Supplemental material: Multiple testing of conditional independence hypotheses using information-theoretic approach

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1 Proofs of Lemma 1 and Theorem 1

Lemma 1. *We have (i)*

$$JMI = 0 \iff H_0 = \cap_i H_{0i} \text{ holds.}$$

(ii) The following representation is valid

$$JMI = I(X,Y) + \frac{1}{p}\sum_{i=1}^{p}(I(X,Z_i|Y) - I(X,Z_i))$$

(iii)

$$\frac{1}{2}\sum_{i=1}^{p}\Big(\sum_{x,y,z_i}|p(x,y,z_i) - p(x|z_i)p(y|z_i)p(z_i)|\Big)^2 \le p\times JMI \le \sum_{i=1}^{p}\log(\chi_i^2+1)$$

and both inequalities are tight when H_0 holds.

Proof. The proof of (i) is almost immediate in the view of our short discussion of properties of CMI. Namely, as the summands in the definition of JMI are non-negative, JMI equals 0 only when all $I(X,Y|Z_i)$ are 0 and this is equivalent to $X \perp Y|Z_i$ for $i = 1,\ldots,p$ in the view of information inequality (see Cover and Thomas (2006)). The proof of (ii) follows by applying chain rule (4) twice.
In order to prove (iii) observe that concavity of logarithmic function and Jensen's inequality imply for any $i = 1,\ldots,p$

$$\begin{aligned} I(X,Y|Z_i) &= \sum_{x,y,z_i} p(x,y,z_i)\log\Big(\frac{p(x,y|z_i)}{p(x|z_i)p(y|z_i)}\Big) \le \log\Big(\sum_{x,y,z_i}\frac{p^2(x,y,z_i)}{p(x|z_i)p(y|z_i)p(z_i)}\Big) \\ &= \log\Big(\sum_{x,y,z_i}\frac{(p(x,y,z_i)-p(x|z_i)p(y|z_i)p(z_i))^2}{p(x|z_i)p(y|z_i)p(z_i)} + 1\Big) = \log(\chi_i^2+1). \end{aligned}$$

Summing over $i = 1,\ldots,p$ yields the RHS inequality. LHS is a direct consequence of Pinsker inequality (cf. e.g. Tsybakov (2009)).

Theorem 1. *(i) Assume that the global null H_0 holds. Then*

$$2n\widehat{JMI} \xrightarrow{d} \sum_{i=1}^{K}\lambda_i(M)Z_i^2, \tag{1}$$

where Z_i are independent $N(0,1)$ random variables and $\lambda_i(M), i=1,\ldots,K$ are eigenvalues of matrix M with the elements

$$M_{x,y,z}^{x',y',z'} = \frac{1}{p}p(x',y',z')\sum_{i=1}^{p}\Bigg[\frac{\mathbb{I}(z_i=z_i')}{p(z_i)} - \frac{\mathbb{I}(x=x',z_i=z_i')}{p(x,z_i)} - \frac{\mathbb{I}(y=y',z_i=z_i')}{p(z_i)} + \frac{\mathbb{I}(x=x',y=y',z_i=z_i')}{p(x,y,z_i)}\Bigg]. \quad (2)$$

Moreover, the trace of M equals $p^{-1}(|\mathcal{X}|-1)(|\mathcal{Y}|-1)\sum_i|\mathcal{Z}_i|$.
(ii) Assume that the alternative $H_1=\cup_{i=1}^{p}H_{0,i}^c$ to the global null is valid and Y is binary. Then

$$\sigma^2_{\widehat{JMI}} = \mathrm{Var}\Big(\frac{1}{p}\log\prod_{i=1}^{p}\frac{p(X,Y,Z_i)p(Z_i)}{p(X,Z_i)p(Y,Z_i)}\Big) > 0$$

and

$$n^{1/2}(\widehat{JMI}-JMI)\xrightarrow{d}N(0,\sigma^2_{\widehat{JMI}}) \quad (3)$$

Proof. (i) Let $f(p)=p^{-1}\sum_{i=1}^{p}p(x,y,z_i)\log(p(x,y,z_i)p(z_i)/p(x,z_i)p(y,z_i))$, where $p=p(x,y,z_1,\ldots,z_p)$. Note that when H_0 holds then $\sigma^2_{\widehat{JMI}}=0$ and it follows from the delta method (cf Corollary 1 in Kubkowski et al. (2020)) that the asymptotic distribution of $2n\widehat{JMI}$ is the distribution of Z^TMZ where $Z\in R^p$ has $N(0,I)$ distribution, $M=H\Sigma$, $\Sigma_{xyz}^{x'y'z'}=p(x',y',z')(I(x=x',y=y',z=z')-p(x,y,z))/n$ and $H=D^2f(p)$ is the Hessian of $f(p)$. By direct calculation we have

$$Df(p)_{xyz} = \frac{1}{p}\sum_{i=1}^{p}\log\left(\frac{p(x,y,z_i)p(z_i)}{p(x,z_i)p(y,z_i)}\right),$$

where $z=(z_1,\ldots,z_p)$

$$H_{xyz}^{x'y'z'} = D^2f(p)_{xyz}^{x'y'z'} = \frac{1}{p}\sum_{i=1}^{p}\Bigg[\frac{\mathbb{I}(z_i=z_i')}{p(z_i)} - \frac{\mathbb{I}(x=x',z_i=z_i')}{p(x)} - \frac{\mathbb{I}(y=y',z_i=z_i')}{p(z_i)} + \frac{\mathbb{I}(x=x',y=y',z_i=z_i')}{p(x,y,z_i)}\Bigg]$$

and M is obtained by the direct multiplication of H and Σ resulting in (2). The trace of M equals

$$\frac{1}{p}\sum_{i=1}^{p}\sum_{x,y,z}\left(p(x,y|z_i)-p(y|z_i)+1\right),$$

thus after performing summations we obtain the value given above.
(ii) is proved in Corollary 1 in Kubkowski et al (2020).

2 Supplementary figures

Figures 1 and 2 show the behaviour of the true asymptotic distribution of $\widehat{JMI}$ and its estimate.The left column depicts boxplots of sorted eigenvalues $\lambda_i(\hat{M})$ and compares them with $\lambda_i(M)$. The middle column compares averaged CDFs corresponding to $\lambda_i(\widehat{M})$ and 90% confidence bands for the true CDF based on them with the true asymptotic CDF and the empirical CDF based on $\widehat{JMI}$ values. The right column shows actual type I errors versus the assumed level α based on $N=5000$ repetitions of the experiment. In Figure 1, we show again the results from the main text for Model B and estimated type I errors and we added remaining results for Model A and C. In Figure 2 we show the results for independent variables X, Y and

$Z_1, Z_2, \ldots, Z_p$ sampled from Bernoulli distribution with probability of success 0.5 for $p = 3, 5, 7$. The results are based on $N = 5000$ experiments.

Figure 3 shows ROC-type curves for all three procedures considered in the article. ROC-type curves are based on two models: the one for which H_0 holds and the second for which H_1 is true, and the report *the actual* type I error and the power approximated by means of simulations for varying α. In this way y values of three ROC curves for the fixed x value correspond to the power for *the same* actual type I error.

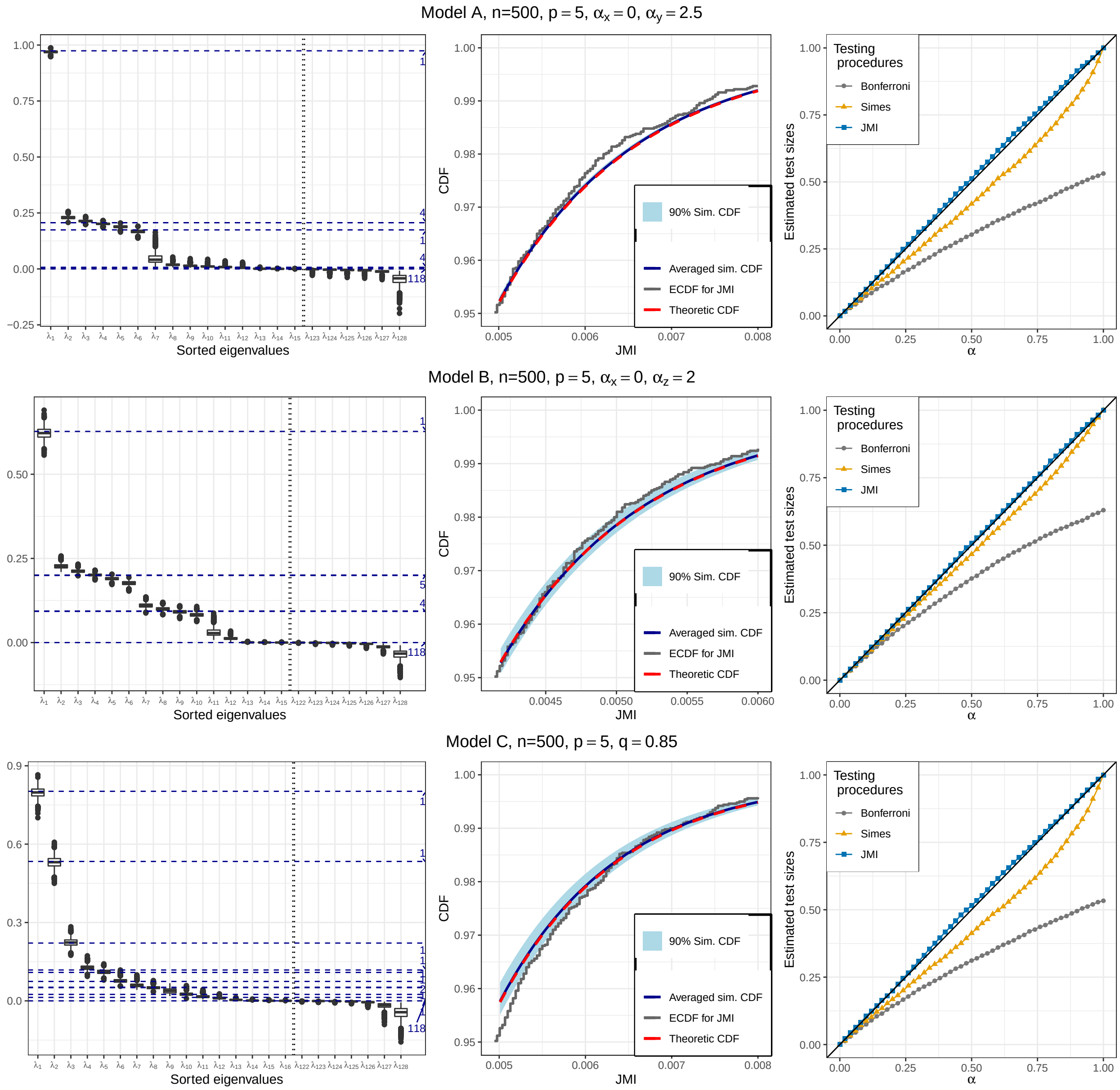

Fig. 1: Left panel: Box-plots of the empirical values $\lambda_i(\widehat{M}), i = 1, \ldots, 128$ for Models A, B and C based on $N = 5000$ repetitions. True eigenvalues are marked by the horizontal lines and are equal to

- 0.974 (multiplicity 1), 0.206 (multiplicity 4), 0.174 (multiplicity 1), 0.006 (multiplicity 4), 0 (multiplicity 118) for Model A,
- 0.627 (multiplicity 1), 0.2 (multiplicity 5), 0.093 (multiplicity 4), 0 (multiplicity 118) for Model B,
- 0.013, 0.025, 0.051, 0.052, 0.074, 0.109, 0.118, 0.221, 0.534, 0.802, (multiplicity 1), 0 (multiplicity 118) for Model C.

The central panel: values of theoretical CDF, the empirical CDF of $\widehat{JMI}$ and the average of CDFs corresponding to $\lambda_i(\hat{M})$ for the values of JMI grater than 0.95 quantile of $\widehat{JMI}$. Right panel: Actual type I errors against assumed level α.

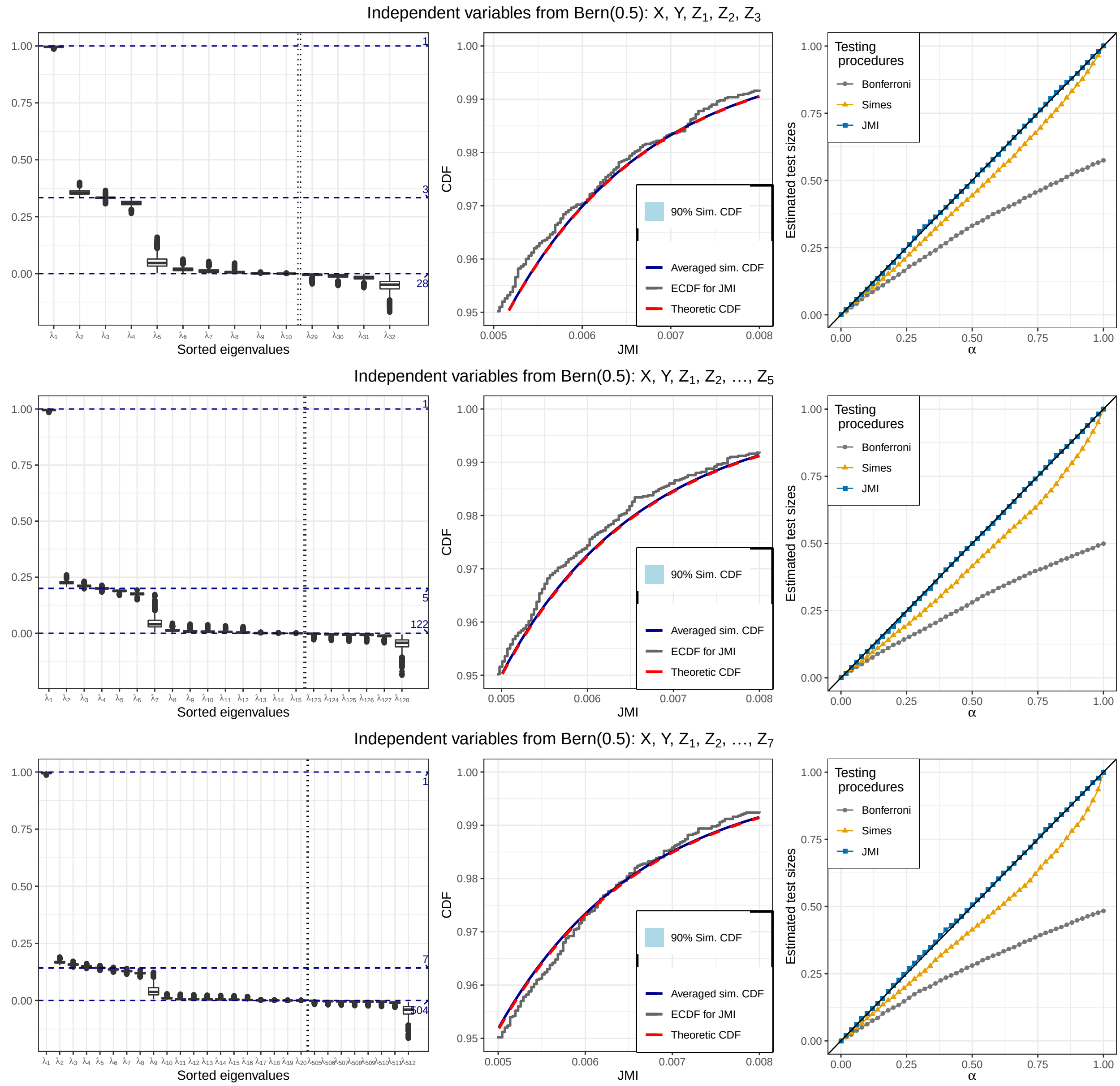

Fig. 2: Left panel: Box-plots of the empirical values $\lambda_i(\hat{M})$, $i = 1, \ldots, 2^{p+2}$ for a model, in which X, Y, $Z_1, Z_2, \ldots, Z_p$ for $p = 3, 5, 7$ are iid Bernoulli variables with probability of success 0.5 based on $N = 5000$ repetitions. True eigenvalues are marked by the horizontal lines and are equal to

- 1 (multiplicity 1), 0.333 (multiplicity 3), 0 (multiplicity 28) for $p = 3$,
- 1 (multiplicity 1), 0.2 (multiplicity 5), 0 (multiplicity 122) for $p = 5$,
- 1 (multiplicity 1), 0.143 (multiplicity 5), 0 (multiplicity 504) for $p = 7$.

The central panel: values of theoretical CDF, the empirical CDF of $\widehat{JMI}$ and the average of CDFs corresponding to $\lambda_i(\hat{M})$ for the values of JMI greater than 0.95 quantile of $\widehat{JMI}$. Right panel: Actual type I errors against assumed level α. The setting corresponds to Model A with parameters: $\alpha_x = 0$, $\alpha_y = 0$ and Model B with parameters $\alpha_z = 0$ and any α_x for $p = 3, 5, 7$.

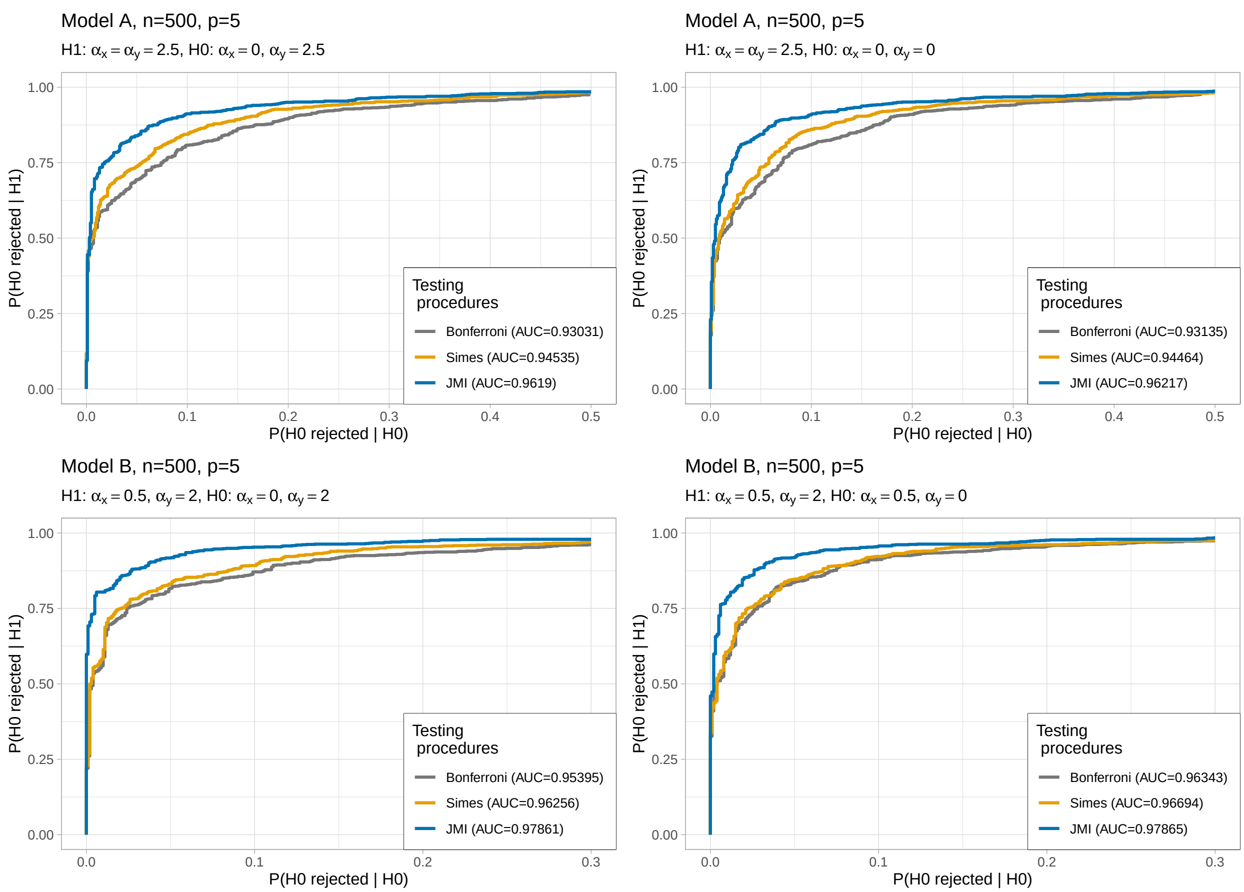

Fig. 3: ROC-type curves and the corresponding values of AUC for models A, B and C for H_0 and H_1 indicated in headers. In the first column null hypotheses indicates that X is independent of Y and all Z_i, in the second all variables are pairwise independent. The results are based on $N = 1000$ tests for the data generated from a model, in which H0 holds and $N = 1000$ tests for the data sampled from a model, in which H0 is violated. In both cases sample sizes equal $n = 500$. Plots in the first column are also shown in the main text.

References

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