

314 **Supplementary Materials for "K-Nearest-Neighbor Local Sampling Based**
315 **Conditional Independence Testing"**

316 **A Theoretical results**

317 **A.1 Proof of Lemma 1**

Proof. Recall that Z is a random vector taking values in Euclidean space $(\mathbb{R}^{d_z}, \|\cdot\|_2)$, where d_z is the dimension of Z and $\|\cdot\|_2$ is Euclidean distance. Z_1, Z_2, \dots, Z_n are i.i.d. random vectors according to $p(z)$. For a fixed $z \in \mathbb{R}^{d_z}$, we denote by $Z_n^{(1)}(z), \dots, Z_n^{(n)}(z)$ a reordering of Z_1, Z_2, \dots, Z_n according to the increasing values of $\|Z_i - z\|_2$, that is,

$$\|Z_n^{(1)}(z) - z\|_2 \leq \dots \leq \|Z_n^{(n)}(z) - z\|_2.$$

318 Define the set $G = \{z \in \mathbb{R}^{d_z} \mid \forall \delta > 0, P(\{\omega : Z(\omega) \in S_z(\delta)\}) > 0\}$, where $S_z(\delta) = \{x \in$
319 $\mathbb{R}^{d_z} \mid \|x - z\|_2 \leq \delta\}$. For convenience, we omit ω in probability in the following paper. For example,
320 write $P(Z \in S_z(\delta))$ instead of $P(\{\omega : Z(\omega) \in S_z(\delta)\})$. By definition, for $z \in G, \forall \delta > 0,$
321 $P(Z \in S_z(\delta)) > 0$. Let G^c be the complement of G . Then, for $z \in G^c, \exists r_z > 0$, s.t. $\forall r < r_z,$
322 $P(Z \in S_z(r)) = 0$. Note that $P(\|Z_n^{(k)}(z) - z\|_2 > \delta) = P(Z_n^{(k)}(z) \notin S_z(\delta))$.

323 In order to prove $\|Z_n^{(k)}(Z) - Z\|_2 \rightarrow 0$ a.s., it is sufficient to prove $\forall \delta > 0,$
324 $\lim_{n \rightarrow \infty} P(\sup_{m \geq n} \|Z_m^{(k)}(Z) - Z\|_2 > \delta) = 0$. We can obtain

$$\begin{aligned} P(\sup_{m \geq n} \|Z_m^{(k)}(Z) - Z\|_2 > \delta) &\leq P(\{\sup_{m \geq n} \|Z_m^{(k)}(Z) - Z\|_2 > \delta\} \cap \{Z \in G\}) + P(Z \in G^c) \\ &= \int_G P(\sup_{m \geq n} \|Z_m^{(k)}(z) - z\|_2 > \delta) p(z) dz + P(Z \in G^c) \\ &\leq \int_G \sum_{m \geq n} P(Z_m^{(k)}(z) \notin S_z(\delta)) p(z) dz + P(Z \in G^c). \end{aligned} \quad (11)$$

325 First, consider the first term of (11). We have

$$\begin{aligned} P(Z_m^{(k)}(z) \notin S_z(\delta)) &= P(Z_m^{(1)}(z), Z_m^{(2)}(z), \dots, Z_m^{(m)}(z) \notin S_z(\delta)) \\ &\quad + P(Z_m^{(1)}(z) \in S_z(\delta), Z_m^{(2)}(z), \dots, Z_m^{(m)}(z) \notin S_z(\delta)) \\ &\quad + P(Z_m^{(1)}(z), Z_m^{(2)}(z) \in S_z(\delta), Z_m^{(3)}(z), \dots, Z_m^{(m)}(z) \notin S_z(\delta)) \\ &\quad + \dots + P(Z_m^{(1)}(z), \dots, Z_m^{(k-1)}(z) \in S_z(\delta), Z_m^{(k)}(z), \dots, Z_m^{(m)}(z) \notin S_z(\delta)). \end{aligned}$$

326 By setting $P(Z \in S_z(\delta)) = \gamma$, we have

$$\begin{aligned} P(Z_m^{(k)}(z) \notin S_z(\delta)) &= (1 - \gamma)^m + C_m^1 \gamma (1 - \gamma)^{m-1} + C_m^2 \gamma^2 (1 - \gamma)^{m-2} + \dots \\ &\quad + C_m^{k-1} \gamma^{k-1} (1 - \gamma)^{m-k+1}. \end{aligned} \quad (12)$$

327 Consider the j -th term of (12). Let $C_1 := \gamma^j / j!$, $C_2 := C_1 e^j$ and $C_3 := C_2 e^j (1 - \gamma)^{-j}$. By using
328 Stirling's approximation, we have

$$\begin{aligned} \lim_{m \rightarrow \infty} C_m^j \gamma^j (1 - \gamma)^{m-j} &= \lim_{m \rightarrow \infty} \frac{m!}{(m-j)! j!} \gamma^j (1 - \gamma)^{m-j} \\ &= \lim_{m \rightarrow \infty} C_1 \frac{\sqrt{2\pi m} (\frac{m}{e})^m}{\sqrt{2\pi(m-j)} (\frac{m-j}{e})^{m-j}} (1 - \gamma)^{m-j} \\ &= \lim_{m \rightarrow \infty} C_2 \sqrt{\frac{m}{(m-j)}} \frac{m^m}{(m-j)^{m-j}} (1 - \gamma)^{m-j} \\ &= \lim_{m \rightarrow \infty} C_2 e^j (m+j)^j (1 - \gamma)^m \\ &= \lim_{m \rightarrow \infty} C_2 e^j m^j (1 - \gamma)^{m-j} \\ &= \lim_{m \rightarrow \infty} C_3 m^j (1 - \gamma)^m. \end{aligned}$$

329 Thus, there exists $C_4 > 0$ such that $P(Z_m^{(k)}(z) \notin S_z(\delta)) \leq C_4 m^{k-1} (1-\gamma)^m$ when m is large
 330 enough. It holds that

$$\frac{C_4 m^{k-1} (1-\gamma)^m}{m^{-2}} = C_4 m^{k+1} (1-\gamma)^m \rightarrow 0, \quad \text{as } m \rightarrow +\infty.$$

Thus, for $z \in G$ and n large enough, $\forall \delta > 0$, we have $P(Z_m^{(k)}(z) \notin S_z(\delta)) = o(m^{-2})$ and

$$\sum_{m \geq n} P(Z_m^{(k)}(z) \notin S_z(\delta)) \leq \sum_{m \geq n} \frac{1}{m^2},$$

331 which shows $\lim_{n \rightarrow \infty} \sum_{m \geq n} P(Z_m^{(k)}(z) \notin S_z(\delta)) = 0$ for $z \in G$. So by Lebesgue dominated
 332 convergence theorem, we obtain $\lim_{n \rightarrow \infty} \int_G \sum_{m \geq n} P(Z_m^{(k)}(z) \notin S_z(\delta)) p(z) dz = 0$.

Second, we consider the second term of (11). To prove that $P(Z \in G^c) = 0$, we aim to construct a countable open cover of G^c and show that the probability of the random vector Z falling into each of these open balls is zero. By the property of G^c , for every $z \in G^c$, there exists $r_z > 0$ such that for all $r < r_z$, $P(Z \in S_z(r)) = 0$. Furthermore, using the separability of Euclidean space and the density of the rational number set, we can approximate z using points from \mathbb{Q}^{d_z} with \mathbb{Q} being the rational number set. Therefore, for every $z \in G^c$, there exist $x \in \mathbb{Q}^{d_z} \cap S_z(\frac{r_z}{3})$ and $r \in \mathbb{Q} \cap (\frac{r_z}{3}, \frac{2r_z}{3})$, such that $z \in S_x(r) \subseteq S_z(r_z)$. Because $P(Z \in S_z(r_z)) = 0$, we conclude that $P(Z \in S_x(r)) = 0$. Define

$$\mathcal{F} := \{S_x(r) \mid \exists z \in G^c, \text{ such that } z \in S_x(r) \subseteq S_z(r_z) \text{ with } x \in \mathbb{Q}^{d_z} \text{ and } r \in \mathbb{Q}\}.$$

333 Note that the elements in set \mathcal{F} are mutually distinct. By the construction of $S_x(r)$, \mathcal{F} forms a
 334 countable open cover of G^c , and the probability of Z falling into each open ball in \mathcal{F} is zero. Using
 335 the monotonicity and countable additivity properties of probability, we have $P(Z \in G^c) \leq P(Z \in$
 336 $\cup_{S_x(r) \in \mathcal{F}} S_x(r)) \leq \sum_{S_x(r) \in \mathcal{F}} P(Z \in S_x(r)) = 0$. Thus, we conclude that $P(Z \in G^c) = 0$.

337 We therefore conclude that, $\forall \delta > 0$, $\lim_{n \rightarrow \infty} P(\sup_{m \geq n} \|Z_m^{(k)}(Z) - Z\|_2 > \delta) = 0$. This finish the
 338 proof.

339 A.2 Proof of Theorem 2

340 *Proof.* By Pinsker's inequality, we have

$$d_{TV}\{p(x|Z), \hat{p}(x|Z)\} \leq \sqrt{D_{KL}\{p(x|Z), \hat{p}(x|Z)\}}/2.$$

341 Note that $I\{\xi = 1\} + \dots + I\{\xi = k\} = 1$. By the definition of $\hat{p}(x|Z)$, we obtain

$$\begin{aligned} D_{KL}\{p(x|Z), \hat{p}(x|Z)\} &= \int p(x|Z) \log \left\{ \frac{p(x|Z)}{p(x|Z_n^{(1)})^{I\{\xi=1\}} \times \dots \times p(x|Z_n^{(k)})^{I\{\xi=k\}}} \right\} dx \\ &= \int p(x|Z) \log \prod_{l=1}^k \frac{p(x|Z)^{I\{\xi=l\}}}{p(x|Z_n^{(l)})^{I\{\xi=l\}}} dx \\ &= \sum_{l=1}^k I\{\xi = l\} \int p(x|Z) \log \frac{p(x|Z)}{p(x|Z_n^{(l)})} dx \\ &= \sum_{l=1}^k I\{\xi = l\} D_{KL}\{p(x|Z) \| p(x|Z_n^{(l)})\}. \end{aligned}$$

342 Then, by Taylor's expansion, we have

$$\begin{aligned} &D_{KL}\{p(x|Z) \| p(x|Z_n^{(l)})\} \\ &= D_{KL}\{p(x|Z) \| p(x|Z)\} + \frac{\partial}{\partial z'} D_{KL}\{p(x|Z) \| p(x|z')\} \Big|_{z'=Z} (Z_n^{(l)} - Z) \\ &\quad + \frac{1}{2} (Z_n^{(l)} - Z)^T \frac{\partial^2}{\partial z' \partial z'^T} D_{KL}\{p(x|Z) \| p(x|z')\} \Big|_{z'=a} (Z_n^{(l)} - Z), \end{aligned}$$

343 where $a = \lambda Z + (1 - \lambda)Z_n^{(l)}$ with $0 \leq \lambda \leq 1$.

344 Note that $D_{KL}\{p(x|Z)||p(x|Z)\} = \int p(x|Z) \log \frac{p(x|Z)}{p(x|Z)} dx = 0$. By Lemma 1 and Assumptions 1
345 and 2, we have

$$\begin{aligned} \frac{\partial}{\partial z'} D_{KL}\{p(x|Z)||p(x|z')\} \Big|_{z'=Z} &= - \int p(x|Z) \cdot \frac{\partial}{\partial z'} \log p(x|z') \Big|_{z'=Z} dx \\ &= - \frac{\partial}{\partial z'} \int p(x|z') dx \Big|_{z'=Z} = 0 \end{aligned}$$

346 and

$$\frac{\partial^2}{\partial z' \partial z'^T} D_{KL}\{p(x|Z)||p(x|z')\} \Big|_{z'=a} = - \int p(x|Z) \cdot \frac{\partial^2}{\partial z' \partial z'^T} \log p(x|z') \Big|_{z'=a} dx = I_a(Z).$$

347 This means

$$D_{KL}\{p(x|Z)||p(x|Z_n^{(l)})\} = \frac{1}{2}(Z_n^{(l)} - Z)^T I_a(Z)(Z_n^{(l)} - Z).$$

348 Note that $Z_n^{(l)} \rightarrow Z$ a.s. implies that $Z_n^{(l)}$ converges to Z in probability. Then $\forall \delta > 0$, for ϵ defined
349 in Assumption 1, we have

$$\begin{aligned} P(D_{KL}\{p(x|Z)||p(x|Z_n^{(l)})\} > \delta) &\leq P(\{D_{KL}\{p(x|Z)||p(x|Z_n^{(l)})\} > \delta\} \cap \{\|Z_n^{(l)} - Z\|_2 \leq \epsilon\}) \\ &\quad + P(\|Z_n^{(l)} - Z\|_2 > \epsilon) \\ &\leq P\left(\frac{1}{2}\beta\|Z_n^{(l)} - Z\|_2^2 > \delta\right) + P(\|Z_n^{(l)} - Z\|_2 > \epsilon) \\ &= o(1). \end{aligned}$$

350 Thus, $D_{KL}\{p(x|Z)||p(x|Z_n^{(l)})\} = o_p(1)$.

351 Because $I\{\xi = l\} \leq 1$ for $l = 1, 2, \dots, k$, and k is finite, we obtain

$$D_{KL}\{p(x|Z), \hat{p}(x|Z)\} = \sum_{l=1}^k I\{\xi = l\} D_{KL}\{p(x|Z)||p(x|Z_n^{(l)})\} = o_p(1).$$

352 Finally, we conclude that $d_{TV}\{p(x|Z), \hat{p}(x|Z)\} \leq \sqrt{D_{KL}\{p(x|Z), \hat{p}(x|Z)\}/2} = o_p(1)$.

353 A.3 Proof of Theorem 3

354 To prove Theorem 3, the following two lemmas are needed.

Lemma 5. Let \dot{X} be drawn from $\hat{p}(\cdot|Z)$, independently of Y . $\dot{X}^{(1)}, \dots, \dot{X}^{(B)}$ are i.i.d. samples drawn from the k -nearest-neighbor local sampling mechanism based on (\dot{X}, Y, Z) . For any statistic T , the $B + 1$ statistics

$$T(\dot{X}, Y, Z), T(\dot{X}^{(1)}, Y, Z), \dots, T(\dot{X}^{(B)}, Y, Z)$$

355 are exchangeable conditionally on Y and Z .

356 *Proof.* We have that the $B+1$ triples $(\dot{X}, Y, Z), (\dot{X}^{(1)}, Y, Z), \dots, (\dot{X}^{(B)}, Y, Z)$ are i.i.d. samples
357 drawn from the same mechanism after conditionally on $\dot{X}_{(0)}, Y$ and Z , where $\dot{X}_{(0)}$ is the order statistic
358 of \dot{X} . Note that, T is measurable. Thus, $T(\dot{X}, Y, Z), T(\dot{X}^{(1)}, Y, Z), \dots, T(\dot{X}^{(B)}, Y, Z)$ are
359 i.i.d. after conditionally on $\dot{X}_{(0)}, Y$ and Z . Conditionally on $\dot{X}_{(0)}, Y$ and Z , denote their cumulative
360 conditional distribution as $F(\cdot|\dot{X}_{(0)}, Y, Z)$. Denote \dot{X} as $\dot{X}^{(0)}$. Then, for any $t_0, \dots, t_B \in \mathbb{R}$ and

361 any permutation $\pi = (\pi_{(0)}, \dots, \pi_{(B)})$ of the indices $\{0, 1, \dots, B\}$, we have

$$\begin{aligned}
& P(T(\dot{\mathbf{X}}^{(0)}, \mathbf{Y}, \mathbf{Z}) \leq t_0, T(\dot{\mathbf{X}}^{(1)}, \mathbf{Y}, \mathbf{Z}) \leq t_1, \dots, T(\dot{\mathbf{X}}^{(B)}, \mathbf{Y}, \mathbf{Z}) \leq t_B | \mathbf{Y}, \mathbf{Z}) \\
&= E_{\dot{\mathbf{X}}_0 | \mathbf{Y}, \mathbf{Z}} \{P(T(\dot{\mathbf{X}}^{(0)}, \mathbf{Y}, \mathbf{Z}) \leq t_0, T(\dot{\mathbf{X}}^{(1)}, \mathbf{Y}, \mathbf{Z}) \leq t_1, \dots, T(\dot{\mathbf{X}}^{(B)}, \mathbf{Y}, \mathbf{Z}) \leq t_B | \dot{\mathbf{X}}_0, \mathbf{Y}, \mathbf{Z})\} \\
&= E_{\dot{\mathbf{X}}_0 | \mathbf{Y}, \mathbf{Z}} \{P(T(\dot{\mathbf{X}}^{(0)}, \mathbf{Y}, \mathbf{Z}) \leq t_0 | \dot{\mathbf{X}}_0, \mathbf{Y}, \mathbf{Z}), \dots, P(T(\dot{\mathbf{X}}^{(B)}, \mathbf{Y}, \mathbf{Z}) \leq t_B | \dot{\mathbf{X}}_0, \mathbf{Y}, \mathbf{Z})\} \\
&= E_{\dot{\mathbf{X}}_0 | \mathbf{Y}, \mathbf{Z}} \left\{ \prod_{i=0}^B F(t_i | \dot{\mathbf{X}}_0, \mathbf{Y}, \mathbf{Z}) \right\} \\
&= E_{\dot{\mathbf{X}}_0 | \mathbf{Y}, \mathbf{Z}} \{P(T(\dot{\mathbf{X}}^{(\pi_{(0)})}, \mathbf{Y}, \mathbf{Z}) \leq t_0, \dots, T(\dot{\mathbf{X}}^{(\pi_{(B)})}, \mathbf{Y}, \mathbf{Z}) \leq t_B | \dot{\mathbf{X}}_0, \mathbf{Y}, \mathbf{Z})\} \\
&= P(T(\dot{\mathbf{X}}^{(\pi_{(0)})}, \mathbf{Y}, \mathbf{Z}) \leq t_0, \dots, T(\dot{\mathbf{X}}^{(\pi_{(B)})}, \mathbf{Y}, \mathbf{Z}) \leq t_B | \mathbf{Y}, \mathbf{Z}).
\end{aligned}$$

362 Thus, the desired result follows.

363 Let $\stackrel{d}{=}$ denotes equality in distribution. We present the following Lemma:

364 **Lemma 6.** For any two bi-tuples (U, V) and (U', V') , if $\forall \mathbf{u}, (V|U = \mathbf{u}) \stackrel{d}{=} (V'|U' = \mathbf{u})$, we
365 have $d_{TV}\{(U, V), (U', V')\} = d_{TV}(U, U')$.

366 *Proof.* Denote the joint density functions of (U, V) and (U', V') by $p_{U, V}(\mathbf{u}, \mathbf{v})$ and $p_{U', V'}(\mathbf{u}', \mathbf{v}')$,
367 respectively. According to the equivalent definition of the TV distance, we obtain

$$\begin{aligned}
d_{TV}\{(U, V), (U', V')\} &= \frac{1}{2} \iint |p_{U, V}(\mathbf{u}, \mathbf{v}) - p_{U', V'}(\mathbf{u}, \mathbf{v})| d\mathbf{u} d\mathbf{v} \\
&= \frac{1}{2} \iint |p_{V|U}(\mathbf{v}|\mathbf{u})p_U(\mathbf{u}) - p_{V'|U'}(\mathbf{v}|\mathbf{u})p_{U'}(\mathbf{u})| d\mathbf{u} d\mathbf{v} \\
&= \frac{1}{2} \iint p_{V|U}(\mathbf{v}|\mathbf{u}) |p_U(\mathbf{u}) - p_{U'}(\mathbf{u})| d\mathbf{u} d\mathbf{v} \\
&= \frac{1}{2} \int \left[\int p_{V|U}(\mathbf{v}|\mathbf{u}) d\mathbf{v} \right] |p_U(\mathbf{u}) - p_{U'}(\mathbf{u})| d\mathbf{u} \\
&= \frac{1}{2} \int |p_U(\mathbf{u}) - p_{U'}(\mathbf{u})| d\mathbf{u} \\
&= d_{TV}(U, U').
\end{aligned}$$

368 Now we present the proof of Theorem 3:

369 *Proof.* Let $\widetilde{\mathbf{X}}^{(1)}, \dots, \widetilde{\mathbf{X}}^{(B)}$ be i.i.d. drawn from the k -nearest-neighbor local sampling mechanism,
370 see Algorithm 3. Now let $\dot{\mathbf{X}}$ be an additional sample drawn from $\widehat{p}(\cdot | \mathbf{Z})$ independently of \mathbf{Y} . Let
371 $\dot{\mathbf{X}}^{(1)}, \dots, \dot{\mathbf{X}}^{(B)}$ be i.i.d. drawn from the k -nearest-neighbor local sampling mechanism after we
372 observe $\dot{\mathbf{X}}$ instead of \mathbf{X} . Because $(\dot{\mathbf{X}}^{(1)}, \dots, \dot{\mathbf{X}}^{(B)})$, conditionally on $\dot{\mathbf{X}}, \mathbf{Y}$ and \mathbf{Z} , is generated
373 from the same mechanism as $(\widetilde{\mathbf{X}}^{(1)}, \dots, \widetilde{\mathbf{X}}^{(B)})$, conditionally on \mathbf{X}, \mathbf{Y} and \mathbf{Z} , for all $\mathbf{x} \in \mathbb{R}^n$, we
374 have

$$((\widetilde{\mathbf{X}}^{(1)}, \dots, \widetilde{\mathbf{X}}^{(B)}) | \mathbf{X} = \mathbf{x}, \mathbf{Y}, \mathbf{Z}) \stackrel{d}{=} ((\dot{\mathbf{X}}^{(1)}, \dots, \dot{\mathbf{X}}^{(B)}) | \dot{\mathbf{X}} = \mathbf{x}, \mathbf{Y}, \mathbf{Z}).$$

375 Then, by applying Lemma 6, we obtain

$$\begin{aligned}
& d_{TV}\{(\mathbf{X}, \widetilde{\mathbf{X}}^{(1)}, \dots, \widetilde{\mathbf{X}}^{(B)} | \mathbf{Y}, \mathbf{Z}), (\dot{\mathbf{X}}, \dot{\mathbf{X}}^{(1)}, \dots, \dot{\mathbf{X}}^{(B)} | \mathbf{Y}, \mathbf{Z})\} \\
&= d_{TV}\{(\mathbf{X} | \mathbf{Y}, \mathbf{Z}), (\dot{\mathbf{X}} | \mathbf{Y}, \mathbf{Z})\} = d_{TV}\{p(\cdot | \mathbf{Z}), \widehat{p}(\cdot | \mathbf{Z})\}.
\end{aligned}$$

376 Define $\chi_\alpha^B := \left\{ (\mathbf{x}, \mathbf{x}^{(1)}, \dots, \mathbf{x}^{(B)}) \mid \left[1 + \sum_{b=1}^B 1\{T(\mathbf{x}^{(b)}, \mathbf{Y}, \mathbf{Z}) \geq T(\mathbf{x}, \mathbf{Y}, \mathbf{Z})\} \right] / (1 + B) \leq \alpha \right\}$,

377 where $1(\cdot)$ is the indicator function. Note that in our case, the statistic T is selected to be $\widehat{\text{CMI}}$. Then,

378 it follows that

$$\begin{aligned}
P(p \leq \alpha | \mathbf{Y}, \mathbf{Z}) &= P((\mathbf{X}, \widetilde{\mathbf{X}}^{(1)}, \dots, \widetilde{\mathbf{X}}^{(B)}) \in \chi_\alpha^B | \mathbf{Y}, \mathbf{Z}) \\
&= P((\dot{\mathbf{X}}, \dot{\mathbf{X}}^{(1)}, \dots, \dot{\mathbf{X}}^{(B)}) \in \chi_\alpha^B | \mathbf{Y}, \mathbf{Z}) + P((\mathbf{X}, \widetilde{\mathbf{X}}^{(1)}, \dots, \widetilde{\mathbf{X}}^{(B)}) \in \chi_\alpha^B | \mathbf{Y}, \mathbf{Z}) \\
&\quad - P((\dot{\mathbf{X}}, \dot{\mathbf{X}}^{(1)}, \dots, \dot{\mathbf{X}}^{(B)}) \in \chi_\alpha^B | \mathbf{Y}, \mathbf{Z}) \\
&\leq P((\dot{\mathbf{X}}, \dot{\mathbf{X}}^{(1)}, \dots, \dot{\mathbf{X}}^{(B)}) \in \chi_\alpha^B | \mathbf{Y}, \mathbf{Z}) \\
&\quad + d_{TV}\{(\mathbf{X}, \widetilde{\mathbf{X}}^{(1)}, \dots, \widetilde{\mathbf{X}}^{(B)} | \mathbf{Y}, \mathbf{Z}), (\dot{\mathbf{X}}, \dot{\mathbf{X}}^{(1)}, \dots, \dot{\mathbf{X}}^{(B)} | \mathbf{Y}, \mathbf{Z})\} \\
&= P((\dot{\mathbf{X}}, \dot{\mathbf{X}}^{(1)}, \dots, \dot{\mathbf{X}}^{(B)}) \in \chi_\alpha^B | \mathbf{Y}, \mathbf{Z}) + d_{TV}\{p(\cdot | \mathbf{Z}), \widehat{p}(\cdot | \mathbf{Z})\}.
\end{aligned}$$

379 Applying Lemma 5 and the property of rank test, we obtain $P((\dot{\mathbf{X}}, \dot{\mathbf{X}}^{(1)}, \dots, \dot{\mathbf{X}}^{(B)}) \in \chi_\alpha^B | \mathbf{Y}, \mathbf{Z}) \leq$
380 α . Finally, we have $P(p \leq \alpha | \mathbf{Y}, \mathbf{Z}) \leq \alpha + d_{TV}\{p(\cdot | \mathbf{Z}), \widehat{p}(\cdot | \mathbf{Z})\}$.

Because the TV distance is bounded by 1, marginalizing the above inequality over \mathbf{Y} and \mathbf{Z} and applying Theorem 2 and Lebesgue dominated convergence theorem lead to

$$P(p \leq \alpha | H_0) \leq \alpha + E(d_{TV}\{p(\cdot | \mathbf{Z}), \widehat{p}(\cdot | \mathbf{Z})\}) = \alpha + o(1).$$

381 A.4 Proof of Theorem 4

Here we present the assumptions given in [6] that ensure the consistency of CMI estimator. We denote the point (x, y, z) as $\omega \in \mathbb{R}^{d_x} \times \mathbb{R}^{d_y} \times \mathbb{R}^{d_z}$. Let $f(\omega) = p(x, y, z)$ be the joint density function of (X, Y, Z) , $g(\omega) = p(x, z)p(y|z)$ be the joint density function of (X, Y, Z) under H_0 , and $\phi(\omega) = \phi(x, y, z)$ be the joint density of (X, Y', Z) produced by Algorithm 1. The classifier in Algorithm 2 is trained using the label probability $\gamma_\theta(\omega) := P_\theta(l = 1 | \omega)$ with parameter θ . According to Algorithm 2, $P(l = 1) = P(l = 0) = 1/2$. Define the population binary-cross entropy loss over the joint distribution of data and label as

$$\text{BCE}(\gamma_\theta) = -\{E_{Wl}(l \log \gamma_\theta(W) + (1 - l) \log(1 - \gamma_\theta(W)))\}.$$

382 Let $\gamma'(\omega) := \gamma_{\theta'}(\omega)$ be the point-wise minimizer of binary-cross entropy loss based on $f(\omega)$ and
383 $\phi(\omega)$, and $\gamma''(\omega) := \gamma_{\theta''}(\omega)$ be the point-wise minimizer of binary-cross entropy loss based on $f(\omega)$
384 and $g(\omega)$.

385 **Assumption (A1):** $f(\cdot)$ and $\phi(\cdot)$ admit densities in a compact subset $\mathcal{W} \subset \mathbb{R}^{d_x} \times \mathbb{R}^{d_y} \times \mathbb{R}^{d_z}$.

386 **Assumption (A2):** For some constant $\alpha, \zeta > 0$, $\alpha \leq f(\omega)$, $\phi(\omega) \leq \zeta$, $\forall \omega$.

387 **Assumption (A3):** $\gamma'(\omega), \gamma''(\omega) \in [\tau, 1 - \tau]$ and clip predictions such that $\gamma_\theta(\omega) \in [\tau, 1 - \tau] \forall \omega, \theta$,
388 with $0 < \tau \leq \alpha / (\alpha + \zeta)$.

389 **Assumption (A4):** The classifier class \mathcal{C}_θ is parametrized by θ within a compact domain $\Theta \subset \mathbb{R}^h$.
390 There exists a constant K such that $\|\theta\|_2 \leq K$, and the classifier's output is L -Lipschitz with respect
391 to θ .

392 **Assumption (A5):** $\int p(z)^{1-1/d} dz \leq C_5$, $\forall d \geq 2$, where C_5 is a constant.

393 We denote the CMI estimator $\widehat{\text{CMI}}$ based on Algorithm 2 as $\widehat{D}_{KL}^{(n)}(f||\phi)$. The true CMI of (X, Y, Z)
394 is $\text{CMI} := I(X; Y|Z) = D_{KL}(f||g)$. Then we have the following Lemma:

395 **Lemma 7.** Under Assumptions 1 and 2 and (A1)-(A5), we have $\widehat{D}_{KL}^{(n)}(f||\phi) \xrightarrow{P} D_{KL}(f||g)$.

396 *Proof.* By the definition of convergence in probability, it is sufficient to prove $\forall \delta > 0, \forall \eta > 0, \exists N$,
397 when $n > N$, $P(|\widehat{D}_{KL}^{(n)}(f||\phi) - D_{KL}(f||g)| > \delta) < \eta$.

398 Note that

$$\begin{aligned}
&P(|\widehat{D}_{KL}^{(n)}(f||\phi) - D_{KL}(f||g)| > \delta) \\
&= P(|\widehat{D}_{KL}^{(n)}(f||\phi) - D_{KL}(f||\phi) + D_{KL}(f||\phi) - D_{KL}(f||g)| > \delta).
\end{aligned}$$

399 Applying Theorem 1 in [6], we have $\widehat{D}_{KL}^{(n)}(f||\phi) - D_{KL}(f||\phi) \xrightarrow{P} 0$, which means for $\delta/2 > 0$ and
400 $\eta > 0, \exists N_1$, when $n > N_1$, $P(|\widehat{D}_{KL}^{(n)}(f||\phi) - D_{KL}(f||\phi)| > \delta/2) < \eta$.

401 Now consider the term $D_{KL}(f||\phi) - D_{KL}(f||g)$. Applying Lemma 3 in [6], we have $\gamma'(\omega)/\{1 -$
 402 $\gamma'(\omega)\} = f(\omega)/\phi(\omega)$ and $\gamma''(\omega)/\{1 - \gamma''(\omega)\} = f(\omega)/g(\omega)$. Then, by the definition of KL
 403 divergence, it follows that

$$\begin{aligned}
 |D_{KL}(f||\phi) - D_{KL}(f||g)| &= \left| E_{f(\omega)} \log \frac{f(\omega)}{\phi(\omega)} - E_{f(\omega)} \log \frac{f(\omega)}{g(\omega)} \right| \\
 &= \left| E_{f(\omega)} \left(\log \frac{\gamma'(\omega)}{1 - \gamma'(\omega)} - \log \frac{\gamma''(\omega)}{1 - \gamma''(\omega)} \right) \right| \\
 &\leq E_{f(\omega)} \left| \log \frac{1 - \gamma'(\omega)}{\gamma'(\omega)} - \log \frac{1 - \gamma''(\omega)}{\gamma''(\omega)} \right| \\
 &\leq \frac{1 - \tau}{\tau} E_{f(\omega)} \left| \frac{1 - \gamma'(\omega)}{\gamma'(\omega)} - \frac{1 - \gamma''(\omega)}{\gamma''(\omega)} \right| \\
 &= \frac{1 - \tau}{\tau} E_{f(\omega)} \left| \frac{\phi(\omega) - g(\omega)}{f(\omega)} \right| \\
 &= \frac{1 - \tau}{\tau} \iiint |\phi(x, y, z) - g(x, y, z)| dx dy dz \\
 &= \frac{2(1 - \tau)}{\tau} d_{TV}(\phi, g).
 \end{aligned}$$

404 The second inequality follows from Lagrange's mean value theorem and Assumption (A3).

Applying Theorem 1 in [9], $\forall \epsilon_1 \leq \epsilon$ with ϵ being defined in Assumption 1, we have $d_{TV}(\phi, g) \leq b(n)$, where

$$b(n) = \frac{1}{2} \sqrt{\frac{\beta C_5 2^{1/d_z} \Gamma(1/d_z)}{4 (n \gamma_{d_z})^{1/d_z} d_z} + \frac{\beta \epsilon_1 G(2c_{d_z} \epsilon_1^2)}{4}} + \exp\left(-\frac{1}{2} n \gamma_{d_z} c_{d_z} \epsilon_1^{d_z+2}\right) + G(2c_{d_z} \epsilon_1^2).$$

405 Here, β is defined in Assumption 1, C_5 is defined in Assumption (A5), d_z is the dimension of Z ,
 406 $\Gamma(\cdot)$ is the gamma function, γ_{d_z} is the volume of the unit radius l_2 ball in \mathbb{R}^{d_z} , c_{d_z} is defined in
 407 Assumption 2, and $\forall \delta > 0$, $G(\delta) = P(p(Z) \leq \delta)$.

408 Because ϵ_1 can be arbitrary small, we conclude that $\lim_{n \rightarrow \infty} b(n) = 0$. So we arrive at
 409 $\lim_{n \rightarrow \infty} |D_{KL}(f||\phi) - D_{KL}(f||g)| = 0$, which means for $\delta/2 > 0$, $\exists N_2$, when $n > N_2$,
 410 $|D_{KL}(f||\phi) - D_{KL}(f||g)| < \delta/2$.

411 Then for $\delta > 0$ and $\eta > 0$, take $N = \max(N_1, N_2)$, when $n > N$,

$$\begin{aligned}
 &P(|\widehat{D}_{KL}^{(n)}(f||\phi) - D_{KL}(f||\phi) + D_{KL}(f||\phi) - D_{KL}(f||g)| > \delta) \\
 &\leq P(|\widehat{D}_{KL}^{(n)}(f||\phi) - D_{KL}(f||\phi)| + |D_{KL}(f||\phi) - D_{KL}(f||g)| > \delta) \\
 &\leq P(|\widehat{D}_{KL}^{(n)}(f||\phi) - D_{KL}(f||\phi)| > \delta/2) < \eta
 \end{aligned}$$

412 holds. This finish the proof.

413 We therefore conclude that $\widehat{\text{CMI}}$ is a consistent estimator of CMI. When considering $\widehat{\text{CMI}}^{(b)}$ based
 414 on the sample $(\widetilde{\mathbf{X}}^{(b)}, \mathbf{Y}, \mathbf{Z})$ ($b = 1, \dots, B$) drawn from the k -nearest-neighbor local sampling
 415 mechanism as depicted in Algorithm 3, we can state: Under Assumptions 1, 2, (A1)-(A3) with
 416 $f(\omega)$ and $\phi(\omega)$ replaced by densities of the distribution of (\widetilde{X}, Y, Z) and the corresponding 1-NN
 417 distribution, respectively, and Assumptions (A4)-(A5), $\forall b = 1, \dots, B$, $\widehat{\text{CMI}}^{(b)}$ is a consistent
 418 estimator of $\text{CMI}^{(b)}$, where $\text{CMI}^{(b)} = I(\widetilde{X}^{(b)}; Y|Z)$. Now let's present the proof of Theorem 4.

419 *Proof.* Write $P(\cdot|H_1)$ as $P_{H_1}(\cdot)$. By Markov inequality, it follows that

$$\begin{aligned}
P_{H_1}(p > \alpha) &= P_{H_1}\left(\frac{1 + \sum_{b=1}^{B_n} 1(\widehat{\text{CMI}}^{(b)} \geq \widehat{\text{CMI}})}{1 + B_n} > \alpha\right) \\
&\leq \frac{1}{\alpha(1 + B_n)} E_{H_1}\left(1 + \sum_{b=1}^{B_n} 1(\widehat{\text{CMI}}^{(b)} \geq \widehat{\text{CMI}})\right) \\
&= \frac{1}{\alpha(1 + B_n)} + \frac{B_n}{\alpha(1 + B_n)} P_{H_1}(\widehat{\text{CMI}}^{(1)} \geq \widehat{\text{CMI}}) \\
&\leq \frac{1}{\alpha(1 + B_n)} + \frac{1}{\alpha} P_{H_1}(\widehat{\text{CMI}}^{(1)} \geq \widehat{\text{CMI}}).
\end{aligned}$$

420 Because $\tilde{X}^{(1)} \perp\!\!\!\perp Y|Z$, $\text{CMI}^{(1)} = I(\tilde{X}^{(1)}; Y|Z) = 0$. Then, $\forall \delta > 0$,

$$\begin{aligned}
P_{H_1}(\widehat{\text{CMI}}^{(1)} \geq \widehat{\text{CMI}}) &\leq P_{H_1}(\{\widehat{\text{CMI}} \leq \widehat{\text{CMI}}^{(1)}\} \cap \{|\widehat{\text{CMI}}^{(1)} - \text{CMI}^{(1)}| \leq \delta\}) \\
&\quad + P_{H_1}(|\widehat{\text{CMI}}^{(1)} - \text{CMI}^{(1)}| > \delta) \\
&\leq P_{H_1}(\widehat{\text{CMI}} \leq \delta) + P_{H_1}(|\widehat{\text{CMI}}^{(1)} - \text{CMI}^{(1)}| > \delta).
\end{aligned}$$

421 Next, we have

$$\begin{aligned}
P_{H_1}(\widehat{\text{CMI}} \leq \delta) &\leq P_{H_1}(\{\widehat{\text{CMI}} \leq \delta\} \cap \{|\widehat{\text{CMI}} - \text{CMI}| \leq \delta\}) + P_{H_1}(|\widehat{\text{CMI}} - \text{CMI}| > \delta) \\
&\leq P_{H_1}(\text{CMI} - \delta \leq \widehat{\text{CMI}} \leq \delta) + P_{H_1}(|\widehat{\text{CMI}} - \text{CMI}| > \delta).
\end{aligned}$$

422 Thus, we conclude that

$$\begin{aligned}
P_{H_1}(p \leq \alpha) &\geq 1 - \frac{1}{\alpha(1 + B_n)} - \frac{1}{\alpha} [P_{H_1}(\text{CMI} - \delta \leq \widehat{\text{CMI}} \leq \delta) \\
&\quad + P_{H_1}(|\widehat{\text{CMI}} - \text{CMI}| > \delta) + P_{H_1}(|\widehat{\text{CMI}}^{(1)} - \text{CMI}^{(1)}| > \delta)].
\end{aligned}$$

Under H_1 , $\text{CMI} > 0$. Take $\delta = \text{CMI}/4 > 0$, we obtain

$$\lim_{n \rightarrow \infty} P_{H_1}(p \leq \alpha) \rightarrow 1.$$

423 B Additional Empirical Results

424 B.1 The choice of the neighbor order k

425 To investigate the impact of the parameter k on our proposed approach, we employ a linear uniform
426 model. To accomplish this, we generate synthetic data in the following manner:

$$\begin{aligned}
H_0 : X &= \epsilon_x, \quad Y = \epsilon_y, \quad \text{and } Z \sim \text{Uniform}(-1, 1), \\
H_1 : X &= \epsilon_x, \quad Y = \alpha X + 0.5\epsilon_y, \quad \text{and } Z \sim \text{Uniform}(-1, 1),
\end{aligned} \tag{13}$$

427 where ϵ_x and ϵ_y are generated independently from the uniform distribution over the interval $[-1, 1]$.
428 The parameter α is randomly generated within the range of $[0, 2]$. As is shown in Figure 3, our
429 method achieves effective control of type I error and exhibits the highest power under H_1 across all
430 dimensions when $k = 7$. Therefore, we consistently set $k = 7$ in all experiments.

431 B.2 Empirical results for Scenario (13)

432 We demonstrate the effectiveness of our approach and compare it with alternative methods in Scenario
433 (13). The results are shown in Figure 4, which pertains to high-dimensional Z , and Figure 5, which
434 focuses on low-dimensional Z . The results consistently demonstrate that our test achieves favorable
435 performance in terms of the type I error and power under H_1 . Although LPCIT, CMiknn, and
436 NNSCIT effectively control the type I error, they exhibit noticeably lower power compared to our
437 method, when the dimension exceeds 60, often by a substantial margin. Furthermore, KCIT, GCIT,
438 and CCIT all yield high power under H_1 , but they either always or sometimes suffer from inflated
439 type I errors.

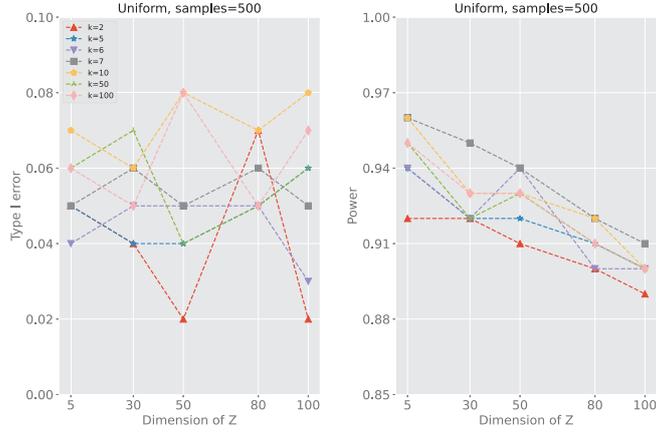


Figure 3: Comparison of the type I error (lower is better) and power under H_1 (higher is better) for our test in Scenario (13) across different values of k .

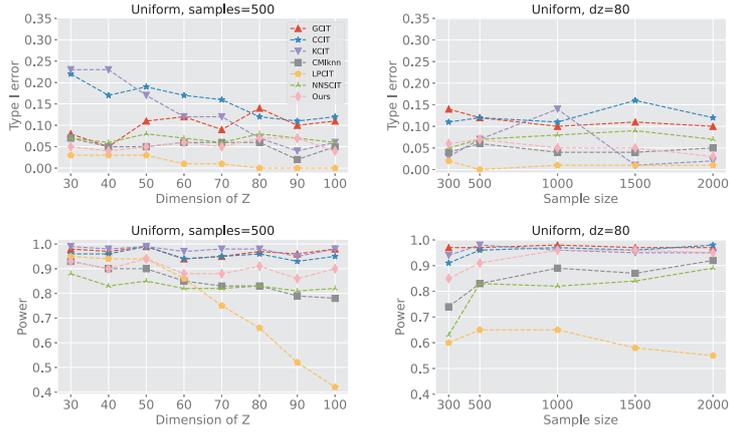


Figure 4: Comparison of the type I error (lower is better) and power under H_1 (higher is better) of our test with six SOTA tests in Scenario (13). **Left:** The results when varying the dimension of Z . **Right:** The results when varying the sample size.

440 B.3 Additional empirical results for Scenario I

441 In Figure 6, we present the type I error and power under H_1 in low dimensions of Z ranging from
 442 5 to 30 for Scenario I (Eq. (9)) with Gaussian or Laplace noises. It can be observed that our test
 443 and LPCIT consistently achieve good and stable performance in terms of type I error and power
 444 under H_1 , when the dimensionality of Z is lower than 30. On the other hand, GCIT, CCIT, and KCIT
 445 exhibit high power under H_1 but fail to control the type I error. NNSCIT and CMiknn demonstrate
 446 relatively good control of type I errors but lack sufficient power under H_1 .

447 B.4 Computational efficiency analysis

448 Figure 7 shows the timing performance of all methods for a single test under Scenario I with Laplace
 449 noises. Our test is found to be highly computationally efficient even when dealing with large
 450 sample sizes and high-dimensional conditioning sets. In contrast, CMiknn and CCIT for sample

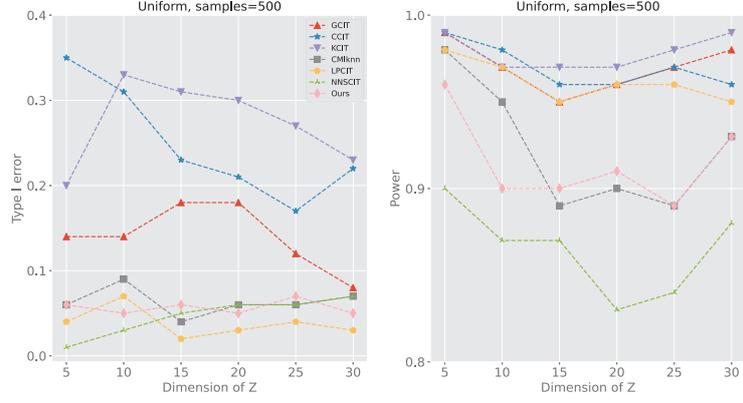


Figure 5: Comparison of the type I error (lower is better) and power under H_1 (higher is better) of our test with six SOTA tests in Scenario (13).

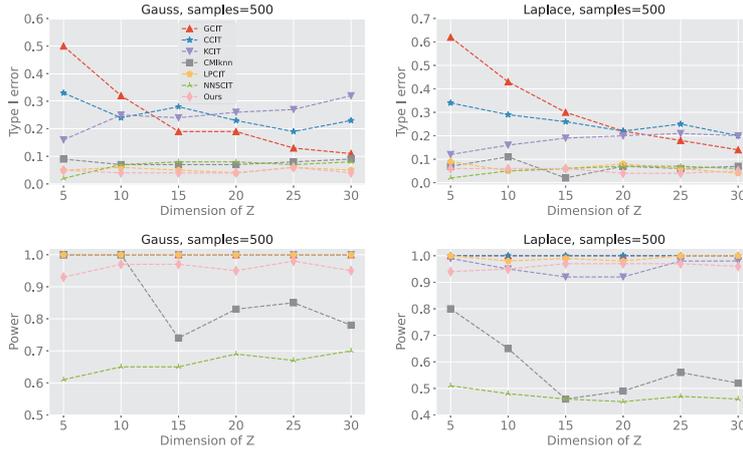


Figure 6: Comparison of the type I error (lower is better) and power under H_1 (higher is better) of our method with six SOTA methods on the post-nonlinear model under Gaussian or Laplace distributions in Scenario I. **Left:** The results under Gaussian distribution. **Right:** The results under Laplace distribution.

451 sizes exceeding 1000, and LPCIT for dimension of Z higher than 50 are impractical due to their
 452 prohibitively long running time.

453 B.5 The detailed experimental setup for Scenario III

454 For the chain structure $Y \rightarrow Z \rightarrow X$, we generate synthetic data as follows:

$$H_0 : Y \sim N(1, 1), Z = Ya + \epsilon_1, X = Z^T b + \epsilon_2,$$

$$H_1 : Y \sim N(1, 1), Z = Ya + \epsilon_1, X = Z^T b + Y + \epsilon_2,$$

455 where a and b are both d_z -dimensional, the entries of a and b are both randomly and uniformly sampled
 456 from $[0, 0.3]$, ϵ_1 is generated from a d_z -dimensional standard multivariate Gaussian distribution, and
 457 ϵ_2 is sampled from a standard Gaussian distribution.

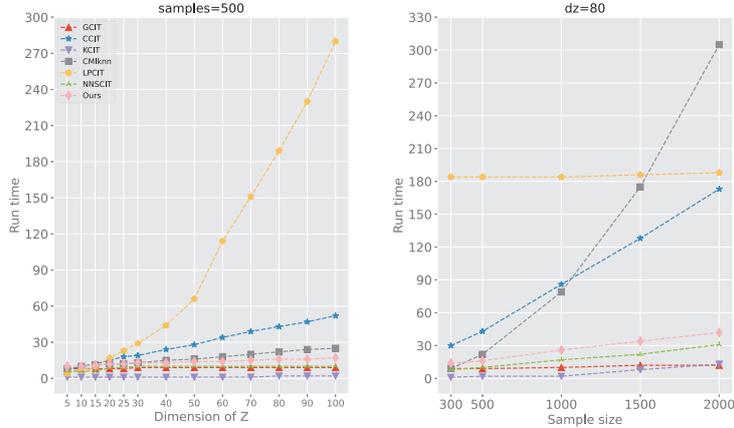


Figure 7: Running times in seconds as a function of sample size or dimension of Z on the post-nonlinear model under Laplace distribution in Scenario I. **Left:** The results when varying the dimension of Z . **Right:** The results when varying the sample size.

458 C Real Data Analysis

459 In order to showcase the superior performance of our test, we conduct a comparative evaluation
 460 against other state-of-the-art (SOTA) CI tests using real datasets. We assess the effectiveness of our
 461 method along with six SOTA approaches on two specific datasets: the ABALONE dataset [1] and the
 462 Flow-Cytometry dataset [8].

463 C.1 Real ABALONE dataset

464 The ABALONE dataset [1] comprises measurements obtained from a study conducted to
 465 predict the age of abalones based on their physical characteristics. The dataset is pub-
 466 licly available at the UCI Machine Learning Repository and can be downloaded from
 467 <https://archive.ics.uci.edu/ml/datasets/abalone>. In our evaluation, we consider the graph structure
 468 recovered by [4] as the ground truth, as depicted in Figure 4 of their paper. This graph represents
 469 the causal relationships among the 8 variables in the dataset. We specifically select 35 CI relations
 470 and 35 non-CI relations from this graph. The philosophy used is that a node X is independent of all
 471 other nodes Y in the graph when conditioned on its parents, children, and parents of children [2, 9].
 472 Additionally, if there exists a direct edge between node X and node Y in the graph, they are never
 473 conditionally independent given any other set of variables. As a result, the conditioning set Z can be
 474 arbitrarily selected from the remaining nodes. The dataset consists of 4177 samples, and d_z varies
 475 from 1 to 6.

476 In order to evaluate the performance of various tests, we utilize precision, recall, and F-score as
 477 evaluation metrics. Precision is calculated as $TP/(TP+FP)$, where TP represents the number of true CI
 478 instances correctly identified, and FP represents the number of non-CI instances incorrectly identified
 479 as CI. Recall is calculated as $TP/(TP+FN)$, where FN represents the number of CI instances not
 480 identified. The F-score is then computed as the harmonic mean of precision and recall, given by $2 \times$
 481 $\text{precision} \times \text{recall} / (\text{precision} + \text{recall})$ [3]. TN represents the number of correctly identified true
 482 non-CI instances. Table 1 presents the results for all methods. It should be noted that we do not record
 483 the results for GCIT as it does not correctly identify any CI relations. Our approach successfully
 484 identifies 31 CI relations and 32 non-CI relations, achieving the highest F-score among the testing
 485 methods, while maintaining high precision and recall.

486 C.2 Real Flow-Cytometry dataset

487 The Flow-Cytometry dataset is a widely used benchmark in the field of causal structure learning
 488 [7, 10]. This dataset captures the expression levels of proteins and phospholipids in human cells [8].

Table 1: The TP, TN, precision (pre), recall (rec) and F-score of our test and six SOTA methods for the real ABALONE dataset.

Method	TP	TN	Pre	Rec	F-score
KCIT	5	35	1	0.1429	0.2501
CCIT	12	34	0.9231	0.3429	0.5
CMlknn	22	35	1	0.6286	0.7720
LPCIT	5	35	1	0.1429	0.2501
NNSCIT	33	6	0.5323	0.9429	0.6805
Ours	31	32	0.9118	0.8857	0.8986

489 The data can be obtained from the website <https://www.science.org/doi/10.1126/science.1105809>. In
490 our evaluation, we consider the consensus graph proposed in [5] as the ground truth, which has also
491 been adopted by [9] for verifying CI relations. Figure 5(a) in [5] illustrates the causal relationships
492 among the 11 proteins in the dataset. Following the philosophy outlined in Section C.1, we select 50
493 CI relations and 40 non-CI relations from this graph. The number of samples is 1755 and d_z varies
494 from 1 to 9.

495 Table 2 presents the results for all tests. Our method outperforms other approaches by correctly
496 identifying 47 CI relations and achieving the highest recall and F-score.

Table 2: The TP, TN, precision (pre), recall (rec) and F-score of our test and six SOTA methods for the real Flow-Cytometry dataset.

Method	TP	TN	Pre	Rec	F-score
KCIT	32	30	0.7619	0.64	0.6957
CCIT	33	29	0.75	0.66	0.7021
CMlknn	41	26	0.7455	0.82	0.7810
GCIT	40	24	0.7143	0.8	0.7547
LPCIT	38	25	0.7170	0.76	0.7379
NNSCIT	33	26	0.7021	0.66	0.6804
Ours	47	23	0.7344	0.94	0.8246

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