

1 **Technical detail.** Well caught! The situation regarding [17] is even worse than Reviewer 3 highlighted: in infinite  
 2 dimensional spaces, one cannot simply exchange trace and expectation by assuming linearity. The good news, however,  
 3 is that we can prove  $\text{tr}(T_1) < \infty$  under the mild assumptions in Hypotheses 2 and 3, rescuing the theorems in both [17]  
 4 and our work. We will include this proof and discussion in the document, and alert the authors of [17] to this issue.

5 In Hypotheses 2 and 3, we assume that instrument space  $\mathcal{Z}$  is separable, and that RKHS  $\mathcal{H}_\mathcal{Z}$  has continuous, bounded  
 6 kernel  $k_\mathcal{Z}$  with feature map  $\phi(z)$ . By Proposition 3,  $\mathcal{H}_\mathcal{Z}$  is separable, i.e. it has countable orthonormal basis  $\{e_i\}_{i=1}^\infty$ .  
 7 Consider the space  $\mathcal{L}_2(\mathcal{H}_\mathcal{Z}, \mathcal{H}_\mathcal{Z})$  of Hilbert-Schmidt operators  $A : \mathcal{H}_\mathcal{Z} \rightarrow \mathcal{H}_\mathcal{Z}$  with inner product  $\langle A, B \rangle_{\mathcal{L}_2} =$   
 8  $\sum_{i=1}^\infty \langle Ae_i, Be_i \rangle_{\mathcal{H}_\mathcal{Z}}$ . Recall tensor product notation: for  $a, b, c \in \mathcal{H}_\mathcal{Z}$ ,  $[a \otimes b]c = \langle b, c \rangle_{\mathcal{H}_\mathcal{Z}}a$ . By Parseval's identity, we  
 9 have two helpful results:  $\|a \otimes b\|_{\mathcal{L}_2}^2 = \|a\|_{\mathcal{H}_\mathcal{Z}}^2 \|b\|_{\mathcal{H}_\mathcal{Z}}^2$  so  $a \otimes b \in \mathcal{L}_2(\mathcal{H}_\mathcal{Z}, \mathcal{H}_\mathcal{Z})$  [G, eq. 3.6]; and if  $C \in \mathcal{L}_2(\mathcal{H}_\mathcal{Z}, \mathcal{H}_\mathcal{Z})$   
 10 then  $\langle C, a \otimes b \rangle_{\mathcal{L}_2} = \langle a, Cb \rangle_{\mathcal{H}_\mathcal{Z}}$  [G, eq. 3.7].

First, we verify the existence of covariance operator  $T_1 \in \mathcal{L}_2(\mathcal{H}_\mathcal{Z}, \mathcal{H}_\mathcal{Z})$  satisfying  $\langle T_1, A \rangle_{\mathcal{L}_2} = \mathbb{E}\langle \phi(Z) \otimes \phi(Z), A \rangle_{\mathcal{L}_2}$ . By Riesz representation theorem,  $T_1$  exists if the RHS is a bounded linear operator. Linearity follows by definition. Boundedness of  $k_\mathcal{Z}$  in Hypothesis 3 implies  $\mathbb{E}[k_\mathcal{Z}(Z, Z)] < \infty$  and hence

$$|\mathbb{E}\langle \phi(Z) \otimes \phi(Z), A \rangle_{\mathcal{L}_2}| \leq \mathbb{E}|\langle \phi(Z) \otimes \phi(Z), A \rangle_{\mathcal{L}_2}| \leq \|A\|_{\mathcal{L}_2} \mathbb{E}\|\phi(Z) \otimes \phi(Z)\|_{\mathcal{L}_2} = \|A\|_{\mathcal{L}_2} \mathbb{E}[k_\mathcal{Z}(Z, Z)] < \infty$$

11 Second, we verify  $T_1$  is indeed a covariance operator with  $\text{tr}(T_1) < \infty$ .

$$\begin{aligned} \langle f, T_1 g \rangle_{\mathcal{H}_\mathcal{Z}} &= \langle T_1 f, g \rangle_{\mathcal{L}_2} = \mathbb{E}\langle \phi(Z) \otimes \phi(Z), f \otimes g \rangle_{\mathcal{L}_2} = \mathbb{E}\langle f, \phi(Z) \rangle_{\mathcal{H}_\mathcal{Z}} \langle g, \phi(Z) \rangle_{\mathcal{H}_\mathcal{Z}} = \mathbb{E}[f(Z)g(Z)] \\ \text{tr}(T_1) &= \sum_{i=1}^\infty \langle e_i, T_1 e_i \rangle_{\mathcal{H}_\mathcal{Z}} = \sum_{i=1}^\infty \mathbb{E}\langle e_i, \phi(Z) \rangle_{\mathcal{H}_\mathcal{Z}}^2 = \mathbb{E} \sum_{i=1}^\infty \langle e_i, \phi(Z) \rangle_{\mathcal{H}_\mathcal{Z}}^2 = \mathbb{E}\|\phi(Z)\|_{\mathcal{H}_\mathcal{Z}}^2 = \mathbb{E}[k_\mathcal{Z}(Z, Z)] < \infty \end{aligned}$$

12 where the second line uses definition of trace, the penultimate expression in the first line, monotone convergence  
 13 theorem [43, Theorem A.3.5] with upper bound  $\|\phi(z)\|^2$ , Parseval's identity, and boundedness of  $k_\mathcal{Z}$ .

14 **Limitations.** Extensive use of IV estimation in applied economic research has revealed a common pitfall: weak  
 15 instrumental variables. A weak instrument satisfies Hypothesis 1, but the relationship between a weak instrument  $Z$  and  
 16 input  $X$  is negligible;  $Z$  is essentially irrelevant. In this case, IV estimation becomes highly erratic [B]. In [St], the  
 17 authors formalize this phenomenon with local analysis. We recommend that practitioners resist the temptation to use  
 18 many weak instruments, and instead use few strong instruments such as those described in the introduction.

19 **Experiments.** We provide implementation details for KernelIV and its  
 20 competitors in Appendix 7.10.2, including kernel choice and kernel hyperpa-  
 21 rameter tuning. Theorem 4 details the performance of KIV with suboptimal  
 22  $n/m$ , parametrized by  $a$ . In Figure 9, we present a *linear* design [14] with  
 23  $h(x) = 4x - 2$ . We will include Figure 5 in the main text, and move linear and  
 24 sigmoid designs to the appendix. In Figure 10, we provide a robustness study  
 25 of KernelIV applied to the sigmoid design with  $n + m = 1000$ , varying  
 26 hyperparameter values for Gaussian kernel  $k_\mathcal{X}$ . For comparison, our tuning  
 27 procedure selects value 0.3. We will increase figure sizes.

28 **Exposition.** We will define  $e$  as unmeasured, confounding noise, and relate  
 29  $n/m$  to statistical efficiency earlier on. In Hypotheses 5 and 9, we will define  
 30 the power of an operator in terms of its eigendecomposition. We will move  
 31 the decay schedule for  $\lambda$  from Appendix 7.6 to Theorem 2. We define  $\Omega_{\mu(z)}$   
 32 in line 257, but we will restate this definition in Definition 2 and Hypothesis  
 33 7 for clarity. We will replace ‘a.s.’ with ‘almost surely’ in Hypothesis 8.

34 **References.** We agree it is important to cite early work on mean embeddings  
 35 by [Sm] as summarized in [M]. We will ensure all references are cited in  
 36 the main text. We cite groups of papers for the following reasons: [24, 25]  
 37 introduce  $E$  and  $\mu$ , which in our paper we argue are equivalent; [25, 26]  
 38 and likewise [32, 33, 34] were published at the same time; [39, 40] contain  
 39 different theorems that we generalize into Theorems 6 and 5 en route to  
 40 Theorem 2; [46, 47] contain an original consistency argument and a stronger minimax optimality argument, respectively.

41 [B] J Bound, DA Jaeger, and RM Baker. Problems with IV estimation when the correlation between the instruments  
 42 and the endogenous explanatory variable is weak. *JASA*, 90(430):443–450, 1995. [G] A Gretton. RKHS in ML: Testing  
 43 statistical dependence. Adv. topics in ML lecture notes, UCL Gatsby Unit, 2018. [M] K Muandet, K Fukumizu, BK  
 44 Sriperumbudur, and B Schölkopf. Kernel mean embedding of distributions: A review and beyond. *FTML*, 10(1-2):1-141,  
 45 2017. [Sm] A Smola, A Gretton, L Song, and B Schölkopf. A Hilbert space embedding for distributions. In *ALT*, pages  
 46 13–31, 2007. [St] D Staiger and JH Stock. IV regression with weak instruments. *Econometrica*, 65(3):557–586, 1997.

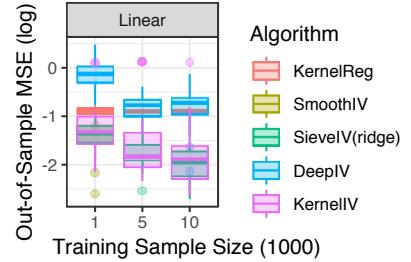


Figure 9: Linear design

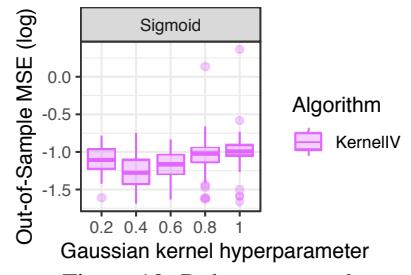


Figure 10: Robustness study