hat{\mathcal{F}}$, h is continuous and bounded by $M_\mathcal{X}$. So based on the definition of $C_b(\mathcal{X})$ in (16), $h \in C_b(\mathcal{X})$. Thus, $\hat{\mathcal{F}} \subseteq C_b(\mathcal{X})$.

Having both side of the inclusion we conclude that $\hat{\mathcal{F}} = C_b(\mathcal{X})$. One can prove $\hat{\mathcal{G}} = C_b(\mathcal{Z})$ similarly.

$\square$

Applying the universality of kernels from Assumption 2 we can prove the following lemma:

Lemma 6. *Let X, Z be random variables residing in metric spaces $\mathcal{X}$, $\mathcal{Z}$ with separable RKHSs $\mathcal{F}$, $\mathcal{G}$ induced by kernel functions k_X and k_Z, respectively, for which Assumption 2 holds. Let $\hat{\mathcal{F}}$ and $\hat{\mathcal{G}}$ be the rescaled RKHSs defined in* (17)*. Then:*

$$\frac{M_{\mathcal{X}} M_{\mathcal{Z}}}{M_{\mathcal{F}} M_{\mathcal{G}}} \sup_{s\in\mathcal{F}, t\in\mathcal{G}} \mathrm{Cov}[s(X), t(Z)] = \sup_{s\in\hat{\mathcal{F}}, t\in\hat{\mathcal{G}}} \mathrm{Cov}[s(X), t(Z)] = \sup_{s\in C_b(\mathcal{X}), t\in C_b(\mathcal{Z})} \mathrm{Cov}[s(X), t(Z)], \tag{20}$$

where $C_b(\mathcal{X}), C_b(\mathcal{Z})$ are defined in (16)*.*

Proof. The right equality of Lemma 6 immediately follows by Lemma 5:

$$\sup_{s\in\hat{\mathcal{F}}, t\in\hat{\mathcal{G}}} \mathrm{Cov}[s(X), t(Z)] = \sup_{s\in C_b(\mathcal{X}), t\in C_b(\mathcal{Z})} \mathrm{Cov}[s(X), t(Z)]. \tag{21}$$

Applying Lemma 4 on $\mathcal{F}, \mathcal{G}, \tilde{\mathcal{F}}, \tilde{\mathcal{G}}$, we have:

$$\sup_{s\in\mathcal{F}, t\in\mathcal{G}} \mathrm{Cov}[s(X), t(Z)] = M_{\mathcal{F}} M_{\mathcal{G}} \sup_{s\in\tilde{\mathcal{F}}, t\in\tilde{\mathcal{G}}} \mathrm{Cov}[s(X), t(Z)]. \tag{22}$$

Note that from (17) and (14), we have that the corresponding normalized space for $\hat{\mathcal{F}}$ is:

$$\left\{ \frac{h}{M_{\mathcal{X}}} : h \in \hat{\mathcal{F}} \right\} = \left\{ \frac{M_{\mathcal{X}}}{M_{\mathcal{F}}} \frac{h}{M_{\mathcal{X}}} : h \in \mathcal{F} \right\} = \left\{ \frac{h}{M_{\mathcal{F}}} : h \in \mathcal{F} \right\} = \tilde{\mathcal{F}}. \tag{23}$$

Similarly, the normalized space for $\hat{\mathcal{G}}$ is:

$$\left\{ \frac{g}{M_{\mathcal{Z}}} : g \in \hat{\mathcal{G}} \right\} = \left\{ \frac{g}{M_{\mathcal{G}}} : g \in \mathcal{G} \right\} = \tilde{\mathcal{G}}. \tag{24}$$

Equation (23) implies that the normalized space induced from $\hat{\mathcal{F}}$ coincides with the normalized space induced from $\mathcal{F}$. Similarly, Equation (24) implies the normalized spaces for $\mathcal{G}$ and $\hat{\mathcal{G}}$ also coincide. Moreover, for all $\hat{h} \in \hat{\mathcal{F}}$, $||\hat{h}||_\infty \le M_{\mathcal{X}}$ and for all $\hat{g} \in \hat{\mathcal{G}}$, $||\hat{g}||_\infty \le M_{\mathcal{Z}}$. Hence, applying Lemma 4 on $\hat{\mathcal{F}}, \hat{\mathcal{G}}, \tilde{\mathcal{F}}, \tilde{\mathcal{G}}$, we have:

$$\sup_{s\in\hat{\mathcal{F}}, t\in\hat{\mathcal{G}}} \mathrm{Cov}[s(X), t(Z)] = M_{\mathcal{X}} M_{\mathcal{Z}} \sup_{s\in\tilde{\mathcal{F}}, t\in\tilde{\mathcal{G}}} \mathrm{Cov}[s(X), t(Z)]. \tag{25}$$

By dividing Equation (22) and (25), we prove the left part of Lemma 6:

$$\frac{M_{\mathcal{X}} M_{\mathcal{Z}}}{M_{\mathcal{F}} M_{\mathcal{G}}} \sup_{s\in\mathcal{F}, t\in\mathcal{G}} \mathrm{Cov}[s(X), t(Z)] = \sup_{s\in\hat{\mathcal{F}}, t\in\hat{\mathcal{G}}} \mathrm{Cov}[s(X), t(Z)]. \tag{26}$$

□

By combining Theorem 3 and Lemma 6, we have the following result:

$$\frac{M_{\mathcal{X}} M_{\mathcal{Z}}}{M_{\mathcal{F}} M_{\mathcal{G}}} \mathrm{HSIC}(X, Z) \ge \sup_{s\in C_b(\mathcal{X}), t\in C_b(\mathcal{Z})} \mathrm{Cov}[s(X), t(Z)]. \tag{27}$$

Recall that h_θ is a neural network from $\mathcal{X}$ to $\mathcal{Y}$, such that it can be written as composition of $g \circ f$, where $f : \mathcal{X} \to \mathcal{Z}$ and $g : \mathcal{Z} \to \mathcal{Y}$. Moreover, $h_\theta \in C_b(\mathcal{X})$ and $g \in C_b(\mathcal{Z})$. Using the fact that the supremum on a subset of a set is smaller or equal than the supremum on the whole set, we conclude that:

$$\begin{aligned} \frac{M_{\mathcal{X}} M_{\mathcal{Z}}}{M_{\mathcal{F}} M_{\mathcal{G}}} \mathrm{HSIC}(X, Z) &\ge \sup_\theta \mathrm{Cov}[h_\theta(X), g(Z))] \\ &= \sup_\theta \mathrm{Cov}[h_\theta(X), g \circ f(X)] \\ &= \sup_\theta \mathrm{Var}[h_\theta(X)]. \end{aligned} \tag{28}$$

□

C Proof of Theorem 2

Proof. Let $t_i : \mathbb{R}^{d_X} \to \mathbb{R}$, $i = 1, 2, ..., d_X$ be the following truncation functions:

$$t_i(X) = \begin{cases} -R, & \text{if } X_i < -R, \\ X_i, & \text{if } -R \leq X_i \leq R, \\ R, & \text{if } X_i > R. \end{cases} \tag{29}$$

where $0 < R < \infty$ and X_i is the i-th dimension of X. Functions t_i are continous and bounded in $\mathcal{X}$, and

$$t_i \in C_{b'}(\mathcal{X}), \quad \text{where} \quad C_{b'}(\mathcal{X}) = \{t \in C(\mathcal{X}) : \|t\|_\infty \leq R\} \tag{30}$$

Moreover, g satisfies Assumptions 1 and 2. Similar to the proof of Theorem 1, by combining Theorem 3 and Lemma 6, we have that:

$$\begin{aligned} \frac{RM_{\mathcal{Z}}}{M_{\mathcal{F}}M_{\mathcal{G}}} \operatorname{HSIC}(X,Z) &\geq \sup_{t \in C_{b'}(\mathcal{X}),\, g \in C_b(\mathcal{Z})} \operatorname{Cov}[t(X), g(Z)] \\ &\geq \operatorname{Cov}[t_i(X), h_\theta(X)], \quad i = 1, \ldots, d_X. \end{aligned} \tag{31}$$

Moreover, the following lemma holds:

Lemma 7. *Let $X \sim \mathcal{N}(0, \sigma^2\mathbf{I})$ and $t_i(X)$ defined by* (29)*. For all h_θ that satisfy Assumption 1, we have:*

$$\operatorname{Cov}[X_i, h_\theta(X)] - \operatorname{Cov}[t_i(X), h_\theta(X)] \leq \frac{2M_{\mathcal{X}}\sigma}{\sqrt{2\pi}} \exp(-\frac{R^2}{2\sigma^2}), \quad \textit{for all } i = 1, 2, \ldots, d_X. \tag{32}$$

Proof.

$$\text{LHS} = \int_{-\infty}^{\infty} (x_i - t_i(x)) h_\theta(x) \frac{1}{\sqrt{2\pi\sigma^2}} \exp(-\frac{x_i^2}{2\sigma^2}) dx_i \tag{33a}$$

$$= \frac{1}{\sqrt{2\pi\sigma^2}} \left(\int_{-\infty}^{-R} (x_i + R) h_\theta(x) \exp(-\frac{x_i^2}{2\sigma^2}) dx_i + \int_{R}^{\infty} (x_i - R) h_\theta(x) \exp(-\frac{x_i^2}{2\sigma^2}) dx_i \right) \tag{33b}$$

$$\leq \frac{2M_{\mathcal{X}}}{\sqrt{2\pi\sigma^2}} \int_R^\infty (x_i - R) \exp(-\frac{x_i^2}{2\sigma^2}) dx_i \tag{33c}$$

$$= \frac{2M_{\mathcal{X}}}{\sqrt{2\pi\sigma^2}} \int_R^\infty x_i \exp(-\frac{x_i^2}{2\sigma^2}) dx_i - \frac{2M_{\mathcal{X}}R}{\sqrt{2\pi\sigma^2}} \int_R^\infty \exp(-\frac{x_i^2}{2\sigma^2}) dx_i \tag{33d}$$

$$\leq \frac{2M_{\mathcal{X}}}{\sqrt{2\pi\sigma^2}} \int_R^\infty x_i \exp(-\frac{x_i^2}{2\sigma^2}) dx_i \tag{33e}$$

$$= \frac{2M_{\mathcal{X}}\sigma}{\sqrt{2\pi}} \exp(-\frac{R^2}{2\sigma^2}), \tag{33f}$$

where (33a), (33b), (33d), (33f) are direct results from definition or simple calculation, (33c) comes from the fact that $M_{\mathcal{X}} = \max \|h_\theta(X)\|_\infty$ and the symmetry of two integrals, and (33e) is due to the non-negativity of the probability density function. □

Combining Lemma 7 with (31), we have the following result:

$$\frac{RM_{\mathcal{Z}}}{M_{\mathcal{F}}M_{\mathcal{G}}} \operatorname{HSIC}(X,Z) + \frac{2M_{\mathcal{X}}\sigma}{\sqrt{2\pi}} \exp(-\frac{R^2}{2\sigma^2}) \geq \operatorname{Cov}[X_i, h_\theta(X)], \quad \text{for all } i = 1, \ldots, d_X. \tag{34}$$

We can further bridge HSIC to adversarial robustness directly by taking advantage of the following lemma:

Lemma 8 (Stein's Identity [15]). *Let $X = (X_1, X_2, \dots X_{d_X})$ be multivariate normally distributed with arbitrary mean vector μ and covariance matrix Σ. For any function $h(x_1, \dots, x_{d_X})$ such that $\frac{\partial h}{\partial x_i}$ exists almost everywhere and $\mathbb{E}|\frac{\partial}{\partial x_i}| < \infty$, $i = 1, \dots, d_X$, we write $\nabla h(X) = (\frac{\partial h(X)}{\partial x_1}, \dots, \frac{\partial h(X)}{\partial x_{d_X}})^\top$. Then the following identity is true:*

$$\mathrm{Cov}[X, h(X)] = \Sigma E[\nabla h(X)]. \tag{35}$$

Specifically,

$$\mathrm{Cov}\left[X_1, h\left(X_1, \dots, X_{d_X}\right)\right] = \sum_{i=1}^{d_X} \mathrm{Cov}\left(X_1, X_i\right) E\left[\frac{\partial}{\partial x_i} h\left(X_1, \dots, X_{d_X}\right)\right] \tag{36}$$

Given that $X \sim \mathcal{N}(0, \sigma^2 \mathbf{I})$, Lemma 8 implies:

$$\mathrm{Cov}\left[X_i, h_\theta\left(X\right)\right] = \sigma^2 \mathbb{E}\left[\frac{\partial}{\partial x_i} h_\theta\left(X\right)\right]. \tag{37}$$

Combining (34) and (37), we have:

$$\frac{R M_{\mathcal{Z}}}{M_{\mathcal{F}} M_{\mathcal{G}}} \mathrm{HSIC}(X, Z) + \frac{2 M_{\mathcal{X}} \sigma}{\sqrt{2\pi}} \exp(-\frac{R^2}{2\sigma^2}) \geq \sigma^2 \mathbb{E}\left[\frac{\partial}{\partial x_k} h_\theta\left(X\right)\right]. \tag{38}$$

Note that a similar derivation could be repeated exactly by replacing $h_\theta(X)$ with $-h_\theta(X)$. Thus, for every $i = 1, 2, \dots, d_X$, we have:

$$\frac{R M_{\mathcal{Z}}}{M_{\mathcal{F}} M_{\mathcal{G}}} \mathrm{HSIC}(X, Z) + \frac{2 M_{\mathcal{X}} \sigma}{\sqrt{2\pi}} \exp(-\frac{R^2}{2\sigma^2}) \geq \sigma^2 \mathbb{E}\left[\left|\frac{\partial}{\partial x_i} h_\theta\left(X\right)\right|\right]. \tag{39}$$

Summing up both sides in (39) for $i = 1, 2, \dots, d_X$, we have:

$$\frac{d_X R M_{\mathcal{Z}}}{M_{\mathcal{F}} M_{\mathcal{G}}} \mathrm{HSIC}(X, Z) + \frac{2 d_X M_{\mathcal{X}} \sigma}{\sqrt{2\pi}} \exp(-\frac{R^2}{2\sigma^2}) \geq \sigma^2 \mathbb{E}\left[\sum_{i=1}^{d_X}\left|\frac{\partial}{\partial x_i} h_\theta\left(X\right)\right|\right]. \tag{40}$$

On the other hand, for $\delta \in \mathcal{S}_r$, by Taylor's theorem:

$$\begin{aligned}
\mathbb{E}[|h_\theta(X+\delta) - h_\theta(X)|] &\leq \mathbb{E}[|\delta^\top \nabla_X h_\theta(X)|] + o(r) && \text{(41a)} \\
&\leq \mathbb{E}\left[\|\delta\|_\infty \|\nabla_X h_\theta(X)\|_1\right] + o(r) && \text{(41b)} \\
&\leq r \mathbb{E}\left[\sum_{i=1}^{d_X}\left|\frac{\partial}{\partial x_i} h_\theta\left(X\right)\right|\right] + o(r), && \text{(41c)}
\end{aligned}$$

where (41b) is implied by Hölder's inequality, and (41c) is implied by the triangle inequality.

Combining (40) and (41), we have:

$$\frac{r d_X R M_{\mathcal{Z}}}{\sigma^2 M_{\mathcal{F}} M_{\mathcal{G}}} \mathrm{HSIC}(X, Z) + \frac{2 r d_X M_{\mathcal{X}}}{\sqrt{2\pi}\sigma} \exp(-\frac{R^2}{2\sigma^2}) + o(r) \geq \mathbb{E}[|h_\theta(X+\delta) - h_\theta(X)|]. \tag{42}$$

Let $R = \sigma\sqrt{-2\log o(1)}$ where, here, $o(1)$ stands for an arbitrary function $w : \mathbb{R} \to \mathbb{R}$ s.t.

$$\lim_{r \to 0} w(r) = 0. \tag{43}$$

Then, we have $\frac{2 r d_X M_{\mathcal{X}}}{\sqrt{2\pi}\sigma} \exp(-\frac{R^2}{2\sigma^2}) = o(r)$, because:

$$\begin{aligned}
\lim_{r \to 0} \frac{2 r d_X M_{\mathcal{X}}}{\sqrt{2\pi}\sigma} \exp(-\frac{R^2}{2\sigma^2})/r &= \lim_{r \to 0} \frac{2 d_X M_{\mathcal{X}}}{\sqrt{2\pi}\sigma} \exp(\log o(1)) \\
&= \lim_{r \to 0} \frac{2 d_X M_{\mathcal{X}}}{\sqrt{2\pi}\sigma} o(1) \\
&= 0
\end{aligned} \tag{44}$$

Thus, we conclude that:

$$\frac{r\sqrt{-2\log o(1)} d_X M_{\mathcal{Z}}}{\sigma M_{\mathcal{F}} M_{\mathcal{G}}} \mathrm{HSIC}(X, Z) + o(r) \geq \mathbb{E}[|h_\theta(X+\delta) - h_\theta(X)|]. \tag{45}$$

□

D Licensing of Existing Assets

We provide the licensing information of each existing asset below:

Datasets.

- *MNIST mnist* is licensed under the Creative Commons Attribution-Share Alike 3.0 license.
- *CIFAR-10* and *CIFAR-100* [12] are licensed under the MIT license.

Models.

- The implementations of *LeNet* [17] and *ResNet-18* [11] in our paper are licensed under BSD 3-Clause License.
- The implementation of *WideResNet-28-10* [35] is licensed under the MIT license.

Algorithms.

- The implementations of *SWHB* [16], *PGD* [17], *TRADES* [36] are licensed under the MIT license.
- The implementation of *VIB* [1] is licensed under the Apache License 2.0.
- There are no licenses for *MART* [30] and *XIC* [9].

Adversarial Attacks. The implementations of *FGSM* [8], *PGD* [17], *CW* [3] and *AutoAttack* [5] are all licensed under the MIT license.

E Algorithm Details and Hyperparameter Tuning

Non-adversarial learning, information bottleneck based methds:

- *Cross-Entropy (CE)*, which includes only loss $\mathcal{L}$.
- *Stage-Wise HSIC Bottleneck (SWHB)* [16]: This is the original HSIC bottleneck. It does not include full backpropagation over the HSIC objective: early layers are fixed stage-wise, and gradients are computed only for the current layer.
- *XIC* [9]: To enhance generalization over distributional shifts, this penalty includes inputs and residuals (i.e., $\mathrm{HSIC}(X, Y - h(X))$).
- *Variational Information Bottleneck (VIB)* [1]: this is a variational autoencoder that includes a mutual information bottleneck penalty.

Adversarial learning methods:

- *Projected Gradient Descent (PGD)* [17]: This optimizes $\mathcal{L}_r$, given by (3) via projected gradient ascent over $\mathcal{S}_r$.
- *TRADES* [36]: This uses a regularization term that minimizes the difference between the predictions of natural and adversarial examples to get a smooth decision boundary.
- *MART* [30]: Compared to TRADES, MART pays more attention to adversarial examples from misclassified natural examples and add a KL-divergence term between natural and adversarial examples to the binary cross-entropy loss.

We use code provided by authors, including the recommended hyperparameter settings and tuning strategies. In both SWHB and HBaR, we apply Gaussian kernels for X and Z and a linear kernel for Y. For Gaussian kernels, we set $\sigma = 5\sqrt{d}$, where d is the dimension of the corresponding random variable.

We report all tuning parameters in Table 4. In particular, we report the parameter settings on the 4-layer LeNet [17] for MNIST, ResNet-18 [11] and WideResNet-28-10 [35] for CIFAR-10, and WideResNet-28-10 [35] for CIFAR-100 with the basic HBaR and when combining HBaR with state-of-the-art (i.e., PGD, TRADES, MART) adversarial learning.

For HBaR, to make a fair comparison with SWHB [16], we build our code, along with the implementation of PGD and PGD+HBaR, upon their framework. When combining HBaR with other state-of-the-art adversarial learning (i.e., TRADES and MART), we add our HBaR implemention to the MART framework and use recommended hyperparameter settings/tuning strategies from MART and TRADES. To make a fair comparison, we use the same network architectures among all methods with the same random weight initialization and report last epoch results.

Table 4: Parameter Summary for MNIST, CIFAR-10, and CIFAR-100. λ_x and λ_y are balancing hyperparameters for HBaR; λ is balancing hyperparameter for TRADES and MART.

Dataset	param.	HBaR	PGD	PGD+HBaR	TRADES	TRADES+HBaR	MART	MART+HBaR
MNIST	λ_x	1	-	0.003	-	0.001	-	0.001
	λ_y	50	-	0.001	-	0.005	-	0.005
	λ	-			5	5	5	5
	batch size	256			256			
	optimizer	adam			sgd			
	learning rate	0.0001			0.01			
	lr scheduler	divided by 2 at the 65-th and 90-th epoch			divided by 10 at the 20-th and 40-th epoch			
	# epochs	100			50			
CIFAR-10/100	λ_x	0.006	-	0.0005	-	0.0001	-	0.0001
	λ_y	0.05	-	0.005	-	0.0005	-	0.0005
	λ	-			5	5	5	5
	batch size	128			128			
	optimizer	adam			sgd			
	learning rate	0.01			0.01			
	lr scheduler	cosine annealing			divided by 10 at the 75-th and 90-th epoch			
	# epochs	300	95		95			

F Sensitivity of Regularization Hyperparameters λ_x and λ_y

We provide a comprehensive ablation study on the sensitivity of λ_x and λ_y on MNIST and CIFAR-10 dataset with (Table 5 and 6) and without (Table 7 and 8) adversarial training. As a conclusion, (a) we set the weight of cross-entropy loss as 1, and empirically set λ_x and λ_y according to the performance on a validation set. (b) For MNIST with adversarial training, we empirically discover that $\lambda_x : \lambda_y$ ranging around $5 : 1$ provides better performance; for MNIST without adversarial training, $\lambda_x = 1$ and $\lambda_y = 50$, inspired by SWHB (Ma et al., 2020), provide the best performance. (c) for CIFAR-10 (and CIFAR-100), with and without adversarial training, $\lambda_x : \lambda_y$ ranging from $1 : 5$ to $1 : 10$ provides better performance.

Table 5: **MNIST by LeNet with adversarial training**: Ablation study on HBaR regularization hyperparameters λ_x and λ_y trained by HBaR +TRADES over the metric of natural test accuracy (%) and adversarial test robustness (PGD^{40} and AA, %).

λ_x	λ_y	Natural	PGD^{40}	AA
0.003	0.001	98.66	94.35	91.57
0.003	0	98.92	93.05	90.95
0	0.001	98.86	91.77	88.21
0.0025	0.0005	98.96	94.52	91.42
0.002	0.0005	98.92	94.13	91.33
0.0015	0.0005	98.93	94.06	91.43
0.001	0.0005	98.95	93.76	91.14
0.001	0.0002	98.92	94.61	91.37
0.0008	0.0002	98.94	94.15	91.07
0.0006	0.0002	98.91	94.13	90.72
0.0004	0.0002	98.90	93.96	90.56

Table 6: **CIFAR-10 by WideResNet-28-10 with adversarial training**: Ablation study on HBaR regularization hyperparameters λ_x and λ_y trained by HBaR +TRADES over the metric of natural test accuracy (%), and adversarial test robustness (PGD^{20} and AA, %).

λ_x	λ_y	Natural	PGD^{20}	AA
0.0001	0.0005	85.61	56.51	53.53
0.0001	0	80.19	49.49	45.33
0	0.0005	84.74	55.00	51.50
0.001	0.005	85.70	55.74	52.78
0.0005	0.005	84.42	55.95	52.66
0.00005	0.0005	85.37	56.43	53.40

Table 7: **MNIST by LeNet without adversarial training**: Ablation study on HBaR regularization hyperparameters λ_x and λ_y over the metric of $\mathrm{HSIC}(X, Z_M)$, $\mathrm{HSIC}(Y, Z_M)$, natural test accuracy (%), and adversarial test robustness (PGD^{40}, %).

λ_x	λ_y	HSIC (X, Z_M)	HSIC (Y, Z_M)	Natural	PGD^{40}
CE only		45.29	8.73	99.23	0.00
0.0001	0	21.71	8.01	99.28	0.00
0.001	0	5.82	6.57	99.36	0.00
0.01	0	3.22	4.28	99.13	0.00
0	1	56.45	9.00	98.92	0.00
0.001	0.05	53.70	8.99	99.13	0.03
0.001	0.01	10.44	8.51	99.37	0.00
0.001	0.005	8.86	8.24	99.38	0.00
0.01	0.5	16.13	8.90	99.14	5.00
0.1	5	15.81	8.90	98.96	7.72
1	50	15.68	8.89	98.90	8.33
1.1	55	15.90	8.88	98.88	6.99
1.2	60	15.76	8.89	98.95	7.24
1.5	75	15.62	8.89	98.94	8.23
2	100	15.41	8.89	98.91	7.00

Table 8: **CIFAR-10 by ResNet-18 without adversarial training**: Ablation study on HBaR regularization hyperparameters λ_x and λ_y over the metric of $\mathrm{HSIC}(X, Z_M)$, $\mathrm{HSIC}(Y, Z_M)$, natural test accuracy (%), and adversarial test robustness (PGD^{20}, %).

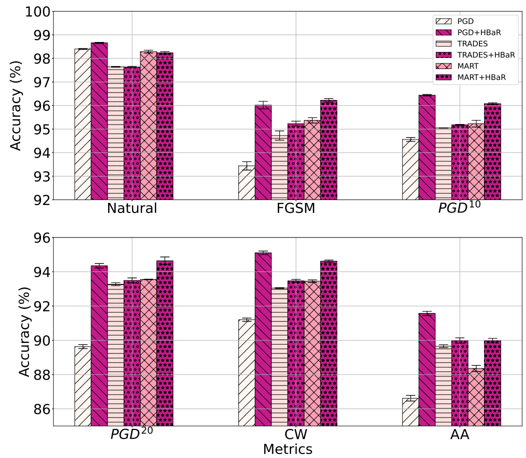
λ_x	λ_y	HSIC (X, Z_L)	HSIC (Y, Z_L)	Natural	PGD^{20}
CE only		3.45	4.76	95.32	8.57
0.001	0.05	43.48	8.93	95.36	2.91
0.002	0.05	43.15	8.92	95.55	2.29
0.003	0.05	41.95	8.90	95.51	3.98
0.004	0.05	30.12	8.77	95.45	5.23
0.005	0.05	11.56	8.45	95.44	23.73
0.006	0.05	6.07	8.30	95.35	34.85
0.007	0.05	4.81	8.24	95.13	15.80
0.008	0.05	4.44	8.21	95.13	8.43
0.009	0.05	3.96	8.14	94.70	10.83
0.01	0.05	4.09	7.87	92.33	2.90

Table 9: **MNIST by LeNet**: Mean and Standard deviation of natural test accuracy (in %) and adversarial robustness ((in %) on FGSM, PGD, CW, and AA attacked test examples) of adversarial learning baselines and combining HBaR with each correspondingly.

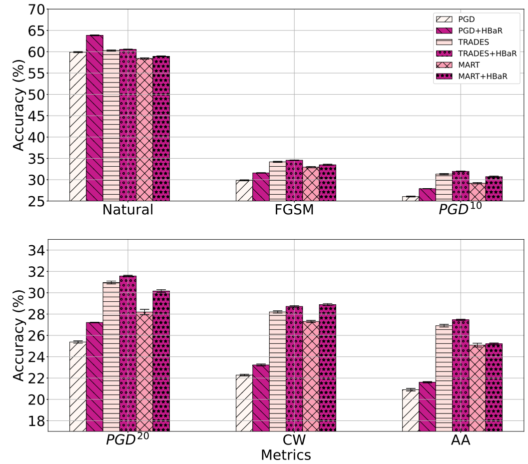
Methods	MNIST by LeNet					
	Natural	FGSM	PGD^{20}	PGD^{40}	CW	AA
PGD	98.40 ± 0.018	93.44 ± 0.177	94.56 ± 0.079	89.63 ± 0.117	91.20 ± 0.097	86.62 ± 0.166
HBaR + PGD	**98.66** ± 0.026	**96.02** ± 0.161	**96.44**±0.030	**94.35**±0.130	**95.10**±0.106	**91.57**±0.123
TRADES	**97.64**±0.017	94.73±0.196	95.05±0.006	93.27±0.088	93.05±0.025	89.66±0.085
HBaR + TRADES	**97.64**±0.030	**95.23**±0.106	**95.17**±0.023	**93.49**±0.147	**93.47**±0.089	**89.99**±0.155
MART	**98.29**±0.059	95.57±0.113	95.23±0.144	93.55±0.018	93.45±0.077	88.36±0.179
HBaR + MART	98.23±0.054	**96.09**±0.074	**96.08**±0.035	**94.64**±0.125	**94.62**±0.06	**89.99**±0.13

G Error Bar for Combining HBaR with Adversarial Examples

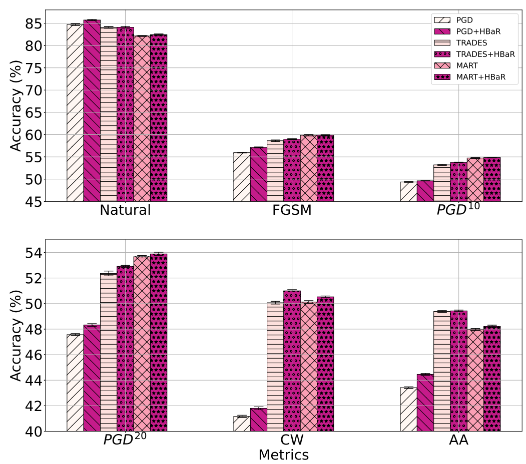
We show how HBaR can be used to improve robustness when used as a regularizer, as described in Section 4.2, along with state-of-the-art adversarial learning methods. We run each experiment by five times. Figure 5 illustrates mean and standard deviation of the natural test accuracy and adversarial robustness against various attacks on CIFAR-10 by ResNet-18 and WideResNet-28-10. Table 9, 10, 11, and 12 show the detailed standard deviation. Combined with the adversarial training baselines, HBaR consistently improves adversarial robustness against all types of attacks with small variance.



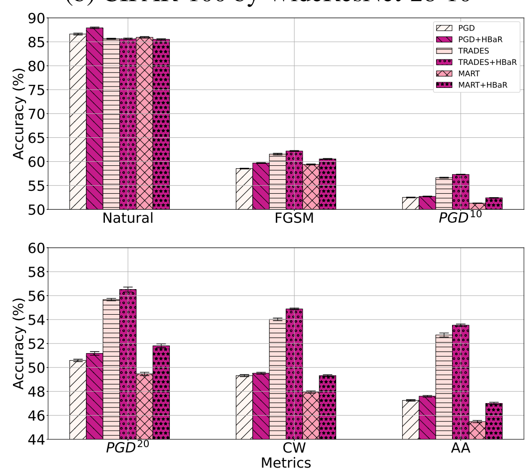
(a) MNIST by LeNet



(b) CIFAR-100 by WideResNet-28-10



(c) CIFAR-10 by ResNet-18



(d) CIFAR-10 by WideResNet-28-10

Figure 5: Error bar of natural test accuracy (in %) and adversarial robustness ((in %) on FGSM, PGD, CW, and AA attacked test examples) on MNIST by LeNet, CIFAR-100 by WideResNet-28-10, CIFAR-10 by ResNet-18 and WideResNet-28-10 of adversarial learning baselines and combining HBaR with each correspondingly.

Table 10: **CIFAR-10 by ResNet-18**: Mean and Standard deviation of natural test accuracy (in %) and adversarial robustness ((in %) on FGSM, PGD, CW, and AA attacked test examples) of adversarial learning baselines and combining HBaR with each correspondingly.

Methods	CIFAR-10 by ResNet-18					
	Natural	FGSM	PGD^{10}	PGD^{20}	CW	AA
PGD	84.71±0.16	55.95±0.097	49.37±0.075	47.54±0.080	41.17±0.086	43.42±0.064
HBaR + PGD	**85.73**±0.166	**57.13**±0.099	**49.63**±0.058	**48.32**±0.103	**41.80**±0.116	**44.46**±0.169
TRADES	84.07±0.201	58.63±0.167	53.21±0.118	52.36±0.189	50.07±0.106	49.38±0.069
HBaR + TRADES	**84.10**±0.104	**58.97**±0.093	**53.76**±0.080	**52.92**±0.175	**51.00**±0.085	**49.43**±0.064
MART	82.15±0.117	59.85±0.154	54.75±0.089	53.67±0.088	50.12±0.106	47.97±0.156
HBaR + MART	**82.44**±0.156	**59.86**±0.132	**54.84**±0.051	**53.89**±0.135	**50.53**±0.069	**48.21**±0.100

Table 11: **CIFAR-10 by WideResNet-28-10**: Mean and Standard deviation of natural test accuracy (in %) and adversarial robustness ((in %) on FGSM, PGD, CW, and AA attacked test examples) of adversarial learning baselines and combining HBaR with each correspondingly.

Methods	CIFAR-10 by WideResNet-28-10					
	Natural	FGSM	PGD^{10}	PGD^{20}	CW	AA
PGD	86.63±0.186	58.53±0.073	52.21±0.084	50.59±0.096	49.32±0.089	47.25±0.124
HBaR + PGD	**87.91**±0.102	**59.69**±0.097	**52.72**±0.081	**51.17**±0.152	**49.52**±0.174	**47.60**±0.131
TRADES	**85.66**±0.103	61.55±0.134	56.62±0.097	55.67±0.098	54.02±0.106	52.71±0.169
HBaR + TRADES	85.61±0.0133	**62.20**±0.102	**57.30**±0.059	**56.51**±0.136	**54.89**±0.098	**53.53**±0.127
MART	**85.94**±0.156	59.39±0.109	51.30±0.052	49.46±0.136	47.94±0.098	45.48±0.100
HBaR + MART	85.52±0.136	**60.54**±0.071	**53.42**±0.142	**51.81**±0.177	**49.32**±0.131	**46.99**±0.137

Table 12: **CIFAR-100 by WideResNet-28-10**: Mean and Standard deviation of natural test accuracy (in %) and adversarial robustness ((in %) on FGSM, PGD, CW, and AA attacked test examples) of adversarial learning baselines and combining HBaR with each correspondingly.

Methods	CIFAR-100 by WideResNet-28-10					
	Natural	FGSM	PGD^{20}	PGD^{40}	CW	AA
PGD	59.91±0.116	29.85±0.117	26.05±0.106	25.38±0.129	22.28±0.079	20.91±0.133
HBaR + PGD	**63.84**±0.105	**31.59**±0.054	**27.90**±0.030	**27.21**±0.025	**23.23**±0.088	**21.61**±0.061
TRADES	60.29±0.122	34.19±0.132	31.32±0.134	30.96±0.135	28.20±0.097	26.91±0.172
HBaR + TRADES	**60.55**±0.065	**34.57**±0.068	**31.96**±0.067	**31.57**±0.079	**28.72**±0.071	**27.46**±0.098
MART	58.42±0.164	32.94±0.160	29.17±0.166	28.19±0.252	27.31±0.096	25.09±0.179
HBaR + MART	**58.93**±0.102	**33.49**±0.144	**30.72**±0.130	**30.16**±0.133	**28.89**±0.118	**25.21**±0.111

H Limitations

One limitation of our method is that the robustness gain, though beating other IB-based methods, is modest when training with only natural examples. However, the potential of getting adversarial robustness *without* adversarial training is interesting and worth further exploration in the future. Another limitation of our method, as well as many proposed adversarial defense methods, is the uncertain performance to new attack methods. Although we have established concrete theories and conducted comprehensive experiments, there is no guarantee that our method is able to handle novel, well-designed attacks. Finally, in our theoretical analysis in Section 4.3, we have made several assumptions for Theorem 2. While Assumptions 1 and 2 hold in practice, the distribution of input feature is not guaranteed to be standard Gaussian. Although the empirical evaluation supports the correctness of the theorem, we admit that the claim is not general enough. We aim to proof a more general version of Theorem 2 in the future, hopefully agnostic to input distributions. We will keep track of the advances in the adversarial robustness field and further improve our work correspondingly.

I Potential Societal Negative Impact

Although HBaR has great potential as a general strategy to enhance the robustness for various machine learning systems, we still need to be aware of the potential negative societal impacts it might result in. For example, over-confidence in the *adversarially-robust* models produced by HBaR as well as other defense methods may lead to overlooking their potential failure on newly-invented attack methods; this should be taken into account in safety-critical applications like healthcare [6] or security [26]. Another example is that, one might get insights from the theoretical analysis of our method to design stronger adversarial attacks. These attacks, if fall into the wrong hands, might cause severe societal problems. Thus, we encourage our machine learning community to further explore this field and be judicious to avoid misunderstanding or misusing of our method. Moreover, we propose to establish more reliable adversarial robustness checking routines for machine learning models deployed in safety-critical applications. For example, we should test these models with the latest adversarial attacks and make corresponding updates to them annually.