Consistency of the Maximal Information Coefficient Estimator

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Abstract

The Maximal Information Coefficient (MIC) of Reshef et al. [Res11] is a statistic for measuring dependence between variable pairs in large datasets. In this note, we prove that MIC is a consistent estimator of the corresponding population statistic MIC_*. This corrects an error in an argument of Reshef et al. [RRF$^+$16], which we describe.

1 Introduction

The Maximal Information Coefficient (MIC) of n two-dimensional data points is a statistic introduced by Reshef et al. [RRF$^+$11] for measuring the dependence between pairs of variables. In later work [RRF$^+$16], the authors introduced the MIC_* statistic, which is defined analogously to MIC but for jointly-distributed pairs of random variables. Both statistics are based upon measuring the mutual information of the discrete distributions specified by imposing finite grids over the data (respectively, the joint distributions).

Given a dataset D_n of n points drawn iid from a jointly-distributed pair of random variables (X, Y), the authors of [RRF$^+$16] sought to show that the MIC statistic is a *consistent estimator* of MIC_* (i.e., that $\text{MIC}(D_n)$ converges in probability to $\text{MIC}_*(X, Y)$ as $n \to \infty$). In this note, we identify and correct an error in an argument of [RRF$^+$16] related to proving this consistency. Our new proof modifies the original approach of Reshef et al., but the result is slightly weaker than the originally-desired claim (the set of parameters for which the consistency holds is smaller). It is left open whether the full consistency claim of [RRF$^+$16] can be recovered.

After introducing some notation in Section 2, we describe the flaw in the original argument of Reshef et al. in Section 3, and then we provide our new proof of consistency in Section 4.

2 Preliminaries

We primarily adopt the notation used by Reshef et al. [RRF$^+$16], and we summarize a few key pieces here. For the sake of brevity, readers should refer to the original paper of Reshef et al. for exact definitions of the MIC and MIC_* statistics.

Let (X, Y) denote a pair of jointly-distributed random variables, and let D_n be a sample of n points drawn iid from (X, Y). If G is a grid partition with $k \geq 2$ rows and $\ell \geq 2$ columns, then $(X,Y)|_G$ denotes the discrete distribution induced by (X,Y) on the $k\ell$ cells of G. We let M denote the MIC$_*$ population characteristic matrix for (X,Y), and we let $\widehat{M}$ denote the MIC sample characterisic matrix for D_n. We say that a grid partition Γ is an *equipartition* of (X,Y) if all rows of $(X,Y)|_\Gamma$ have equal probability mass and all columns of $(X,Y)|_\Gamma$ have equal probability mass. The total variation distance between distributions Π and Ψ is given by

$$D_{\mathrm{TV}}(\Pi,\Psi) = \tfrac{1}{2}\|\Pi - \Psi\|_1.$$

We use $I(X,Y)$ to denote the mutual information of a jointly-distributed pair of random variables (X,Y).

3 Flaw in Original Argument

Here we point out the error in the proof of Lemma 37 from [RRF+16, Appendix A] in the paragraph with header "*Bounding the* $\epsilon_{i,j}$" .

To provide context, we consider a jointly-distributed pair of random variables (X,Y) and a dataset D_n of n points drawn iid from (X,Y) for some $n > 0$. Let Γ be an equipartition of (X,Y) with $kn^{\epsilon/4}$ rows and $\ell n^{\epsilon/4}$ columns for some $k,\ell \geq 2$ and $\epsilon > 0$. Let $C(n) = k\ell n^{\epsilon/2}$ denote the total number of cells in Γ. So $\Pi = (X,Y)|_\Gamma$ and $\Psi = D_n|_\Gamma$ are discrete distributions, and we let $\pi_{i,j}$ and $\psi_{i,j}$ denote their PMFs respectively. Note also that because the n points of D_n are drawn iid from (X,Y), for any cell (i,j) the quantity $n\psi_{i,j}$ is the sum of n iid Bernoulli random variables with mean $\pi_{i,j}$, and so $\mathrm{E}[n\psi_{i,j}] = n\pi_{i,j}$.

The purpose of Lemma 37 is to give a uniform bound on the absolute difference $|I(D_n|_G) - I((X,Y)|_G)|$ for all $k \times \ell$ grids G that holds with high probability. The strategy of the original authors is to obtain this bound by introducing the "common" equipartition grid Γ. The main consequence of the error in Lemma 37 is that the probabilistic guarantee of the subsequent Lemma 38 does not hold as stated, which prevents the overall argument of consistency from going through. We start by pointing out the error in the proof of Lemma 37 before showing an example of its consequences on Lemma 38.

Error in Lemma 37 For every (i,j), the authors define $\epsilon_{i,j} = (\psi_{i,j} - \pi_{i,j})/\pi_{i,j}$, and so

$$|\epsilon_{i,j}| = \left|\frac{\psi_{i,j} - \pi_{i,j}}{\pi_{i,j}}\right| \;\geq\; \delta \quad \Longrightarrow \quad |n\psi_{i,j} - n\pi_{i,j}| \;\geq\; \delta \cdot n\pi_{i,j}. \tag{1}$$

Given that $n\psi_{i,j}$ is the sum of n iid Bernoulli RVs, the authors state the following multiplicative Chernoff bound:

$$\begin{aligned} \Pr[\,|\epsilon_{i,j}| \geq \delta\,] \;=\; \Pr[\,|\psi_{i,j} - \pi_{i,j}| \geq \delta \cdot \pi_{i,j}\,] \;&=\; \Pr[\,|n\psi_{i,j} - n\pi_{i,j}| \geq \delta \cdot n\pi_{i,j}\,] && (2)\\ &\leq\; \exp\left(-\Omega(n\pi_{i,j}\delta^2)\right). && (3) \end{aligned}$$

For reference, we state below the standard two-sided Chernoff bound from Corollary 4.6 in [MU05], which says that

$$\Pr\left[\,|n\psi_{i,j} - n\pi_{i,j}| \geq \delta \cdot n\pi_{i,j}\,\right] \leq 2\exp\left(-\frac{n\pi_{i,j}\cdot\delta^2}{3}\right) \tag{4}$$

for any $0 < \delta < 1$.

Now, the authors set $\delta = \sqrt{\pi_{i,j}}/C(n)^{0.5+\alpha}$ for some $\alpha \geq 0$. Applying the bound from (3) with this value of δ, the authors write

$$\Pr\left[\ |\epsilon_{i,j}|\ \geq\ \frac{\sqrt{\pi_{i,j}}}{C(n)^{0.5+\alpha}}\ \right]\ \leq\ \exp\left(-\Omega\left(\frac{n}{C(n)^{1+2\alpha}}\right)\right), \tag{5}$$

which incorrectly drops a dependence on $\pi_{i,j}$.

A correct application of the true Chernoff bound from (4) instead yields

$$\Pr\left[\ |\epsilon_{i,j}|\ \geq\ \frac{\sqrt{\pi_{i,j}}}{C(n)^{0.5+\alpha}}\ \right] = \Pr\left[\ |n\psi_{i,j} - n\pi_{i,j}|\ \geq\ \frac{\sqrt{\pi_{i,j}}}{C(n)^{0.5+\alpha}}\cdot n\pi_{i,j}\ \right] \tag{6}$$

$$\leq 2\exp\left(-\frac{n\pi_{i,j}}{3}\cdot\frac{\pi_{i,j}}{C(n)^{1+2\alpha}}\right) \tag{7}$$

$$\leq 2\exp\left(-\Omega\left(\frac{n\cdot(\pi_{i,j})^2}{C(n)^{1+2\alpha}}\right)\right). \tag{8}$$

Compared to (5), the term in (8) resulting from the correct application of the Chernoff bound has a dependence on $\pi_{i,j}$. This means that the bound on the error probability of $|\epsilon_{i,j}| \geq \delta$ becomes non-negligible as the value of some $\pi_{i,j}$ goes to 0. We note that since the number of grid cells (i,j) increases with n by the definition of Γ, the value of any $\pi_{i,j}$ can decrease with n. When this occurs, we expect the bound on the probability in (8) to grow undesirably large.

Ramifications on Lemma 38 Using the corrected error probability from (8) for a single $\epsilon_{i,j}$ and taking a union bound over all (i,j) means that the statement of Lemma 37 now holds with total error probability at most

$$2\sum_{(i,j)}\exp\left(-\Omega\left(\frac{n(\pi_{i,j})^2}{C(n)^{1+2\alpha}}\right)\right). \tag{9}$$

This updated probability seems to prevent the proof (as written) of Lemma 38 in [RRF+16] from working in general.

For example, consider the special case where X and Y are independent. Then the discrete distribution $\Pi = (X,Y)|_\Gamma$ has PMF $\pi_{i,j} = 1/C(n)$ for all (i,j) given that Γ is an equipartition.

The overall error term from Lemma 37 in (9) can be rewritten then as

$$2\sum_{(i,j)}\exp\left(-\Omega\left(\frac{(n\cdot(1/C(n))^2}{C(n)^{1+2\alpha}}\right)\right)\ =\ 2\cdot C(n)\exp\left(-\Omega\left(\frac{n}{C(n)^{3+2\alpha}}\right)\right). \tag{10}$$

Now in Lemma 38, the authors consider $k\ell \leq B(n) = O(n^{1-\epsilon})$, and since $C(n) = k\ell n^{\epsilon/2}$, we have

$$C(n) \leq B(n)\cdot n^{\epsilon/2} = O(n^{1-\epsilon/2}) \tag{11}$$

as written on page 34. But this means

$$C(n)^{3+2\alpha} = O\left(n^{(1-\epsilon/2)\cdot(3+2\alpha)}\right). \tag{12}$$

The current strategy in the proof of Lemma 38 relies on bounding the error term in (10) as

$$2 \cdot C(n) \exp\left(-\Omega\left(\frac{n}{C(n)^{3+2\alpha}}\right)\right) \;\le\; O(n) \exp\left(-\Omega\left(n^{u}\right)\right) \tag{13}$$

for some $u > 0$. To achieve such a bound requires $C(n)^{3+2\alpha} = o(n)$, and in turn this requires from (12) that

$$(1-\epsilon/2)(3+2\alpha) = \left(\frac{2-\epsilon}{2}\right)(3+2\alpha) \le 1. \tag{14}$$

Simplifying yields the constraint

$$2\alpha \;\le\; \frac{2}{2-\epsilon} - 3 \;=\; \frac{3\epsilon-4}{2-\epsilon}, \tag{15}$$

and so to require $C(n)^{3+2\alpha} = o(n)$ means we must have

$$\alpha \le \frac{3\epsilon-4}{4-2\epsilon}\,. \tag{16}$$

Now for $0 < \epsilon < 1$, which corresponds to a value of $B(n) = O\left(n^{1-\epsilon}\right)$ which grows with n, we can verify that the right hand side of (16) is always negative. So to obtain the desired error term in (13) constrains α to be negative, which contradicts the requirement of $\alpha > 0$ used in earlier parts of the proof of Lemma 38.

So in the case where the joint distribution (X, Y) is formed by two independent random variables, using the corrected error bound from Lemma 37 in (10) renders the proof of Lemma 38 incorrect. Thus for general joint distributions (X, Y), we should not expect the current technique in the proof of Lemma 38 to work.

4 New Consistency Proof

We now outline an alternative approach to replace Lemmas 35-38 in [RRF+16, Appendix A], which are needed to prove the consistency of the MIC estimator in Theorem 6.

4.1 Overview of Argument

Our main goal is to prove a statement similar to Lemma 38 of [RRF+16], which probabilistically bounds the difference between corresponding entries of M and $\widehat{M}$:

Goal 1. *We want to show that there exists a function $B(n)$ that grows with n such that, for every joint distribution (X, Y) and n, if D_n is a sample of n points drawn iid from (X, Y), then*

$$|M_{k,\ell} - \widehat{M}_{k,\ell}| = o(1)$$

holds simultaneously for all $k\ell \le B(n)$ with probability at least $1 - o(1)$ (where the randomness is over the sampling that determines D_n and the asymptotics are defined wrt increasing n).

If we obtain Goal 1, then the proof of Theorem 6 [RRF+16, Appendix A] (which shows the consistency of the MIC estimator and relies on obtaining Goal 1) can remain unmodified.

4.1.1 Proof Sketch of Goal 1

Recall that for a fixed (k, ℓ) pair (and assuming wlog $k \le \ell$) we have

$$
\begin{aligned}
|M_{k,\ell} - \widehat{M}_{k,\ell}| &= \left| \max_{G:\, k\times\ell} \frac{I((X,Y)|_G)}{\log_2 k} \;-\; \max_{G:\, k\times\ell} \frac{I(D_n|_G)}{\log_2 k} \right| \\
&= \frac{1}{\log_2 k} \cdot \left| \max_{G:\, k\times\ell} I((X,Y)|_G) \;-\; \max_{G:\, k\times\ell} I(D_n|_G) \right| \\
&\le \max_{G:\, k\times\ell} \left| \, I((X,Y)|_G) \;-\; I(D_n|_G) \, \right| . \qquad (17)
\end{aligned}
$$

In other words, expression (17) shows that to bound the difference between $M_{k,\ell}$ and $\widehat{M}_{k,\ell}$, it is sufficient to bound the maximum difference in mutual information between the discrete distributions $(X,Y)|_G$ and $D_n|_G$ for a grid G of size at most $k \times \ell$.

So our strategy for Goal 1 is to first obtain such a bound on expression (17) for a fixed (k, ℓ) that holds with probability at least $1-p$, where $p = o(1/B^2(n))$. Then by taking a union bound over all $k\ell \le B(n)$ (which is at most $B^2(n)$ pairs) and by choosing the function $B(n)$ appropriately, the statement of Goal 1 will hold with total probability at least $1 - o(1)$.

The purpose of the original Lemmas 35-37 in [RRF+16] is to bound this maximum difference in mutual information from (17) for $k \times \ell$ grids, but here we will circumvent Lemma 37 and obtain our goal by adapting the original argument of Lemma 36. The result is a probabilistic $o(1)$ bound on the expression (17), but we note that the bound only holds for $k\ell \le B(n) = O(n^\alpha)$ where $0 < \alpha < 0.5$. This is a slightly weaker guarantee compared to the original statement of Lemma 38 and Theorem 6, which held for $k\ell \le B(n) = O(n^\alpha)$ for $0 < \alpha < 1$.

We first state the following variant of Lemma 36 from [RRF+16, Appendix A], which follows directly from the original proof of the lemma.

Lemma 2 (Variant of [RRF+16, Lemma 36]).

- *Let* Π *and* Ψ *be random variables.*
- *Let* Γ *be a grid with* C *cells.*
- *Let* G *be any grid with* $\beta < C$ *cells.*
- *Let* δ *(resp.* d*) be the total probability mass of* $\Pi|_\Gamma$ *(resp.* $\Psi|_\Gamma$*) falling in cells of* Γ *that are not contained in individual cells of* G*.*
- *Let* G' *be a sub-grid of* Γ *of* β *cells obtained by replacing every horizontal or vertical line in* G *that is not in* Γ *with a closest line in* Γ*.*

Then

$$
\begin{aligned}
|I(\Pi|_G) - I(\Psi|_G)| \;\le\; & O\left(\delta \log_2 (\beta/\delta)\right) \;+ \qquad (18)\\
& O\left(d \log_2 (\beta/d)\right) \;+ \qquad (19)\\
& |I(\Pi|_{G'}) - I(\Psi|_{G'})|. \qquad (20)
\end{aligned}
$$

To apply this lemma, we will suppose $\Pi = (X, Y)$ and (by slight abuse of notation) $\Psi = D_n$, and we consider any $k \times \ell$ grid G where $k\ell \le B(n) = O(n^\alpha)$ for some $\alpha > 0$. We will set Γ to be an *equipartition* of Π into kn^ϵ rows and ℓn^ϵ columns for any $\epsilon > 0$.

With these settings, we obtain a probabilistic bound on $|I(\Pi|_G) - I(\Psi|_G)|$ that holds for every $k \times \ell$ grid G *simultaneously* (where the probability is over the randomness of the sampled points D_n) by deriving probabilistic bounds on (18), (19), and (20) separately and applying a union bound.

Stated formally:

Lemma 3. *Let (X, Y) be a pair of jointly-distributed random variables and let D_n be a dataset of n points sampled iid from (X, Y). For any $\alpha > 0$ and any n, consider any pair (k, ℓ) where $\beta = k\ell \le B(n) = O(n^\alpha)$. Let Γ be an equipartition of (X, Y) into kn^ϵ rows, ℓn^ϵ columns, and $C(n) = k\ell n^{2\epsilon}$ total cells for any $\epsilon > 0$. For any grid G, let G' be a grid of equal size as defined in Lemma 2.*

Then the following probabilistic bounds hold simultaneously for every $k \times \ell$ grid G:

1. *with probability 1:*
$$\delta \le \frac{2}{n^\epsilon} \quad \Longrightarrow \quad O\left(\delta \log_2(\beta/\delta)\right) = O\left(\frac{\log_2 n}{n^\epsilon}\right) \tag{21}$$

2. *with probability at least $1 - p_d$ where $p_d := O(n^\alpha) \cdot e^{-\Omega(n^{1-\epsilon-\alpha})}$:*
$$d \le \frac{4}{n^\epsilon} \quad \Longrightarrow \quad O\left(d \log_2(\beta/d)\right) = O\left(\frac{\log_2 n}{n^\epsilon}\right) \tag{22}$$

3. *with probability at least $1 - p_{G'}$ where $p_{G'} := O(n^{\alpha+2\epsilon-3})$:*
$$|I((X,Y)|_{G'}) - I(D_n|_{G'})| \;=\; O\left(\phi \log_2\left(\frac{n^\alpha}{\phi}\right)\right) \tag{23}$$
where
$$\phi = O\left(\frac{n^{\alpha+2\epsilon} \cdot \log_2^{0.5} n}{n^{0.5}}\right). \tag{24}$$

Granting Lemma 3 as true and applying Lemma 2, we have the following corollary that results in a bound on our original target expression (17):

Corollary 4. *Let (X, Y) be a pair of jointly-distributed random variables and let D_n be a dataset of n points sampled iid from (X, Y), and let p_d and p'_G be defined as in Lemma 3.*

For every $0 < \alpha < 0.5$, there exists some $u > 0$ such that for all n and for all $k\ell \le B(n) = O(n^\alpha)$:
$$|I((X,Y)|_G) - I(D_n|_G)| \;=\; O\left(\frac{1}{n^u}\right) \tag{25}$$
holds for every $k \times \ell$ grid G simultaneously with probability at least
$$1 - (p_d + p_{G'}) \ge 1 - O(n^{-2.5}). \tag{26}$$

Proof. As in the statement of Lemma 3, let Γ be an equipartition of (X, Y) into kn^ϵ rows and ℓn^ϵ columns. When $0 < \alpha < 0.5$, any choice of $0 < \epsilon < 1/4 - \alpha/2$ ensures $\alpha + 2\epsilon < 0.5$, which means that expressions (21), (22), and (23) from Lemma 3 are all $O(n^{-u})$ for some positive constant $u < 0.5 - (\alpha + 2\epsilon)$. So for every $k\ell \le B(n) = O(n^\alpha)$, expression (25) of the corollary follows from applying Lemma 2 with these three bounds. The same setting of α and ϵ also means that $p_{G'} = O(n^{\alpha+2\epsilon-3}) = O(n^{-2.5})$ and $p_d = O(n^\alpha) \cdot e^{-\Omega(n^{1-\epsilon-\alpha})} = O(n^{-2.5})$ (since p_d is $o(n^{-c})$ for any $c > 0$), from which expression (26) of the corollary follows. □

We can now use Corollary 4 to formally state the following theorem which achieves our original Goal 1.

Theorem 5. *Let (X, Y) be a pair of jointly-distributed random variables and let D_n be a dataset of n points sampled iid from (X, Y). For every $0 < \alpha < 0.5$, there exists a constant $u > 0$ such that for all n:*

$$|M_{k,\ell} - \widehat{M}_{k,\ell}| = O\left(\frac{1}{n^u}\right) \tag{27}$$

holds for every (k, ℓ) pair where $k\ell \le B(n) = O(n^\alpha)$ simultaneously with probability at least $1 - O(n^{-1.5})$ (where the randomness is over the sampling that determines D_n).

Proof. Recall expression (17), which says that

$$|M_{k,\ell} - \widehat{M}_{k,\ell}| \;\le\; \max_{G:\, k\times\ell} \;|\; I((X,Y)|_G) \;-\; I(D_n|_G) \;|$$

for a fixed pair (k, ℓ). Then by Corollary 4, for every $0 < \alpha < 0.5$ and every n, there exists some $u > 0$ such that the right hand side of this expression is $O(n^{-u})$ with probability at least $1 - O(n^{-2.5})$ for every (k, ℓ) where $k\ell \le B(n) = O(n^\alpha)$. Given that there are at most $O(n^{2\alpha})$ pairs satisfying $k\ell \le O(n^\alpha)$, it follows from a union bound that $|M_{k,\ell} - \widehat{M}_{k,\ell}| = O(n^{-u})$ for *all* such (k, ℓ) pairs simultaneously with probability $1 - O(n^{2\alpha-2.5}) \ge 1 - O(n^{-1.5})$. □

This gives us the desired result of Goal 1, and it now remains to prove the three parts of Lemma 3.

4.2 Lemma 3 Proof: Parts 1 and 2

Recall that $\Pi = (X, Y)$, $\Psi = D_n$, Γ is an equiparition of Π with kn^ϵ rows and ℓn^ϵ columns, and G is a $k \times \ell$ grid where $k\ell \le B(n) = O(n^\alpha)$ for some $\alpha > 0$. We define δ (resp. d) to be the total mass of $\Pi|_\Gamma$ (resp. $\Psi|_\Gamma$) falling in cells of Γ that are not contained in individual cells of G.

We will prove parts 1 and 2 of Lemma 3 together, which say that:

1. $\delta \le (2/n^\epsilon)$ with probability 1.
2. $d \le (4/n^\epsilon)$ with probability at least $1 - p_d$, where $p_d := O(n^\alpha) \cdot e^{-\Omega(n^{1-\epsilon-\alpha})}$.

Our strategy will be to bound δ by δ', and then to show $d \le 2\delta'$ with probability all but p_d.

Chernoff Bounds [MU05, Chapter 4]

First, we (re)state two standard Chernoff bounds that will be used in this section and the next:

Let $X = X_1 + \dots X_n$, where each X_i is an iid Bernoulli RV with $\mathrm{E}[X_i] = \mu$.

i *Two-sided tail bound*: for any $0 < t < 1$:

$$\Pr\left[\, |X - n\mu| \geq t \cdot n\mu \,\right] \;\leq\; 2 \cdot \exp\left(-\frac{n\mu t^2}{3}\right) \tag{28}$$

ii *Upper tail bound*: for any $0 < t \leq 1$ and $\hat{\mu} \geq \mu = \mathrm{E}[X_i]$:

$$\Pr\left[\, X \geq (1+t) \cdot n\hat{\mu} \,\right] \;\leq\; \exp\left(-\frac{n\hat{\mu} t^2}{3}\right) \tag{29}$$

Bound on δ

By definition, δ is the sum of mass in a subset of columns and rows of $\Pi|_\Gamma$. Let $\pi_{i,j}$ denote the pmf at cell (i,j) of $\Pi|_\Gamma$, let $\pi_{i,*}$ denote the total mass of $\Pi|_\Gamma$ in row i, and let $\pi_{*,j}$ denote the total mass of $\Pi|_\Gamma$ in column j. So

$$\pi_{*,j} = \sum_i \pi_{i,j} = \frac{1}{\ell n^\epsilon}$$
$$\pi_{i,*} = \sum_j \pi_{i,j} = \frac{1}{k n^\epsilon}$$

by the definition of Γ as an equipartition of Π. Now let K be the column indices of Γ containing a column separator of G, and let R be the row indices of Γ containing a row separator of G. Since G is a $k \times \ell$ grid, we must have $|K| \leq \ell$ and $|R| \leq k$. Then (with probability 1):

$$\begin{aligned} \delta &\leq \sum_{j \in K} \pi_{*,j} + \sum_{i \in R} \pi_{i,*} \\ &\leq \ell \cdot \pi_{*,j} + k \cdot \pi_{i,*} \;=\; \frac{\ell}{\ell n^\epsilon} + \frac{k}{k n^\epsilon} \;=\; \frac{2}{n^\epsilon}. \end{aligned}$$

Bound on d with probability $1 - p_d$

Again by definition, d is the sum of mass in a subset of columns and rows of $\Psi|_\Gamma = D_n|_\Gamma$. We let $\psi_{i,j}$ denote the pmf at cell (i,j) of $\Psi|_\Gamma$, and we define $\psi_{*,j}$ and $\psi_{i,*}$ analogously to $\pi_{*,j}$ and $\pi_{i,*}$. We will show that each $\psi_{*,j} \leq 2\pi_{*,j}$ (respectively $\psi_{i,*} \leq 2\pi_{i,*}$) probabilistically.

Observe that $n \cdot \psi_{*,j}$ is a sum of n iid Bernoullis, each with mean $\pi_{*,j}$. So

$$\mathrm{E}[n \cdot \psi_{*,j}] \;=\; n \cdot \pi_{*,j} \;=\; \frac{n}{\ell n^\epsilon} \;=\; \frac{n^{1-\epsilon}}{\ell}. \tag{30}$$

Then by the Chernoff bound (29):

$$\begin{aligned} \Pr\left[n \cdot \psi_{*,j} \geq 2 \cdot (n^{1-\epsilon}/\ell)\right] &\leq \exp\left(-\frac{n^{1-\epsilon}}{3\ell}\right) \\ &\leq \exp\left(-\Omega\left(n^{1-\epsilon-\alpha}\right)\right), \end{aligned}$$

where the final inequality is due to $\ell = O(n^\alpha)$, which follows from the assumption that $k\ell = O(n^\alpha)$. So for each $j \in K$ we have $\psi_{*,j} \leq 2\pi_{*,j}$ with probability all but $e^{-\Omega(n^{1-\epsilon-\alpha})}$. A similar calculation shows that $\psi_{i,*} \leq 2\pi_{i,*}$ for each $i \in R$ with probability all but $e^{-\Omega(n^{1-\epsilon-\alpha})}$.

Combining the two inequalities and taking a union bound shows

$$\begin{aligned} d &\leq \sum_{j\in K} \psi_{*,j} + \sum_{i \in R} \psi_{i,*} \\ &\leq \sum_{j\in K} 2\pi_{*,j} + \sum_{i\in R} 2\pi_{i,*} \;\leq\; 2\left(\frac{2}{n^\epsilon}\right) \;=\; \frac{4}{n^\epsilon} \end{aligned}$$

with probability all but $p_d := O(n^\alpha) \cdot e^{-\Omega(n^{1-\epsilon-\alpha})}$, since $|K| + |R| \leq k + \ell \leq k\ell \leq O(n^\alpha)$ and by using the bound on δ previously established.

4.3 Lemma 3 Proof: Part 3

Recall that given the grid Γ (which is an equipartition of (X, Y) into kn^ϵ rows and ℓn^ϵ columns) and the $k \times \ell$ grid G, the grid G' is a $k \times \ell$ sub-grid of Γ obtained by replacing every horizontal or vertical line in G that is not in Γ with a closet line in Γ.

To prove an upper bound on the quantity $|I((X,Y)|_{G'}) - I(D_n|_{G'})|$, we will use Proposition 40 from Appendix B of [RRF+16], which relates the statistical distance between two discrete distributions to their change in mutual information:

Proposition 6 ([RRF+16, Proposition 40, Appendix B]). *Let Π and Ψ be discrete distributions over $k \times \ell$ grids. If $D_{TV}(\Pi, \Psi) \leq \delta$ for any $0 < \delta \leq 1/4$, then*

$$|I(\Pi) - I(\Psi)| \leq O\left(\delta \log_2\left(\frac{\min\{k, l\}}{\delta}\right)\right).$$

Because $D_{TV}(\Pi, \Psi) = \frac{1}{2}\|\Pi - \Psi\|_1$, and since G' is a subgrid of Γ, it follows by the triangle inequality that

$$D_{TV}((X,Y)|_{G'}, D_n|_{G'}) \;\leq\; D_{TV}((X,Y)|_\Gamma, D_n|_\Gamma).$$

Thus if we obtain a bound $D_{TV}((X,Y)|_\Gamma, D_n|_\Gamma) \leq \phi$, then applying Proposition 6 yields

$$|I((X,Y)|_{G'}) - I(D_n|_{G'})| = O\left(\phi \log_2\left(\frac{\min\{k,\ell\}}{\phi}\right)\right) = O\left(\phi \log_2\left(\frac{n^\alpha}{\phi}\right)\right)$$

by the assumption that $k\ell \leq B(n) = O(n^\alpha)$.

So given (X, Y), the dataset D_n, and the equipartition Γ of $C(n) = k\ell n^{2\epsilon}$ total cells, we will prove the following bound on $D_{TV}((X,Y)|_\Gamma, D_n|_\Gamma)$, which implies Part (3) of Lemma 3.

Lemma 7. *Let (X, Y) be a pair of jointly-distributed random variables and let D_n be a dataset of n points sampled iid from (X, Y). For any $\alpha > 0$ and any n, consider any pair (k, ℓ) where $k\ell \leq B(n) = O(n^\alpha)$. Let Γ be an equipartition of (X, Y) into kn^ϵ rows, ℓn^ϵ columns, and $C(n) = k\ell n^{2\epsilon}$ total cells for any $\epsilon > 0$. Then*

$$D_{TV}((X,Y)|_\Gamma, D_n|_\Gamma) = O\left(\frac{n^{\alpha+2\epsilon} \cdot \log_2^{0.5} n}{n^{0.5}}\right)$$

with probability at least $1 - O(n^{\alpha+2\epsilon-3})$.

Proof. Given (X, Y), a sample D_n of n points drawn iid from (X, Y), and the grid Γ, define the discrete distributions

$$\Pi = (X,Y)|_\Gamma \;\text{ with pmf }\; \pi_{i,j}$$
$$\Psi = D_n|_\Gamma \;\text{ with pmf }\; \psi_{i,j}$$

where $i \in [kn^\epsilon]$ and $j \in [\ell n^\epsilon]$ (note that the use of Π and Ψ here differs slightly from the previous subsection). Also, for every cell (i, j) of Γ, we say that

$$(i,j) \text{ is } \textit{large} \text{ if } \pi_{ij} > \frac{9\log_2 n}{n}$$
$$\text{and } (i,j) \text{ is } \textit{small} \text{ if } \pi_{ij} \le \frac{9\log_2 n}{n},$$

and let L and S denote the sets of *large* and *small* (i, j) cells, respectively.

Now recall that

$$\begin{aligned} D_{TV}(\Pi,\Psi) \;\le\; \|\,\Pi-\Psi\,\|_1 \;&=\; \sum_{(i,j)} |\pi_{i,j}-\psi_{i,j}| \\ &=\; \sum_{(i,j)\in L} |\pi_{i,j}-\psi_{i,j}| \;+\; \sum_{(i,j)\in S} |\pi_{i,j}-\psi_{i,j}|. \end{aligned} \tag{31}$$

By the triangle inequality, we have that

$$\begin{aligned} \sum_{(i,j)\in S} |\pi_{i,j}-\psi_{i,j}| \;&\le\; \sum_{(i,j)\in S} |\pi_{i,j}| + |\psi_{i,j}| \\ &=\; \sum_{(i,j)\in S} |\pi_{i,j}| + \sum_{(i,j)\in S} |\psi_{i,j}|, \end{aligned}$$

and substituting back into (31) gives

$$D_{TV}(\Pi,\Psi) \;\le\; \sum_{(i,j)\in L} |\pi_{i,j}-\psi_{i,j}| \;+\; \sum_{(i,j)\in S} |\pi_{i,j}| \;+\; \sum_{(i,j)\in S} |\psi_{i,j}|. \tag{32}$$

So to bound $D_{TV}(\Pi, \Psi)$, we will bound each term of (32) separately.

Bound on $\sum|\pi - \psi|$ for large (i, j):

Observe that $\psi_{i,j}$ is the fraction of points of D_n contained in cell (i, j) of Γ. Each point has probability $\pi_{i,j}$ of falling in cell (i, j), so $n \cdot \psi_{i,j}$ is the sum of n iid Bernoullis, each with mean $\pi_{i,j}$.

Using the two-sided Chernoff bound from (28), we then have that for any (i, j)

$$\Pr\left[|\; n\psi_{i,j} - n\pi_{i,j}\;| \ge tn\pi_{i,j}\right] \;\le\; 2\cdot\exp\left(-\frac{n\pi_{i,j}\cdot t^2}{3}\right) \tag{33}$$

for any $0 < t < 1$.

Since $\pi_{i,j} > (9 \log_2 n)/n$ for each *large* (i, j), observe that setting $t = 3\sqrt{\frac{\log_2 n}{n\cdot\pi_{i,j}}}$ means that

$$t \;<\; \frac{3\sqrt{\log_2 n}}{\sqrt{n}}\cdot\frac{\sqrt{n}}{\sqrt{9\log_2 n}} = 1,$$

and thus the bound in (33) can be applied[1].

Then for each *large* (i,j), using this setting of $t = 3\sqrt{\frac{\log_2 n}{n \cdot \pi_{i,j}}}$ gives

$$\begin{aligned}\Pr\left[\mid n\psi_{i,j} - n\pi_{i,j} \mid \geq tn\pi_{i,j}\right] \;&\leq\; 2 \cdot \exp\left(-\frac{n\pi_{i,j} \cdot t^2}{3}\right) \\ &\leq\; 2 \cdot \exp\left(-3\log_2 n\right) \;\leq\; \frac{2}{n^3}.\end{aligned}$$

So for each *large* (i,j), with probability at least $1 - 2n^{-3}$ we have

$$\mid n\pi_{i,j} - n\psi_{i,j} \mid \;\leq\; tn\pi_{i,j} \iff \mid \pi_{i,j} - \psi_{i,j} \mid \;\leq\; t\pi_{i,j}$$

which means by our setting of t that

$$\mid \pi_{i,j} - \psi_{i,j} \mid \;\leq\; \frac{3\log_2^{0.5} n}{\sqrt{\pi_{i,j} n}} \cdot \pi_{i,j} \;=\; \frac{3\log_2^{0.5} n}{\sqrt{n}} \cdot \sqrt{\pi_{i,j}} \;\leq\; \frac{3\log_2^{0.5} n}{\sqrt{n}}.$$

Here, the last inequality holds given that $\pi_{i,j} \leq 1$ for any *large* (i,j).

Now summing over all *large* (i,j) and taking a union bound, we have

$$\sum_{(i,j)\in L} \mid \pi_{i,j} - \psi_{i,j} \mid \;\leq\; k\ell n^{2\epsilon} \cdot \frac{3\log_2^{0.5} n}{n^{0.5}} \;\leq\; O\left(\frac{n^{\alpha+2\epsilon} \cdot \log_2^{0.5} n}{n^{0.5}}\right) \tag{34}$$

with probability at least $1 - O(n^{\alpha+2\epsilon-3})$, since $|L| \leq C(n) = k\ell n^{2\epsilon}$ and by the assumption that $k\ell \leq B(n) = O(n^{\alpha})$.

Bound on $\sum|\pi|$ for small (i,j):

Recall that cell (i,j) is *small* if $\pi_{i,j} \leq \frac{9\log_2 n}{n}$, and so with probability 1:

$$\sum_{(i,j)\in S} \pi_{i,j} \;\leq\; \frac{9 \cdot C(n)\log_2 n}{n}.$$

Bound on $\sum|\psi|$ for small (i,j):

Observe that $n \cdot \left(\sum_{(i,j)\in S} \psi_{i,j}\right)$ is the total number of points of D_n contained in *small* (i,j) cells of Γ and is thus the sum of n iid Bernoullis, each with mean $\sum_{(i,j)\in S} \pi_{i,j}$.

So in expectation we have

$$\begin{aligned}\mathrm{E}\left[n \cdot \left(\sum_{(i,j)\in S} \psi_{i,j}\right)\right] \;&=\; n \cdot \left(\sum_{(i,j)\in S} \pi_{i,j}\right) \\ &\leq\; n \cdot \left(\frac{9 \cdot C(n)\log_2 n}{n}\right) \;=\; 9 \cdot C(n)\log_2 n,\end{aligned}$$

where the inequality is due to the bound on $\sum|\pi|$ for *small* (i,j) from the previous step.

[1]The only lower bound constraint on π for large (i,j) comes from ensuring $t < 1$ so that our Chernoff bound variant can be applied. This constraint also determines the $\sqrt{n}$ denominator in (34).

Now using the upper Chernoff bound from (29) and setting $t = 1$ gives

$$\Pr\left[n \cdot \left(\sum_{(i,j)\in S} \psi_{i,j} \right) \geq 18 \cdot C(n) \log_2 n \right] \leq \exp\left(-3k\ell n^{2\epsilon} \cdot \log_2 n\right)$$
$$\leq \exp\left(-\Omega(n^{2\epsilon})\right)$$

since $C(n) = k\ell n^{2\epsilon}$ and $k, \ell \geq 2$.

This means that with probability at least $1 - e^{-\Omega(n^{2\epsilon})}$ we have

$$n \cdot \left(\sum_{(i,j)\in S} \psi_{i,j} \right) < 18 \cdot C(n) \log_2 n$$

and so

$$\sum_{(i,j)\in S} \psi_{i,j} < 18 \cdot \frac{C(n) \log_2 n}{n} = O\left(\frac{n^{\alpha+2\epsilon} \cdot \log_2 n}{n} \right).$$

Final bound on $D_{TV}(\Pi, \Psi)$

To conclude the proof, using the preceding three individual bounds on the terms from (32) we have that

$$\begin{aligned} D_{TV}(\Pi, \Psi) &\leq \sum_{(i,j)\in L} |\pi_{i,j} - \psi_{i,j}| + \sum_{(i,j)\in S} |\pi_{i,j}| + \sum_{(i,j)\in S} |\psi_{i,j}| \\ &\leq O\left(\frac{n^{\alpha+2\epsilon} \cdot \log_2^{0.5} n}{n^{0.5}} \right) + O\left(\frac{n^{\alpha+2\epsilon} \cdot \log_2 n}{n} \right) + O\left(\frac{n^{\alpha+2\epsilon} \cdot \log_2 n}{n} \right) \\ &= O\left(\frac{n^{\alpha+2\epsilon} \cdot \log_2^{0.5} n}{n^{0.5}} \right) \end{aligned}$$

with probability at least $1 - O(n^{\alpha+2\epsilon-3}) - e^{-\Omega(n^{2\epsilon})} \geq 1 - O(n^{\alpha+2\epsilon-3})$. □

5 Conclusion

We emphasize that Theorem 5, which is the core new result needed to prove the consistency of the MIC estimator, yields a slightly weaker result than in the original claim of [RRF+16]. In our theorem, we show that the difference between the corresponding (k, ℓ) entries of $\widehat{M}$ and M is small when $k\ell \leq B(n) = O(n^{\alpha})$ for $0 < \alpha < 0.5$ with high probability. The original claim of Reshef et al. sought to prove the same result for $k\ell \leq B(n) = O(n^{\alpha})$ for $0 < \alpha < 1$. We suspect that the statement of Theorem 5 *does* hold for $0 < \alpha < 1$, but that the techniques used here are insufficient to prove this stronger claim.

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