

HIGHLIGHTS

- ♣ **Problem to solve:** Measuring conditional dependence between two random phenomena when a confounder has a potential influence on the amount of information between them.
- ♣ **Proposed solution:** Novel measure based on incomplete unbiased statistics of degree two.
 - Allows to re-interpret independence as uncorrelatedness on a finite-dimensional feature space.
 - Prunes data according to observations of the confounder itself.
 - Avoids inverting ill-conditioned autocorrelation matrices.

BACKGROUND

- Measuring conditional dependence is an important task in a variety of areas related to data science.
- Empirically estimating conditional dependence is challenging: known methods in the literature require inferring conditional marginal distributions.
 - Numerical issues related to matrix inversions and regularization.
 - Complexity scales cubically with the number of samples.
- Proposal:** *conditional Hilbert-Schmidt independence criterion (C-HSIC)*
 - Translates statistical dependence into correlation: mapping data onto finite-dimensional spaces based on steering vectors [1].
 - Bypasses matrix inversion: conditioning is achieved by pruning pairwise differences of data under the control of the confounder [2].
 - Embraces the HSIC as a particular case when the U-Statistic is complete.

MARGINAL DEPENDENCE AS CORRELATION

- Mapping $\mathbf{d} : \mathbb{R} \rightarrow \mathbb{C}^M$, $[\mathbf{d}(\diamond)]_m \triangleq \frac{1}{\sqrt{M}} G\left(\frac{m}{\sqrt{M}}\right) e^{j2\pi \frac{m}{\sqrt{M}} \diamond}$
- $\lim_{M \rightarrow \infty} \|\mathbf{C}_{u,v}\|_F^2 = 0 \iff x, y \text{ independent}$ (1)
- Data set with L i.i.d. samples of x and y :

$$\begin{cases} \mathbf{U} \triangleq [\mathbf{u}_1, \dots, \mathbf{u}_L] = [\mathbf{d}(x(1)), \dots, \mathbf{d}(x(L))] \\ \mathbf{V} \triangleq [\mathbf{v}_1, \dots, \mathbf{v}_L] = [\mathbf{d}(y(1)), \dots, \mathbf{d}(y(L))] \end{cases}$$
- Marginal dependence measure from empirical covariance matrix:

$$\hat{\mathbf{C}}_{u,v} = \frac{1}{L-1} \mathbf{U} (\mathbf{I} - \frac{1}{L} \mathbf{1}\mathbf{1}^T) \mathbf{V}^H \implies \|\hat{\mathbf{C}}_{u,v}\|_F^2 = \frac{1}{(L-1)^2} \text{Tr}(\mathbf{P} \mathbf{U}^H \mathbf{U} \mathbf{P} \mathbf{V} \mathbf{V}^H) \quad (2)$$

Data centering matrix

Unbounded dimension

$$\|\hat{\mathbf{C}}_{u,v}\|_F^2 \xrightarrow{M \rightarrow \infty} \text{HSIC}(\{x(l)\}; \{y(l)\}) \triangleq \lim_{M \rightarrow \infty} \frac{1}{(L-1)^2} \text{Tr}(\mathbf{P} \mathbf{K} \mathbf{P} \mathbf{Q}) \quad (3)$$

$$\begin{cases} \mathbf{K} \triangleq \lim_{M \rightarrow \infty} \mathbf{U}^H \mathbf{U} \\ \mathbf{Q} \triangleq \lim_{M \rightarrow \infty} \mathbf{V}^H \mathbf{V} \end{cases} \implies [\mathbf{K}]_{l,l'} = \lim_{M \rightarrow \infty} \mathbf{d}^H(x(l)) \mathbf{d}(x(l')) = \kappa(x(l) - x(l'))$$

$$\kappa(\diamond) \triangleq \int_{-\infty}^{\infty} G^2(f) e^{-j2\pi f \diamond} df$$

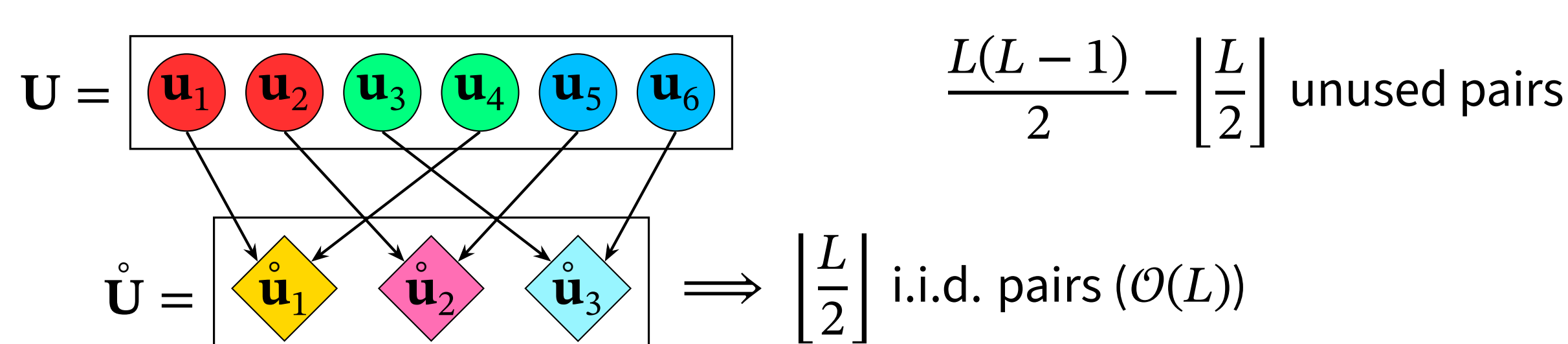
- E.g. Universal Gaussian kernel: $\kappa(\diamond) = \exp(-(\diamond/(\partial L^{-1/5}))^2)$

SAMPLE COVARIANCE MATRIX AS INCOMPLETE U-STATISTIC

- L samples $\implies K_{\max} \triangleq \frac{L(L-1)}{2}$ unique pairs.
- Orderings $f_1(k)$ and $f_2(k)$ for $1 \leq k \leq K \leq K_{\max}$.
- Pairwise differences: $\hat{\mathbf{u}}_k \triangleq \frac{\mathbf{u}_{f_1(k)} - \mathbf{u}_{f_2(k)}}{\sqrt{2}}$, $\hat{\mathbf{v}}_k \triangleq \frac{\mathbf{v}_{f_1(k)} - \mathbf{v}_{f_2(k)}}{\sqrt{2}}$.
- Sample cross-covariance between virtual sources $\hat{\mathbf{u}}$ and $\hat{\mathbf{v}}$:

$$\begin{cases} \hat{\mathbf{U}} \triangleq [\hat{\mathbf{u}}_1, \dots, \hat{\mathbf{u}}_K] \\ \hat{\mathbf{V}} \triangleq [\hat{\mathbf{v}}_1, \dots, \hat{\mathbf{v}}_K] \end{cases} \implies \hat{\mathbf{C}}_{\hat{\mathbf{u}}, \hat{\mathbf{v}}} = \frac{1}{K} \hat{\mathbf{U}} \hat{\mathbf{V}}^H \quad (\text{incomplete U-Statistic}) \quad (4)$$
- $K = K_{\max} \implies \hat{\mathbf{C}}_{\hat{\mathbf{u}}, \hat{\mathbf{v}}} \equiv \hat{\mathbf{C}}_{u,v}$ (complete).

Robustness to pruning



CONDITIONAL DEPENDENCE VIA U-STATISTICS

- Conditional cross-covariance matrix: $\mathbf{C}_{u,v|z} \triangleq \int_{\mathbb{R}} \mathbf{C}_{\hat{\mathbf{u}}, \hat{\mathbf{v}}|z=z} dF_z(z)$.
- Virtual random variable: $\hat{z} \triangleq z_1 - z_2$, with independent $z_1, z_2 \sim z$.
- Alternative conditioning:

$$\begin{aligned} \mathbf{C}_{u,v|z} &= \iint_{\mathbb{R}^2} \mathbf{C}_{\hat{\mathbf{u}}, \hat{\mathbf{v}}|z_1=z_2} dF_z(z_1) dF_z(z_2) = \iint_{\mathbb{R}^2} \mathbf{C}_{\hat{\mathbf{u}}, \hat{\mathbf{v}}|z=0} dF_z(z_1) dF_z(z_2) \\ &= \mathbf{C}_{\hat{\mathbf{u}}, \hat{\mathbf{v}}|z=0} \cdot \iint_{\mathbb{R}^2} dF_z(z_1) dF_z(z_2) = \mathbf{C}_{\hat{\mathbf{u}}, \hat{\mathbf{v}}|z=0} \end{aligned} \quad (5)$$

- Data pruning controlled by close samples of z :

$$\text{sort}_{\uparrow} |z(l) - z(l')|, \quad \forall l \neq l' \implies \{f_1(k), \{f_2(k)\} \implies \hat{\mathbf{C}}_{\hat{\mathbf{u}}, \hat{\mathbf{v}}|z}$$

$$1 \leq \alpha \ll (L-1) \implies K = \lfloor L\alpha/2 \rfloor$$

Conditional HSIC

- Conditional dependence measure: $\|\hat{\mathbf{C}}_{\hat{\mathbf{u}}, \hat{\mathbf{v}}|z}\|_F^2 = \frac{1}{K^2} \text{Tr}(\hat{\mathbf{U}}^H \hat{\mathbf{U}} \hat{\mathbf{V}}^H \hat{\mathbf{V}})$.
- Asymptotically, it approaches the C-HSIC:

$$\|\hat{\mathbf{C}}_{\hat{\mathbf{u}}, \hat{\mathbf{v}}|z}\|_F^2 \xrightarrow{M \rightarrow \infty} \text{C-HSIC}_{\alpha}(\{x(l)\}; \{y(l)\}) \triangleq \frac{1}{4K^2} \text{Tr}(\tilde{\mathbf{K}} \tilde{\mathbf{Q}}) \quad (6)$$

$$\begin{cases} \tilde{\mathbf{K}} \triangleq \mathbf{K}_{1,1} + \mathbf{K}_{2,2} - \mathbf{K}_{1,2} - \mathbf{K}_{1,2}^H \longrightarrow [\mathbf{K}_{\diamond, \blacklozenge}]_{k,k'} = \kappa(x(f_{\diamond}(k)) - x(f_{\blacklozenge}(k'))) \\ \tilde{\mathbf{Q}} \triangleq \mathbf{Q}_{1,1} + \mathbf{Q}_{2,2} - \mathbf{Q}_{1,2} - \mathbf{Q}_{1,2}^H \longrightarrow [\mathbf{Q}_{\diamond, \blacklozenge}]_{k,k'} = \kappa(y(f_{\diamond}(k)) - y(f_{\blacklozenge}(k'))) \end{cases} \quad (7)$$

Numerical illustration

$$\mathcal{M}^+ : \begin{cases} I(x; y) \geq 0 \\ I(x; y|z) = 0 \end{cases}, \quad \mathcal{M}^- : \begin{cases} I(x; y) = 0 \\ I(x; y|z) \geq 0 \end{cases} \quad (8)$$

Figure 1. Model $\mathcal{M}^+$.

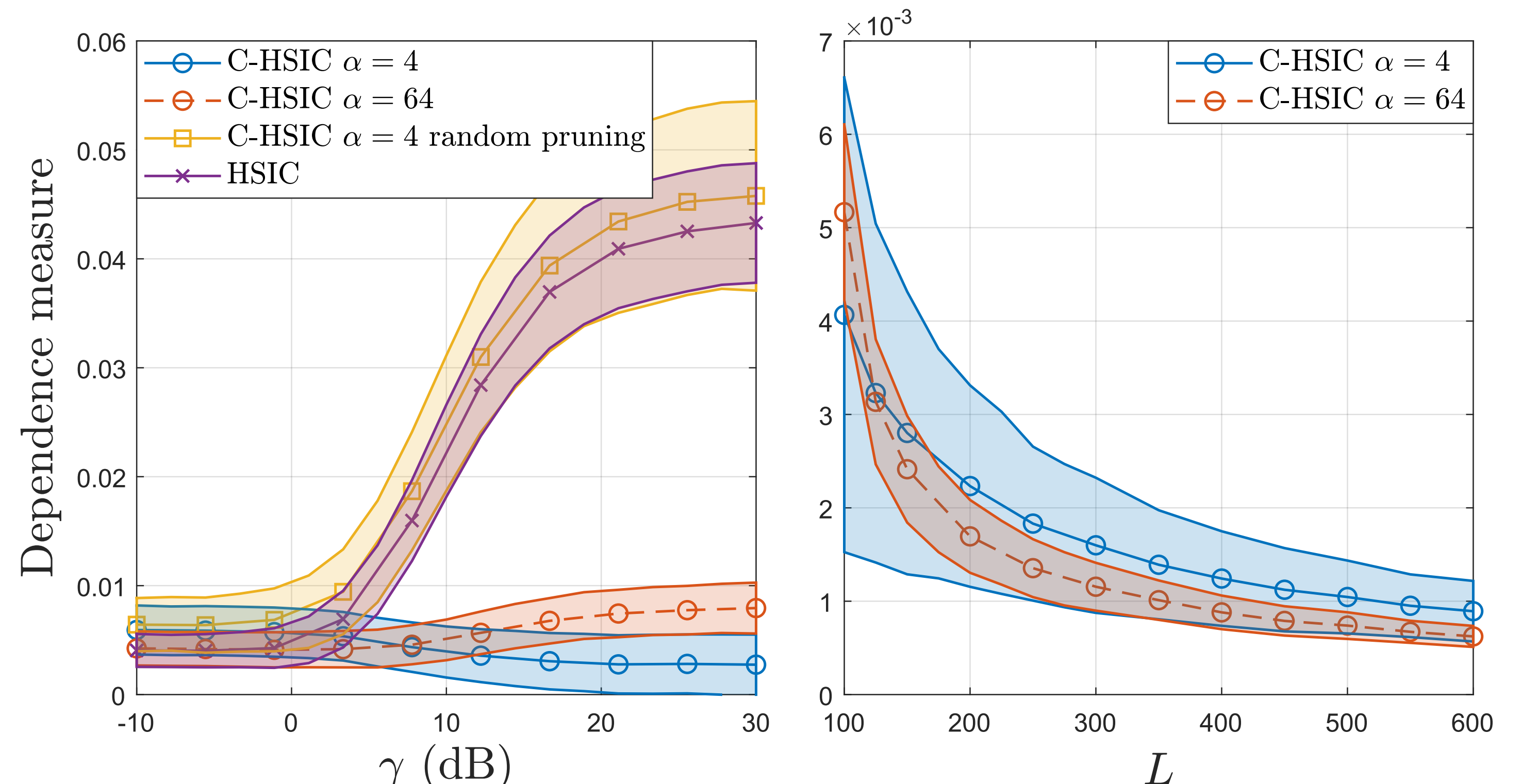
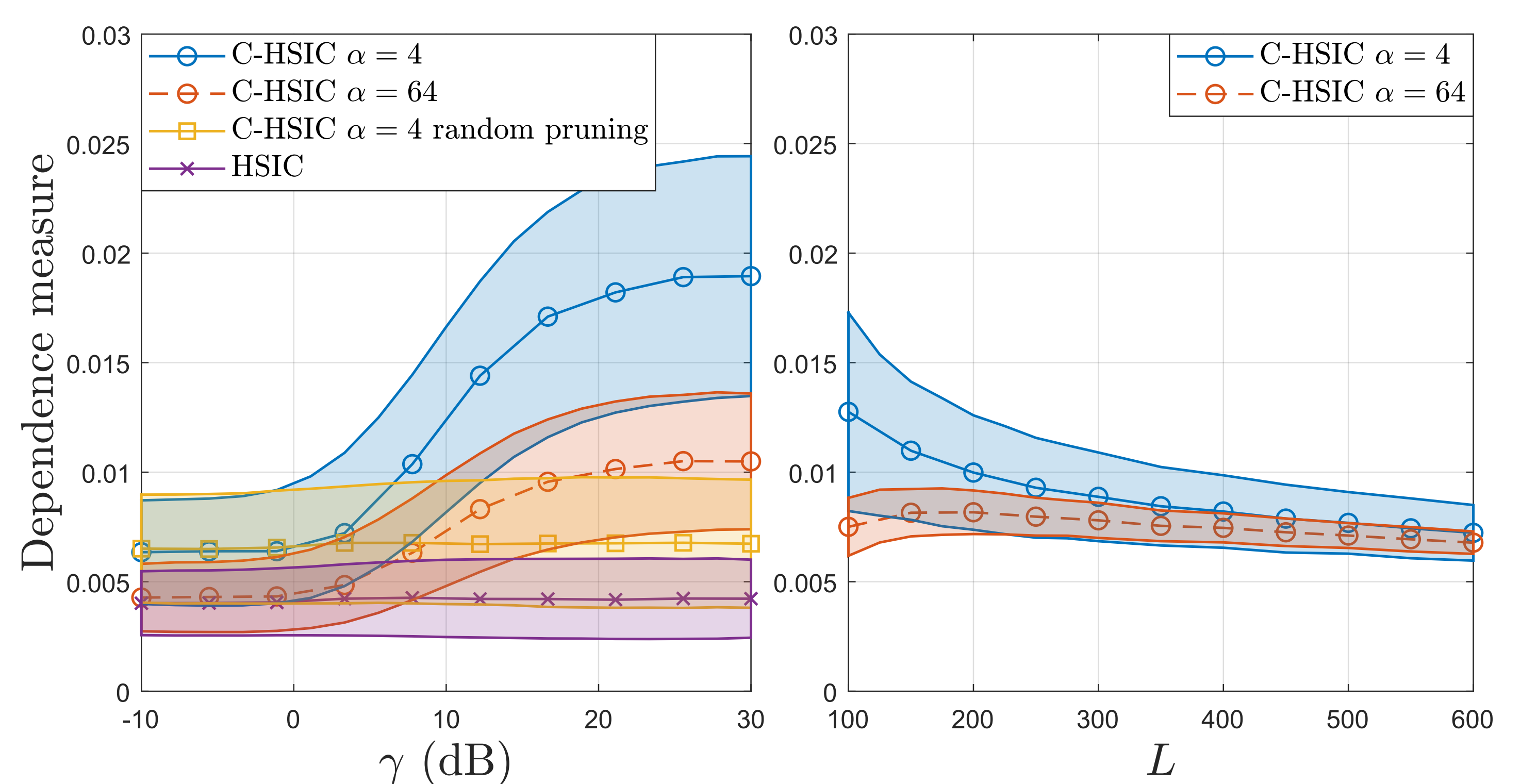


Figure 2. Model $\mathcal{M}^-$.



F. de Cabrera, M. Vilà-Insa, and J. Riba, "Conditional dependence via U-Statistics pruning," *IEEE Signal Processing Letters*, vol. 32, pp. 981–985, 2025, issn: 1558-2361. doi: 10.1109/lsp.2025.3539587

References

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- M. Vila and J. Riba, "A test for conditional correlation between random vectors based on weighted U-Statistics," in *ICASSP 2022 - 2022 IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP)*, IEEE, May 2022, pp. 5792–5796. doi: 10.1109/icassp43922.2022.9747042.

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