

## A ALGORITHMIC COMPARISON

	SDCIT	KCIPT
$H_0$	$\Omega = \Omega_\pi$	$\{\Omega_i^{(1)} = \Omega_{\pi,i}^{(2)}\}_{i=1}^B$
$T$	modified MMD	averaged MMDs
null distribution	half-sampling without replacement	aggregated bootstrap null distributions
# of permutations	1 for $T$ $b + 1$ for null.	$B$ for $T$
# of MM(S)Ds	1 for $T$ $b + 1$ for null.	$B$ for $T$ $Bb$ for null.

Table 2: Comparison of SDCIT and KCIPT

## B TAKING PERMUTATION ERROR INTO ACCOUNT

Our test statistic measures the distance between the original sample (representing  $P_{xyz}$ ) and a pseudo-null sample (representing  $P_{xz}P'_{y|z}$ ), where  $P'_{y|z}$  approximates  $P_{y|z}$ . Ideally, the test statistic and its null distribution will be reliably estimated if permutation error is small and, hence,  $P'_{y|z}$  approximates  $P_{y|z}$  well.

We first relate an MMSD estimate and its corresponding permutation error during the estimate, and provide a means to adjust MMSD estimates. Let  $T$  be an MMSD estimate given  $K_{xz}$ ,  $K_y$ , and  $D$  (see Algorithm 2). Let  $\tau$  be an MMSD estimate assuming  $K_x = \mathbf{1}_{n \times n}$ , that is  $\tau = \text{MMSD}(K_z, K_y, D)$ . In other words,  $\tau$  is the MMSD estimate between  $P'_{y|z}P_z$  and  $P_{y|z}P_z$ . While  $T$  is, roughly, about the conditional dependence between  $X$  and  $Y$  given  $Z$ ,  $\tau$  measures permutation error, i.e., discrepancy between  $(\mathbf{y}, \mathbf{z})$  and  $(\pi\mathbf{y}, \mathbf{z})$ . We illustrate a null distribution  $\{T_i\}_{i=1}^b$  and its associated  $\{\tau_i\}_{i=1}^b$  in Figure 7. We can clearly observe that the distribution of  $\tau$  is centered at 0 but still there are lots of null samples associating non-negligible errors.

We then formulate  $T$  (under a permutation error) is the function of unknown  $T^*$  (under zero permutation error) and  $\tau$ . We assume a linear model  $T = T^* + \beta\tau + \epsilon$  where  $\epsilon$  is assumed a zero-mean Gaussian noise. Given a null distribution  $\{(T_i, \tau_i)\}_{i=1}^b$ , we can learn  $\beta$  by fitting a linear model. Then, the null distribution  $\{T_i\}_{i=1}^b$  is adjusted to  $\{T_i - \beta\tau_i\}_{i=1}^b$  and our test statistic is also adjusted similarly. Such adjustment yields a null distribution with smaller variance as shown in Figure 8. The adjustment slightly improves both power and calibratedness.

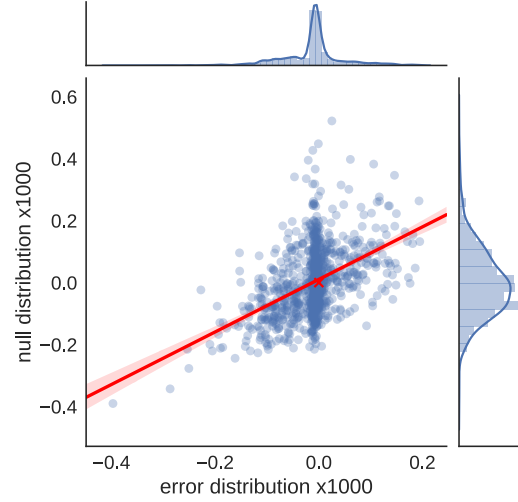


Figure 7: A null distribution and its corresponding errors measured with MMSD. A red cross near origin indicates the test statistic and its corresponding error. A red line indicates a fitted linear model.

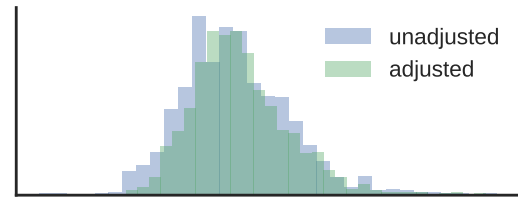


Figure 8: Unadjusted and adjusted null distributions.