

Ground Truth Bias in External Cluster Validity Indices

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Abstract

External *cluster validity indices* (CVIs) are used to quantify the quality of a clustering by comparing the similarity between the clustering and a ground truth partition. However, some external CVIs show a biased behavior when selecting the most similar clustering. Users may consequently be misguided by such results. Recognizing and understanding the bias behavior of CVIs is therefore crucial.

It has been noticed that, some external CVIs exhibit a preferential bias towards a larger or smaller number of clusters which is monotonic (directly or inversely) in the number of clusters in candidate partitions. This type of bias is caused by the functional form of the CVI model. For example, the popular *Rand Index* (RI) exhibits a monotone increasing (NCinc) bias, while the *Jaccard Index* (JI) index suffers from a monotone decreasing (NCdec) bias. This type of bias has been previously recognized in the literature.

In this work, we identify a new type of bias arising from the distribution of the ground truth (reference) partition against which candidate partitions are compared. We call this new type of bias *ground truth* (GT) bias. This type of bias occurs if a change in the reference partition causes a change in the bias

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status (e.g., NCinc, NCdec) of a CVI. For example, NCinc bias in the RI can be changed to NCdec bias by skewing the distribution of clusters in the ground truth partition. It is important for users to be aware of this new type of biased behavior, since it may affect the interpretations of CVI results.

The objective of this article is to study the empirical and theoretical implications of GT bias. To the best of our knowledge, this is the first extensive study of such a property for external CVIs. Our computational experiments show that 5 of 26 pair-counting based CVIs studied in this paper, which are all functions of the RI, exhibit GT bias. Following the numerical examples, we provide a theoretical analysis of GT bias based on the relationship between the RI and quadratic entropy. Specifically, we prove that the quadratic entropy of the ground truth partition provides a computable test which predicts the NC bias status of the RI.

Keywords: External Cluster Validity Indices, Rand Index, Ground Truth Bias, Quadratic Entropy

1. Introduction

Clustering is one of the fundamental techniques in data mining, which helps users explore potentially interesting patterns in unlabeled data. Cluster analysis has been widely used in many areas, ranging from bioinformatics [1] and market segmentation [2] to information retrieval [3] and image processing [4].
5 However, depending on different factors, e.g., different clustering algorithms, initializations, parameter settings (the number of clusters c), many alternative candidate partitions might be discovered for a fixed dataset.

Cluster validity indices (CVIs) are used to quantify the goodness of a partition. Many CVIs have been proposed and successfully used for this task [5, 6, 7, 8]. These measures can be generally divided into two major types: internal
10 and external. If the data are *labeled*, the ground truth partition can be used with an external CVI to explore the match between candidate and ground truth partitions. Since the labeled data may not correspond to clusters proposed by

15 any algorithm, we will refer groups in the ground truth as *subsets*, and algorithmically proposed groups as *clusters*. When the data are *unlabeled* (the real case), an important post-clustering question is how to evaluate different candidate partitions. This job falls to the internal CVIs. One of the most important uses of the external CVIs is to evaluate the comparative quality of internal CVIs
20 on labeled data [9], so that in the real case, some confidence can be placed in a chosen internal CVI to guide us towards realistic clusters found in unlabeled data. *This article is focused on external CVIs.*

External CVIs (or comparison measures), are often interpreted as similarity (or dissimilarity) measures between the ground truth and candidate partitions.
25 The ground truth partition, which is usually generated by an expert in the data domain, identifies the primary substructure of interest to the expert. This partition provides a benchmark for comparison with candidate partitions. The general idea of this evaluation methodology is that the more similar a candidate is to the ground truth (a larger value for the similarity measure), the better this
30 partition approximates the labeled structure in the data.

However, this evaluation methodology implicitly assumes that the similarity measure works correctly, i.e., that a larger similarity score indicates a partition that is really more similar to the ground truth. But this assumption may not always hold. When this assumption is false, the evaluation results will be misleading.
35 One of the reasons that can cause the assumption to be false is that a measure may have bias issues. That is, some measures are biased towards certain clusterings, even though they are not more similar to the ground truth compared to the other candidate partitions being evaluated. This can cause misleading results for users employing these biased measures. Thus, recognizing and understanding the bias behavior of the CVIs is crucial.
40

The *Rand Index* (RI, similarity measure) is a very popular pair-counting based validation measure that has been widely used in many applications [10, 11, 12, 13, 14, 15, 16] in the last five years. It has been noticed that the RI tends to favor candidate partitions with larger numbers of clusters when the number
45 of subsets in the ground truth is fixed [5], i.e., it tends to increase as the number

of clusters increases (we call it NCinc bias in this work, where NC = number of clusters). NC bias means that the CVI’s preference is influenced by the number of clusters in the candidate partitions. For example, some measures may prefer the partition with larger (smaller) number of clusters, i.e., NCinc (NCdec) bias.

50 The following initial example illustrates NC bias for two popular measures, the *Rand Index* (RI) and *Jaccard Index* (JI) measures.

1.1. Example 1 - NC bias of RI and JI

In this example, we illustrate NC bias for RI and JI. We generate a set of candidate partitions randomly with different numbers of clusters and a random

55 ground truth. We use RI and JI to choose the most similar partition from the candidate partitions by comparing the similarity between each of them and the ground truth. As there is no difference in the generation methodology of the candidate partitions, we expect them to be treated equally on average. A measure without NC bias should treat these candidate partitions equally

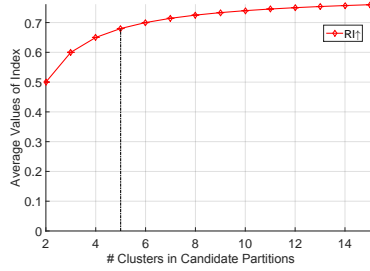
60 without preference to any partition in terms of their different number of clusters. However, if a measure prefers the partition, e.g., with a larger number of clusters (gives higher value to the partition with a larger number of clusters if it is a similarity measure), we say it possess NC bias, more specifically, NCinc bias.

Let U_{GT} be a ground truth partition with c_{true} subsets. Consider a set of

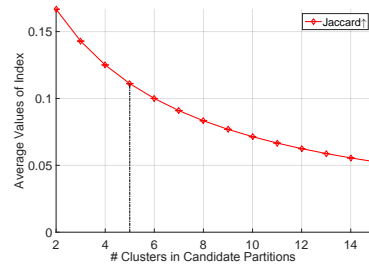
65 $N = 100,000$ objects, let the number of clusters in the candidate partitions c vary from 2 to c_{max} , where $c_{max} = 3 * c_{true}$. We randomly generate a ground truth partition U_{GT} with $c_{true} = 5$. Then for each c , $2 \leq c \leq 15$, we generate 100 partitions randomly, and calculate the RI and JI between U_{GT} and each generated partition. Finally, we compute the average values of these two

70 measures at each value of c . The results are shown in Figure 1. Please note that the RI and JI are max-optimal (larger value is preferred). Evidently RI monotonically increases and JI monotonically decreases as c increases. Figure 1 shows that for this experiment, the RI points to $c = 15$, its maximum over the range of c ; and the JI points to $c = 2$, its maximum over the range of c . Both

75 indices exhibit NC bias (RI shows NCinc bias and JI shows NCdec bias).

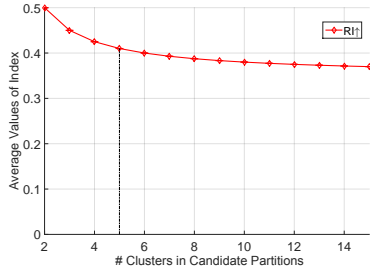


(a) Average RI values with random U_{GT} containing 5 subsets.

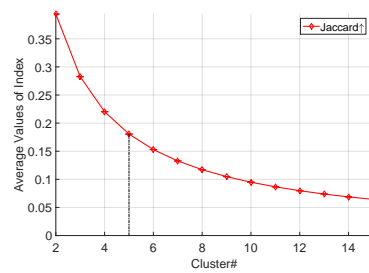


(b) Average JI values with random U_{GT} containing 5 subsets.

Figure 1: The average RI and JI values over 100 partitions at each c with uniformly generated ground truth. The symbol \uparrow means larger values are preferred. Vertical line indicates correct number of clusters.



(a) Average RI values with skewed ground truth.



(b) Average JI values with skewed ground truth.

Figure 2: The average RI and JI values over 100 partitions at each c with skewed ground truth. The symbol \uparrow means larger values are preferred. Vertical line indicates correct number of clusters.

But, does the RI *always* exhibit NCinc bias towards clusterings with a larger numbers of clusters? *The answer is no.* We have discovered that the overall bias of some CVIs, including the RI, may change their NC bias tendencies depending on the distribution of the subsets in the ground truth. The change in the NC bias status of an external CVI due to the different ground truths is called *GT bias*. This kind of changeable bias behavior caused by the ground truth has not been recognized previously in the literature. It is important to be aware of this

phenomenon, since it affects how a user should interpret clustering validation results. Next, we give an example of GT bias (GT = ground truth).

85 **1.2. Example 2 - GT bias of RI**

We use the same protocols as in Example 1, but change the distribution of the subsets in the ground truth by randomly assigning 80% of the objects to the first cluster and then randomly assigning the remaining 20% of the labels to the other four clusters for $c = 2, 3, 4, 5$. Thus, the distribution of the ground
90 truth is heavily skewed (non-uniform). The average values of RI and JI are shown in Figure 2. The shape of JI in Figures 1b and 2b is same: it still decreases monotonically with c , exhibiting NCdec bias, and indicating $c = 2$ as its preferred choice. Turning now to the RI, we see that trend seen in Figure 1a is reversed. The RI in Figure 2a is maximum at $c = 2$, and *decreases* monotonically
95 as c increases. So the NC bias of RI has changed from NCinc bias to NCdec bias. Thus, RI shows GT bias. To summarize, Examples 1 and 2 show that NC bias is possessed by some external CVIs due to monotonic tendencies of the underlying mathematical model. But beyond this, some external CVIs can be influenced by GT bias, which is due to the way the distribution of the ground
100 truth interacts with the elements of the CVI.

The objective of this article is to study the empirical and theoretical implications of GT bias. To the best of our knowledge, this is the first extensive study of this property for external cluster validity indices. In this work, our contributions can be summarized as follows:

- 105 1. We identify the GT bias effect for external validation measures, and also explain its importance.
2. We test and discuss NC bias for 26 popular pair-counting based external validation measures.
3. We prove that RI and related 4 indices suffer from GT bias. And also
110 provide theoretical explanations for understanding why GT bias happens and when it happens on RI and related 4 indices.
4. We present experimental results that support our analysis.

5. We present an empirical example to show that *Adjusted Rand index* (ARI) also suffers from a modified GT bias.

115 The remainder of the paper is organized as follows. In Section 2 we discuss work related to the bias problems of some external validation measures. We introduce relevant notations and definitions of NC bias and GT bias in Section 3. In Section 4, we briefly introduce some background knowledge about 26 pair-counting based external validation measures. In section 5, we test the influence
120 of NC bias and GT bias for these 26 measures. Theoretical analysis of GT bias on the RI is presented in Section 6. An experimental example, showing that ARI has GT bias in certain scenarios, is presented in Section 7. The paper is concluded in Section 8.

2. Related Work

125 Several works have discussed the bias behavior of external CVIs. As the conditions imposed on the discussion of the biased behavior are varied, here we classify these conditions into three categories for convenience of discussion: i) general bias; ii) NC bias; iii) GT bias.

General Bias. It has been noticed that the RI exhibits a monotonic trend as
130 both the number of subsets in the ground truth and the number of clusters in the candidate partitions increases [17, 18, 19]. However, in our case, we consider the monotonic bias behavior of an external CVI as a function of the number of clusters in the candidate partitions when the number of subsets in the ground truth is fixed.

135 Wu et al. [20] observed that some external CVIs were unduly influenced by the well known tendency of k-means to equalize cluster sizes. They noted that certain CVIs tended to prefer approximately balanced k-means solutions even though the ground truth distribution was heavily skewed. The only case considered in [20] was the special case when all of the candidate partitions
140 had the same number of clusters. We will develop the general case, allowing candidate partitions to have different numbers of clusters.

Wu et al. [21] studied the use of the external CVI known as the F-measure for evaluation of clusters in the context of document retrieval. They found that the F-measure tends to assign higher scores to partitions containing a large number
145 of clusters, which they called the “the incremental effect” of the F-measure. These authors also found that the F-measure has a “prior-probability effect”, i.e., the F-measure tends to assign higher scores to partitions with higher prior probabilities for the relevant documents. Wu et al. only discussed using the F-measure for accepting or rejecting proposed documents, they did not consider
150 the multiclass case.

NC Bias. The NC bias problem of some external CVIs has been noticed in the literature [22, 5, 23]. Nguyen et al. [5] pointed out that some external validation measures such as the *mutual information* (MI) (also the work [23]) and the *normalized mutual information* (NMI) suffered from NCinc bias. Based
155 this observation, they proposed adjustments to the information-theoretic based measures. However, they did not notice that the CVIs may show different NC bias behavior with different ground truth partitions.

GT Bias. Milligan and Cooper [22] tested 5 external CVIs, i.e., RI, *Adjusted Rand Index* (ARI, Hubert & Arabie) [24], ARI (Morey & Agresti) [25], Fowlkes
160 & Mallow (FM) [17] and *Jaccard Index* (JI), by comparing partitions with variable numbers of clusters generated by the hierarchical clustering algorithms, against the ground truth. The empirical tests showed that the RI suffered from NCinc bias, and FM and JI suffered from NCdec bias. However, it was mentioned in this work that “... the bias with the Rand index would be to select
165 a solution with a larger number of clusters. The only exception occurred when two clusters were hypothesized to be present in the data. In this case, the bias was reversed.” This empirical observation can be related our work. However, there was no analysis or further discussion about this reversed bias behavior of RI except this isolated observation. In this work, we provide a comprehensive
170 empirical and theoretical study of this kind of changeable bias behavior due to the distribution of the ground truth.

3. Notation and Definitions

In this section, we first introduce the notations used in this work. Then we provide the definitions about the different bias behavior of the external CVIs, i.e., NC bias, GT bias which further has two subtypes, i.e., GT1 bias and GT2 bias.

3.1. Notation

Let D be a set of N objects $\{o_1, \dots, o_N\}$. A convenient way to represent a crisp c -partition of D is with a set of (cN) values $\{u_{ik}\}$ arrayed as a $c \times N$ matrix $U = [u_{ik}]$. Element u_{ik} is the *membership* of o_k in cluster i . We denote the set of all possible c -partitions of D as:

$$M_{hcN} = \{U \in \mathfrak{R}^{cN} \mid \forall i, k, u_{ik} \in \{0, 1\}; \forall k, \sum_{i=1}^c u_{ik} = 1; \forall i, \sum_{k=1}^N u_{ik} > 0\} \quad (1)$$

The cardinality (or size) of cluster i is $\sum_{k=1}^N u_{ik} = n_i$. When all of the n_i are equal to N/c , we say that U is *balanced*.

3.2. Definitions

This section contains definitions for the types of bias exerted on external CVIs by their functional forms (NC bias) and the distribution of the ground truth partition (GT bias). We will call the influence of the number of clusters in ground truth partition, U_{GT} , Type 1 or *GT1 bias*, and the influence of the size distribution of the subsets in U_{GT} Type 2, or *GT2 bias*.

Definition 1. Let $U_{GT} \in M_{hrN}$ be any crisp ground truth partition with r subsets, where $2 \leq r \leq N$. Let $CP = \{V_1, \dots, V_m\}$, where $V_i \in M_{hc_iN}$, be a set of candidate partitions with different numbers of clusters, where $2 \leq c_i \leq N$. We compare U_{GT} with each $V_i \in CP$ using an external *Cluster Validity Index* (CVI) and choose the one that is the best match to U_{GT} . There are two types of external CVIs: max-optimal (larger value is better) similarity measures such as *Rand's index* (RI); and min-optimal (smaller value is better) dissimilarity measures such as the Mirkin metric (refer to Table 3).

We say an external CVI has NC bias if it shows bias behavior with respect to
 195 the *number of clusters* in V_i when comparing $V_i \in CP$ to the ground truth
 U_{GT} . There are three types of NC bias status defined in this work based on our
 numerical experiments ¹

1. if a max-optimal (min-optimal) CVI tends to assign higher (smaller) scores
 to the partition $V_i \in CP$ with larger c_i , then we say this CVI has NCinc
 200 (NC increase) bias;
2. if a max-optimal (min-optimal) CVI tends to assign smaller (higher) scores
 to the partition $V_i \in CP$ with larger values of c_i , then we say this CVI
 has NCdec (NC decrease) bias;
3. if a CVI tends to be indifferent to the values of c_i for the partitions $V_i \in$
 205 CP , we say that this CVI has no NC bias. In this case, we will call the
 lack of bias NCflat.

For example, the RI shows NCinc bias in Figure 4b; JI shows NCdec bias
 in Figure 4c; RI shows NCflat bias in Figure 4a and ARI shows NCflat bias
 in Figure 4e. Next, we define *ground truth bias* (GT bias), which occurs if the
 210 use of a *different ground truth partition* alters the NC bias status of an external
 CVI.

Definition 2. Let Q and Q' denote the NC bias status of an external CVI,
 with respect to two ground truth partitions, U_{GT} and U'_{GT} respectively, so
 $Q, Q' \in \{\text{NCinc}, \text{NCdec}, \text{NCflat}\}$. If $Q \neq Q'$, then this external CVI has *ground*
 215 *truth bias* (GT bias).

For example, given two ground truth partitions $U_{GT} \neq U'_{GT}$, if an external
 CVI shows e.g., NCflat bias with U_{GT} (e.g., Figure 4a), and shows, e.g., NCinc
 bias with U'_{GT} (e.g., Figure 4b), then this CVI has GT bias. Definition 2
 characterizes GT bias as an transition effect on the NC bias status of an external
 220 CVI.

¹There could be other types of NC bias status, e.g., NC fluctuating, which are out of the
 scope of this work and left to be discussed in the future work.

There are quite a few subcases of GT bias depending on the properties of U_{GT} and U'_{GT} relative to each other. In this article we have studied two specific cases of GT bias, i.e., $GT1$ bias and $GT2$ bias. Generally speaking, when an external CVI changes its bias status with respect to two ground truth partitions U_{GT1} and U_{GT2} , we have two cases: i) $GT1$ bias occurs when the subsets in these two ground truth partitions are uniformly distributed but with different numbers of subsets; ii) $GT2$ bias occurs when these two ground truth partitions have same number of subsets but with different distributions. The formal definitions of $GT1$ bias and $GT2$ bias are described as follows.

Definition 3. Let $U_{GT} \in M_{hrN}$ be a balanced crisp ground truth partition with r subsets $\{u_1, \dots, u_r\}$, i.e., $p_i = \frac{|u_i|}{N} = \frac{1}{r}$, and $U'_{GT} \in M_{hr'N}$ be a balanced crisp ground truth partition with r' subsets $\{u'_1, \dots, u'_{r'}\}$, i.e., $p'_i = \frac{|u'_i|}{N} = \frac{1}{r'}$, where $\mathbf{r} \neq \mathbf{r}'$. We say an external CVI has **GT1 bias** if the NC bias status for U_{GT} is different from that of U'_{GT} .

For example, given U_{GT} with 2 balanced subsets, and U'_{GT} with 50 balanced subsets, then if an CVI shows e.g., $NCflat$ bias with U_{GT} , and $NCinc$ bias with U'_{GT} , then this CVI has $GT1$ bias (e.g., Figures 4a and 4b).

Definition 4. Let $U_{GT} \in M_{hrN}$ be a crisp ground truth partition with r subsets $\{u_1, \dots, u_r\}$, $P = \{p_1, \dots, p_r\} = \{\frac{|u_1|}{N}, \dots, \frac{|u_r|}{N}\}$ and $p_2 = p_3 = \dots = p_r = \frac{1-p_1}{r-1}$. Let $U'_{GT} \in M_{hr'N}$ be another crisp ground truth partition with r' subsets $\{u'_1, \dots, u'_{r'}\}$ and $P' = \{p'_1, \dots, p'_{r'}\} = \{\frac{|u'_1|}{N}, \dots, \frac{|u'_{r'}|}{N}\}$, $p'_2 = p'_3 = \dots = p'_{r'} = \frac{1-p'_1}{r'-1}$, where $\mathbf{r} = \mathbf{r}'$ and $\mathbf{p}_1 \neq \mathbf{p}'_1$. We say an external CVI has **GT2 bias** if it exhibits different types of NC bias for U_{GT} and U'_{GT} .

For example, given $U_{GT} \in M_{h5N}$ with $p_1 = 0.1$ and $U'_{GT} \in M_{h5N}$ with $p'_1 = 0.9$, if an external CVI shows, e.g., $NCinc$ bias for U_{GT} and shows e.g., $NCdec$ bias for U'_{GT} , then this CVI has $GT2$ bias (e.g., Figures 5a and 5b).

Figure 3 illustrates the relationship between NC bias and GT bias that is contained in Definitions 1 - 4. In this Figure, CP denotes a set of crisp candidate partitions with different numbers of clusters, and CVI denotes an external CVI .

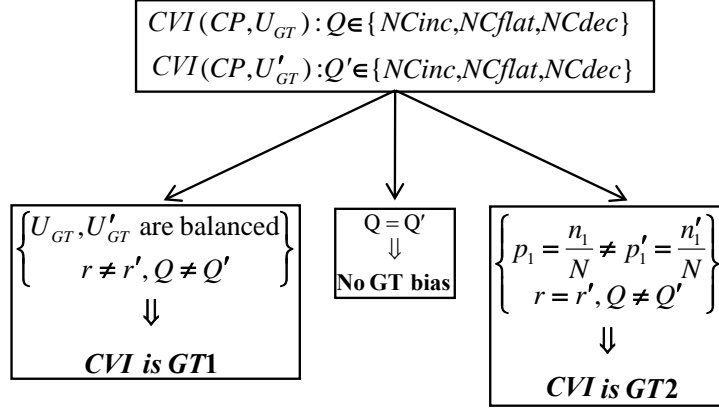


Figure 3: The relationship between NC bias and GT bias in Definitions 1- 4.

250 $U_{GT} \neq U'_{GT}$ are different crisp ground truth partitions and $U_{GT} \in M_{hrN}, U_{GT} \in M_{hr'N}$. We summarized the different bias problems discussed in this work in Table 1.

4. Pair-counting based External Cluster Validity Indices

In this part, we will give some background knowledge briefly about the pair-
 255 counting based cluster validity measures. In addition, we also provide a list of
 26 pair-counting based measures which will be tested for their NC bias and GT
 bias problems.

Pair-counting based comparison CVIs are a group of popular measures based
 on counting the agreements and disagreements between two crisp partitions in
 terms of shared pairs of objects. As in Example 1, we denote the subsets corre-
 260 sponding to the clusters in U and V as $\{u_1, \dots, u_r\}$ and $\{v_1, \dots, v_c\}$. Suppose
 $U \in M_{hrN}$ and $V \in M_{hcN}$ are partitions of D . The contingency table that pairs
 these two partitions is shown in Table 2. Note that the numbers of clusters in
 U and V need not be equal, $r \neq c$.

265 The entry n_{ij} indicates the number of shared object pairs in clusters u_i and
 v_j . The row sum, a_i , is the number of objects in cluster u_i and the column
 sum, b_j , is the number of objects in cluster v_j . The number of pairs of shared

Table 1: Glossaries about different bias discussed in this paper.

Glossary	Explanation
NC bias	An external CVI shows bias behavior with respect to the number of clusters in the compared clusterings.
NCinc bias (NC increase)	One of the NC bias status. An external CVI prefers clusterings with larger number of clusters.
NCdec bias (NC decrease)	One of the NC bias status. An external CVI prefers clusterings with smaller number of clusters.
NCflat bias	One of the NC bias status. An external CVI has no bias for clusterings with respect to the number of clusters.
GT bias	An external CVI shows different NC bias status when varying the ground truth.
GT1 bias	A subtype of GT bias. An external CVI shows different NC bias status for two ground truths with uniform distribution but with different numbers of subsets.
GT2 bias	A subtype of GT bias. An external CVI shows different NC bias status for two ground truths that have the same number of subsets but with different subset distributions.

Table 2: Contingency table based on partitions U and V , $n_{ij} = |u_i \cap v_j|$

		$V \in M_{hcN}$					
		Cluster	\mathbf{v}_1	\mathbf{v}_2	...	\mathbf{v}_c	Sums
$U \in M_{hrN}$	\mathbf{u}_1	n_{11}	n_{12}	...	n_{1c}		a_1
	\mathbf{u}_2	n_{21}	n_{22}	...	n_{2c}		a_2
	\vdots	\vdots	\vdots		\vdots		\vdots
	\mathbf{u}_r	n_{r1}	n_{r2}	...	n_{rc}		a_r
Sums		b_1	b_2	...	b_c		$\sum_{ij} n_{ij} = N$

objects between U and V is divided into four groups: k_{11} , the number of pairs that are in the same cluster in both U and V ; k_{00} , the number of pairs that are in different clusters in both U and V ; k_{10} , the number of pairs that are in the same cluster in U but in different clusters in V ; and k_{01} , the number of pairs that are in different clusters in U but in the same clusters in V . And

275 $k_{11} + k_{10} + k_{01} + k_{00} = \binom{N}{2}$. The sum of $k_{11} + k_{00}$ is interpreted as the total number of *agreements* between U and V , and the sum $k_{10} + k_{01}$ is the total number of disagreements. External CVIs based on pair-counting are computed with these four types of pairs. Please refer to Table 3 for a non-exhaustive list of 26 popular pair-counting based external CVIs [26, 27]. These are the indices which will be discussed in terms of their susceptibility to NC bias and GT bias.

Table 3: Pair-Counting based Comparison Measures (external CVIs)

#	Name/Reference	Symbol	Formula	Find
1	Rand Index [28]	RI	$\frac{k_{11} + k_{00}}{k_{11} + k_{10} + k_{01} + k_{00}}$	Max
2	Adjusted Rand Index Hubert and Arabie [29]	ARI	$\frac{k_{11} - \frac{(k_{11} + k_{10})(k_{11} + k_{01})}{k_{11} + k_{10} + k_{01} + k_{00}}}{\frac{(k_{11} + k_{10}) + (k_{11} + k_{01})}{2} - \frac{(k_{11} + k_{10})(k_{11} + k_{01})}{k_{11} + k_{10} + k_{01} + k_{00}}}$	Max
3	Mirkin [30]	Mirkin	$2(k_{10} + k_{01})$	Min
4	Jaccard Index [31]	JI	$\frac{k_{11}}{k_{11} + k_{10} + k_{01}}$	Max
5	Hubert [32]	H	$\frac{(k_{11} + k_{00}) - (k_{10} + k_{01})}{k_{11} + k_{10} + k_{01} + k_{00}}$	Max
6	Wallace [33]	W1	$\frac{k_{11}}{k_{11} + k_{10}}$	Max
7	Wallace [33]	W2	$\frac{k_{11}}{k_{11} + k_{01}}$	Max
8	Fowlkes & Mallow [17]	FM	$\frac{k_{11}}{\sqrt{(k_{11} + k_{10})(k_{11} + k_{01})}}$	Max
9	Minkowski [34]	MK	$\sqrt{\frac{k_{10} + k_{01}}{k_{11} + k_{10}}}$	Min
10	Hubert's Gamma [6]	Γ	$\frac{k_{11}k_{00} - k_{10}k_{01}}{\sqrt{(k_{11} + k_{10})(k_{11} + k_{01})(k_{01} + k_{00})(k_{10} + k_{00})}}$	Max
11	Yule [35]	Y	$\frac{k_{11}k_{00} - k_{10}k_{01}}{k_{11}k_{10} + k_{01}k_{00}}$	Max
12	Dice [36]	Dice	$\frac{2k_{11}}{2k_{11} + k_{10} + k_{01}}$	Max
13	Kulczynski [37]	K	$\frac{1}{2} \left(\frac{k_{11}}{k_{11} + k_{10}} + \frac{k_{11}}{k_{11} + k_{01}} \right)$	Max
14	McConnaughey [38]	MC	$\frac{k_{11}^2 - k_{10}k_{01}}{(k_{11} + k_{10})(k_{11} + k_{01})}$	Max
15	Peirce [39]	PE	$\frac{k_{11}k_{00} - k_{10}k_{01}}{(k_{11} + k_{01})(k_{10} + k_{00})}$	Max
16	Sokal & Sneath [40]	SS1	$\frac{1}{4} \left(\frac{k_{11}}{k_{11} + k_{10}} + \frac{k_{11}}{k_{11} + k_{01}} + \frac{k_{00}}{k_{10} + k_{00}} + \frac{k_{00}}{k_{01} + k_{00}} \right)$	Max
17	Baulieu [41]	B1	$\frac{\binom{N}{2} - \binom{N}{2}(k_{10} + k_{01}) + (k_{10} - k_{01})^2}{\binom{N}{2}^2}$	Max
18	Russel & Rao [42]	RR	$\frac{k_{11}}{k_{11} + k_{10} + k_{01} + k_{00}}$	Max
19	Fager & McGowan [43]	FMG	$\frac{k_{11}}{\sqrt{(k_{11} + k_{10})(k_{11} + k_{01})}} - \frac{1}{2\sqrt{k_{11} + k_{10}}}$	Max
20	Pearson	P	$\frac{k_{11}k_{00} - k_{10}k_{01}}{(k_{11} + k_{10})(k_{11} + k_{01})(k_{01} + k_{00})(k_{10} + k_{00})}$	Max
21	Baulieu [41]	B2	$\frac{k_{11}k_{00} - k_{10}k_{01}}{\binom{N}{2}^2}$	Max
22	Sokal & Sneath [40]	SS2	$\frac{k_{11}}{k_{11} + 2(k_{10} + k_{01})}$	Max

Continued from previous page

#	Name/Reference	Symbol	Formula	Find
23	Sokal & Sneath [40] Ochiai [44]	SS3	$\frac{k_{11}k_{00}}{\sqrt{(k_{11}+k_{10})(k_{11}+k_{01})(k_{10}+k_{00})(k_{01}+k_{00})}}$	Max
24	Gower & Legendre [45] Sokal & Sneath [40]	GL	$\frac{k_{11}+k_{00}}{k_{11}+\frac{1}{2}(k_{10}+k_{01})+k_{00}}$	Max
25	Rogers & Tanimoto [46]	RT	$\frac{k_{11}+k_{00}}{k_{11}+2(k_{10}+k_{01})+k_{00}}$	Max
26	Goodman & Kruskal [47] Yule [48]	GK	$\frac{k_{11}k_{00}-k_{10}k_{01}}{k_{11}k_{00}+k_{10}k_{01}}$	Max

280 5. Numerical Experiments

In this section, we experimentally test and discuss 26 pair-counting based external cluster validity indices (listed in Table 3) in terms of their preferences to (candidate) partitions with different number of clusters (NC bias). We study whether the behavior of these CVIs can be altered by changing the distribution
285 of ground truth partitions. In particular, we look for cases of GT1 and GT2 bias. We will find that the RI and 4 related CVIs show GT1 and GT2 bias behavior. The theoretical analysis of GT bias performance of the 5 indices will be provided in Section 6. First, we introduce the details of our experimental design.

290 5.1. Experimental Design

The philosophy of our experimental design is described as follows. We generate a set of candidate partitions randomly with different numbers of clusters and we select a random ground truth partition at a specified value of c . An external CVI is used to compare the similarity between each of the candidate
295 partitions and the ground truth. As there is no difference in the generation methodology of the candidate partitions, we expect them to be treated equally on average with a fair CVI, that is, the similarities between each of these candidate partitions and the ground truth should be the same in generally. We then

make a graph, taking the number of clusters of the candidate partitions as the
300 x axis, and the values of the external CVI between the ground truth and the
partition with the specific number of clusters as the y axis. For a fair external
CVI, we expect this graph to be (more or less) flat.

If the line tends to go up as the number of clusters increases, then this CVI
(e.g., similarity measure) shows NCinc bias; if the line tends to go down as
305 the number of clusters increases, then this CVI (e.g., similarity measure) shows
NCdec bias; if the line tends to be flat as the number of clusters increases, then
this CVI (e.g., similarity measure) shows NCflat bias, i.e., no bias.

First we test and discuss the performance of the CVIs with respect to their
NC bias. CVIs that show NCflat behavior are set aside. The remaining CVIs
310 are then tested to see if their NC bias behavior will be influenced or changed
by a change in the ground truth (compared with the same set of candidate
partitions), i.e., will we see GT bias? For example, an external CVI may show
NCinc bias with one ground truth partition and show NCdec bias with another
ground truth partition; or, it may show NCflat bias with one ground truth
315 partition and show NCinc bias with a different ground truth partition.

The distribution of the ground truth partition can be varied in different
ways. In this work, we consider two important factors with respect to the
ground truth: 1) the number of subsets in the ground truth (related to GT1
bias); and 2) the distribution of subsets in the ground truth (related to GT2
320 bias). We designed two sets of experiments for testing the GT1 and GT2 bias
of the 26 pair-counting based external CVIs. More details are as follows.

5.2. Type 1: GT1 bias Testing (Effect of the Cluster Number in the Ground Truth)

We use the same experimental setting as in Example 1. The ground truth
325 partition U_{GT} is randomly generated with c_{true} subsets which are in each case
uniformly distributed in size, where $c_{true} = \{2, 10, 20, 30, 50\}$. Then, we ran-
domly generate 100 candidate partitions with c clusters, where c ranges from 2
to $3*c_{true}$. We performed this experiment on all 26 comparison measures shown

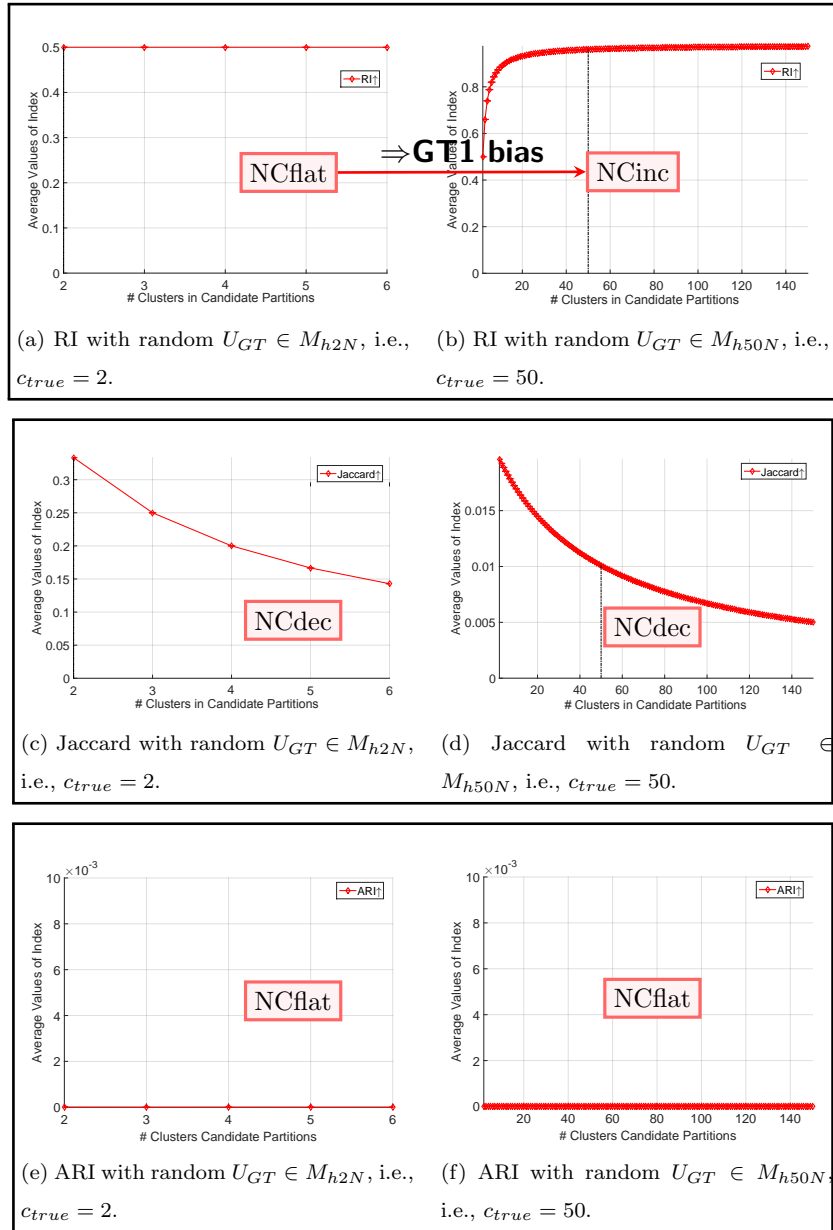


Figure 4: 100 trial average values of the RI, JI and ARI external CVIs with variable ground truth resulting in GT1 bias, $c_{true} = 2, 50$.

330 in Table 3, but due to limited space, we focus our discussion on the results from three representative measures, the RI, JI and ARI (indices #1, #2, and #4 in

Table 3) with $c_{true} = 2, 50$ (Figure 4). The complete results of the numerical experiments discussed in this section can be found in the supplementary document ².

When $c_{true} = 2$, the RI trend is flat, that is, it has NCflat bias. But when
 335 $c_{true} = 50$, the RI favors solutions with larger number of clusters, i.e., it shows
 NCinc bias with $c_{true} = 50$. Thus, the number of clusters in the random ground
 truth partition U_{GT} does influence the NC bias behavior of the RI. According to
 definition 3, this indicates that RI has GT1 bias. Comparing Figures 4c and 4d
 shows that the Jaccard index does not seem to suffer from GT bias due to the
 340 number of subsets in U_{GT} . These two figures show that the JI exhibits NCdec
 bias, decreasing monotonically as c increases from 2 to 6 (Figure 4c) or 2 to 150
 (Figure 4d). Figures 4e and 4f show that the ARI is not monotonic for either
 value of c , and is not affected by the number of clusters in U_{GT} . Thus, ARI has
 NCflat bias. We remark that these observed bias behavior of the tested external
 345 CVIs are based on these experimental settings.

5.3. Type 2: GT2 bias Testing (Effect of the Distribution of Clusters in Ground Truth)

We use an experimental setup similar to that in Example 2. We generate
 a ground truth by randomly assigning 10%, 20%, ..., 90% of the objects to the
 350 first cluster, and then randomly assigning the remaining cluster labels to the
 rest of the data objects. Here $c_{true} = 5$ is discussed. Figure 5 shows the results
 for the RI, JI and ARI with the size of the first cluster either $n_1 = 0.1 * N$ or
 $n_1 = 0.9 * N$.

Figures 5a and 5b show that the RI suffers from GT2 bias according to
 355 definition 4. It is monotone increasing with $n_1 = 10,000$ (NCinc bias), but
 monotone decreasing with $n_1 = 90,000$ (NCdec bias). Note that the graphs
 in Figures 5a and 5b are reflections of each other about the horizontal axis at
 0.5. The Jaccard index in Figures 5c and 5d exhibits the same NC bias status

²The supplementary document is available at <https://sites.google.com/site/yldatascience/>

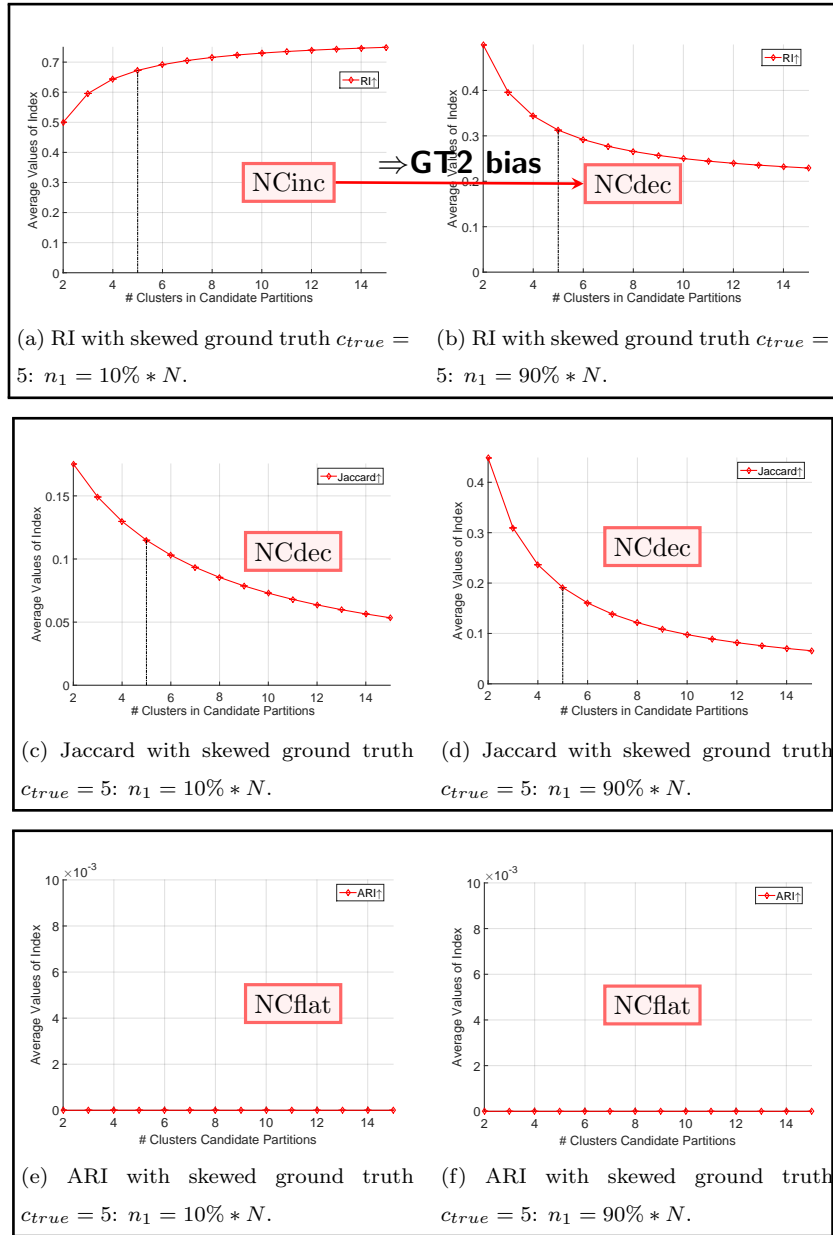


Figure 5: 100 run average values of the RI, JI and ARI with unbalanced ground truth to investigate GT2bias, $c_{true} = 5$. $n_1 = 10\% * N$ (left), $n_1 = 90\% * N$ (right).

as it did in Figures 4c and 4d. Specifically, JI decreases monotonically with c ,
 360 so it still has NCdec bias, but it does not seem to be affected by GT2 bias.
 The ARI in Figures 5e and 5f does not show any influence due to GT2 bias.
 It has NCflat bias under these two sets of experimental settings. So, from our
 empirical results, ARI would appear to be preferable to the RI and the JI in this
 setting. To summarize, these examples illustrate that the RI can suffer from
 365 GT1 bias and GT2 bias; that JI can suffer from NCdec bias but not GT1 bias
 nor GT2 bias; and that ARI does not suffer from NC bias or GT bias, under
 the experimental setup we have used here.

5.4. Summary for All 26 Comparison Measures

The overall results of similar experiments for all 26 indices (refer to supple-
 370 mentary document) in Table 3 led to the conclusion that 5 of the 26 external
 CVIs suffer from GT1 bias and GT2 bias for these experimental settings. These
 measures are *Rand Index* (RI) and

$$\text{Hubert [32]} : H(U, V) = 2RI - 1 \quad (2)$$

$$\text{Gower and Legendre [45]} : GL(U, V) = \frac{2}{1 + 1/RI} \quad (3)$$

$$\text{Rogers and Tanimoto [46]} : RT(U, V) = \frac{1}{2/RI - 1} \quad (4)$$

$$\text{Mirkin [30]} : \text{Mirkin}(U, V) = N(N - 1)(1 - RI) \quad (5)$$

Please note that the external CVIs in equations 2, 3, 4 and 5 are all functions
 of the RI. This observation forms the basis for our analysis in the next section.

375 6. Bias Due to Ground Truth for the Rand Index

In this section, we provide a theoretical analysis for the GT bias, GT1 bias
 and GT2 bias for the Rand Index. More specifically, we will analyze the under-
 lying reason for the GT bias of RI, based on its relationship with the quadratic
 entropy (Equation 8). Then, based on the relationship between RI and the

380 quadratic entropy, we will discuss theoretically about when RI shows GT bias,
 GT1 bias and GT2 bias, according to the distribution of the ground truth and
 the number of subsets in the ground truth.

6.1. Quadratic Entropy and Rand Index

The Havrda-Charvat entropy [49] (Equation 6) is a generalization of the
 385 Shannon entropy (Equation 7). The quadratic entropy (Equation 8) is the
 Havrda-Charvat generalized entropy with $\beta = 2$.

6.1.1. Havrda-Charvat Generalized Entropy

The Havrda-Charvat generalized entropy for a crisp partition U with r clusters
 $U = \{u_1, \dots, u_r\}$ is

$$H_\beta(U) = \frac{1}{1 - 2^{1-\beta}} \left(1 - \sum_{i=1}^r \left(\frac{|u_i|}{N}\right)^\beta\right) \quad (6)$$

where β is any real number > 0 and $\beta \neq 1$. Since H is a continuous function of
 β , when $\beta = 1$

$$H_1(U) = - \sum_{i=1}^r \frac{|u_i|}{N} \log \frac{|u_i|}{N} \quad (7)$$

which is the Shannon entropy $H_S(U)$. When $\beta = 2$ we have quadratic entropy

$$H_2(U) = 2 \left(1 - \sum_{i=1}^r \left(\frac{|u_i|}{N}\right)^2\right) \quad (8)$$

It can be shown that in the case of statistically independent random variables
 U and V

$$H_\beta(U, V) = H_\beta(U) + H_\beta(V) - (1 - 2^{1-\beta})H_\beta(U)H_\beta(V) \quad (9)$$

When $\beta = 2$, Equation 9 becomes

$$H_2(U, V) = H_2(U) + H_2(V) - \frac{1}{2}H_2(U)H_2(V) \quad (10)$$

In [50], Meila showed that the *Variation of Information* (VI) is a metric by
 expressing it as a function of Shannon's entropy. Consider a crisp partition V

with c subsets $V = \{v_1, \dots, v_c\}$, then

$$\begin{aligned} VI(U, V) &= H_S(U|V) + H_S(V|U) \\ &= 2H_S(U, V) - H_S(U) - H_S(V) \end{aligned} \quad (11)$$

The VI is not one of the 26 indices in Table 3, but this information-theoretic CVI can be computed based on the contingency table, and it will help us analyze the GT bias of the 5 external CVIs discussed in Section 5.4.

Simovici [51] showed that replacing Shannon's entropy in Equation 11 by the generalized entropy at Equation 6 still yielded a metric,

$$VI_\beta(U, V) = H_\beta(U|V) + H_\beta(V|U) \quad (12)$$

$$= 2H_\beta(U, V) - H_\beta(U) - H_\beta(V) \quad (13)$$

For $\beta = 2$, this becomes

$$VI_2(U, V) = 2H_2(U, V) - H_2(U) - H_2(V) \quad (14)$$

Based on the above introduced concepts, we next introduce how to derive the relationship between RI and the quadratic entropy (i.e., Havrda-Charvat generalized entropy with $\beta = 2$). This relationship will help us explain why RI shows GT bias.

6.1.2. Quadratic Entropy vs. Rand Index

Let U and V be two crisp partitions of N samples with r clusters and c clusters respectively. Then the relationship between $VI_2(U, V)$ and $RI(U, V)$ can be derived as follows [51].

First, based on Equations 13 and 6, we have $VI_\beta(U, V)$ as

$$VI_\beta(U, V) = 2H_\beta(U, V) - H_\beta(U) - H_\beta(V) \quad (15)$$

$$\begin{aligned} &= \frac{2}{1 - 2^{1-\beta}} \left(1 - \sum_{i=1}^r \sum_{j=1}^c \left(\frac{|u_i \cap v_j|}{N}\right)^\beta\right) - \frac{1}{1 - 2^{1-\beta}} \left(1 - \sum_{i=1}^r \frac{|u_i|}{N}\right)^\beta - \frac{1}{1 - 2^{1-\beta}} \left(1 - \sum_{j=1}^c \left(\frac{|v_j|}{N}\right)^\beta\right) \\ &= \frac{1}{1 - 2^{1-\beta}} \left(2 \left(1 - \sum_{i=1}^r \sum_{j=1}^c \left(\frac{|u_i \cap v_j|}{N}\right)^\beta\right) - \left(1 - \sum_{i=1}^r \left(\frac{|u_i|}{N}\right)^\beta\right) - \left(1 - \sum_{j=1}^c \left(\frac{|v_j|}{N}\right)^\beta\right)\right) \\ &= \frac{1}{N^\beta (1 - 2^{1-\beta})} \left(\sum_{i=1}^r (|u_i|)^\beta + \sum_{j=1}^c (|v_j|)^\beta - 2 \sum_{i=1}^r \sum_{j=1}^c (|u_i \cap v_j|)^\beta\right) \end{aligned}$$

Now setting $\beta = 2$, we get

$$\begin{aligned}
VI_2(U, V) &= \frac{2}{N^2} \left(\sum_{i=1}^r (|u_i|)^2 + \sum_{j=1}^c (|v_j|)^2 - 2 \sum_{i=1}^r \sum_{j=1}^c (|u_i \cap v_j|)^2 \right) \\
&= \frac{2}{N^2} (2k_{10} + 2k_{01}) \\
&= \frac{2}{N} (N - 1)(1 - \mathbf{RI}(U, V))
\end{aligned} \tag{16}$$

400 Equation 16 shows that VI_2 and RI are inversely related. Thus, by analyzing the bias behavior of VI_2 , it will be easy to understand the behavior of RI. Next, we will analyze the GT bias behavior of VI_2 based on the concept of quadratic entropy.

6.2. GT bias of RI

405 In this section, we will first discuss the general case of GT bias for RI by providing a series of theoretical statements for helping understand why RI shows GT bias, and when RI shows GT bias. Then, we will discuss two specific cases, i.e., GT1 bias and GT2 bias for RI and provide related theoretical statements which will explain when RI shows GT1 bias and GT2 bias. The related proofs
410 are provided in Appendix A.

6.2.1. General Case of GT bias

We introduce Lemma 1 to build the foundation for analyzing the GT bias of VI_2 , then *RI*.

Lemma 1. Given $U \in M_{hrN}$ and $V \in M_{hcN}$, two statistically independent crisp partitions of N data objects, we have

$$VI_2(U, V) = H_2(U) + (1 - H_2(U))H_2(V) \tag{17}$$

415 Next, we introduce an important theorem in this paper that demonstrates why RI shows GT bias and when it shows GT bias by judging the relationship between the quadratic entropy of ground truth U_{GT} , $H_2(U_{GT})$ and 1.

Theorem 1. Let $U_{GT} \in M_{hrN}$ be a ground truth partition with r subsets, and let $CP = \{V_1, \dots, V_m\}$ be a set of candidate partitions with different numbers of clusters, where $V_i \in M_{hc_iN}$ contains c_i clusters which are uniformly distributed (balanced), $2 \leq c_i \leq N$. Assuming U_{GT} and $V_i \in CP$ are statistically independent, then RI suffers from GT bias. In addition, according to the relationship between $H_2(U_{GT})$ and 1, we have:

1. if $H_2(U_{GT}) < 1$, RI suffers from NCdec bias (i.e., RI decreases as c_i increases);
2. If $H_2(U_{GT}) = 1$, RI is unbiased, i.e., NCflat bias (i.e., RI has no preferences as c_i increases);
3. if $H_2(U_{GT}) > 1$, RI suffers from NCinc bias (i.e., RI increases as c_i increases).

Given a ground truth partition U_{GT} , Theorem 1 provides a test for the NC bias status of the RI. Compute the quadratic entropy $H_2(U_{GT})$ of the reference matrix U_{GT} and compare it to value 1, and use Theorem 1 to determine the type of bias. Figure 6 illustrates the relationship between $H_2(U_{GT})$ and 1 on the Rand index graphically. Figure 6 is based on the same experimental setting as in Example 2 but with $N = 1000$, and a different distribution P in the ground truth and $c_{true} = 3$. Next, we show that we can also judge the NC bias and GT bias of RI by comparing $\sum_{i=1}^r (p_i)^2$ and $\frac{1}{2}$. Next we introduce the Corollary 1 which is the basis for the following theorems.

Corollary 1. Let $U_{GT} \in M_{hrN}$ be a ground truth partition with r subsets $\{u_1, \dots, u_r\}$, and let $P = \{p_1, \dots, p_r\}$ and $p_i = \frac{|u_i|}{N}$. Let $CP = \{V_1, \dots, V_m\}$ be a set of generated partitions with different numbers of clusters, where $V_i \in M_{hc_iN}$ contains c_i clusters which are balanced, $2 \leq c_i \leq N$. Assuming U_{GT} and $V_i \in CP$ are statistically independent, we have

1. if $\sum_{i=1}^r (p_i)^2 > \frac{1}{2}$, then RI has NCdec bias;
2. if $\sum_{i=1}^r (p_i)^2 = \frac{1}{2}$, then RI has NCflat bias;
3. if $\sum_{i=1}^r (p_i)^2 < \frac{1}{2}$, then RI has NCinc bias.

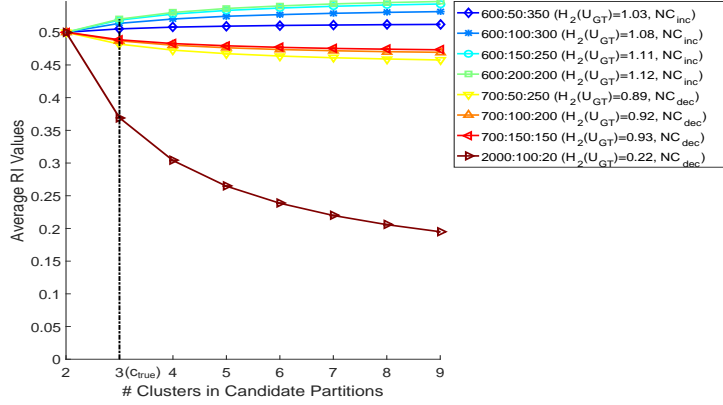


Figure 6: 100 trial average RI values with c_i ranging from 2 to 9 for $c_{true} = 3$. $n_1 : n_2 : n_3$ indicates the sizes of the three clusters and the corresponding $H_2(U_{GT})$ values.

Next, we introduce another theorem which helps us understand how do the prior probabilities $\{p_i\}$ and the number of subsets r in the ground truth U_{GT} influence the NC bias status of RI.

Theorem 2. Let $U_{GT} \in M_{hrN}$ be a ground truth partition with r subsets $\{u_1, \dots, u_r\}$, and let $P = \{p_1, \dots, p_r\}$ and $p_i = \frac{|u_i|}{N}$. Let $P' = \{p'_1, p'_2, \dots, p'_r\}$ denote P sorted into descending order, where $p'_1 \geq p'_2 \dots \geq p'_r$. Let $CP = \{V_1, \dots, V_m\}$ be a set of generated partitions with different numbers of clusters, where $V_i \in M_{hc_iN}$ contains c_i clusters which are balanced, $2 \leq c_i \leq N$. Assuming U_{GT} and $V_i \in CP$ are statistically independent, then RI has GT bias. In addition, depending on P and r , we have:

When $r > 2$

1. if $p'_1 > \frac{1}{2}$, and
 - if $p'_1(p'_1 - \frac{1}{2}) > \sum_{i=2}^r p'_i(\frac{1}{2} - p'_i)$, then RI has NCdec bias;
 - if $p'_1(p'_1 - \frac{1}{2}) = \sum_{i=2}^r p'_i(\frac{1}{2} - p'_i)$, then RI has NCflat bias;
 - if $p'_1(p'_1 - \frac{1}{2}) < \sum_{i=2}^r p'_i(\frac{1}{2} - p'_i)$, then RI has NCinc bias.
2. if $p'_1 = \frac{1}{2}$, then RI has NCinc bias;
3. if $p'_1 < \frac{1}{2}$, then RI has NCinc bias.

When $r = 2$

1. if $p'_1 > \frac{1}{2}$, then RI has NCdec bias;
- 465 2. if $p'_1 = \frac{1}{2}$, then RI has NCflat bias.

Theorem 2 tells us how the ground truth distribution P' and the number of clusters r of U_{GT} affect the Rand index and helps us judge the NC bias status based on P' and r . For example, if $r > 2$, $p'_1 > \frac{1}{2}$ and $p'_1(p'_1 - \frac{1}{2}) > \sum_{i=2}^r p'_i(\frac{1}{2} - p'_i)$, then RI has NCdec bias (e.g., $r = 3$, $p'_1 = \frac{2}{3}$, $p'_2 = \frac{1}{4}$ and 470 $p'_3 = \frac{1}{12}$). If $r = 2$ and $p'_1 = \frac{1}{2}$, then RI has NCflat bias. Thus RI has GT bias.

The above discussion and theoretical analysis are in a more general sense. Next, we discuss GT1 bias and GT2 bias of the RI, which are two specific types of GT bias with certain conditions imposed on the ground truth. This will also help explain and judge the NC bias behavior of the indices in the empirical test 475 shown Section 5.

6.2.2. GT1 bias and GT2 bias

First, we start by introducing a theorem for GT1 bias of RI.

Theorem 3. Let $U_{GT} \in M_{hrN}$ be a crisp ground truth partition with r balanced subsets $\{u_1, \dots, u_r\}$, i.e., $p_i = \frac{|u_i|}{N} = \frac{1}{r}$. Let $CP = \{V_1, \dots, V_m\}$ be a set 480 of generated partitions with different numbers of clusters, where $V_i \in M_{hc_iN}$ contains c_i clusters which are balanced, $2 \leq c_i \leq N$. Assuming U_{GT} and $V_i \in CP$ are statistically independent, then RI suffers from GT1 bias. More specifically,

1. if $r = 2$, then RI has NCflat bias;
- 485 2. if $r > 2$, then RI has NCinc bias.

Theorem 3 provides an explanation of how GT1 bias influences RI. For example, it is easier to understand the behavior of RI shown in the GT1 bias testing in Section 5.2 (Figures 4a and 4b). Next, we introduce a theorem for the GT2 bias of RI.

490 **Theorem 4.** Let $U_{GT} \in M_{hrN}$ be a ground truth partition with r subsets $\{u_1, \dots, u_r\}$. Assume the first cluster u_1 in the ground truth has variable sizes,

and the remaining clusters $\{u_1, \dots, u_r\}$ are uniformly distributed in size across the remaining objects $N - |u_1|$. Let $P = \{p_1, \dots, p_r\}$ and $p_i = \frac{|u_i|}{N}$, $0 < p_i < 1$, and $\sum_{i=1}^r p_i = 1$. So $p_2 = p_3 = \dots = p_r = \frac{1-p_1}{r-1}$. Let $CP = \{V_1, \dots, V_m\}$ be a set of generated partitions with different numbers of clusters, where $V_i \in M_{hc_i N}$ contains c_i clusters which are balanced, $1 \leq i \leq m$. Assuming U_{GT} and $V_i \in CP$ are statistically independent, then RI suffers from GT2 bias. More specifically, let $p^* = \frac{2 + \sqrt{2(r-1)(r-2)}}{2r}$, we have:

When $r > 2$,

1. if $p_1 > p^*$, then RI has NCdec bias;
2. if $p_1 = p^*$, then RI has NCflat bias;
3. if $p_1 < p^*$, then RI has NCinc bias.

When $r = 2$

1. if $p_1 = p^*$, then RI has NCflat bias;
2. if $p_1 \neq p^*$, then RI has NCdec bias.

Theorem 4 provides an explanation of how GT2 bias affects the RI. For ex-

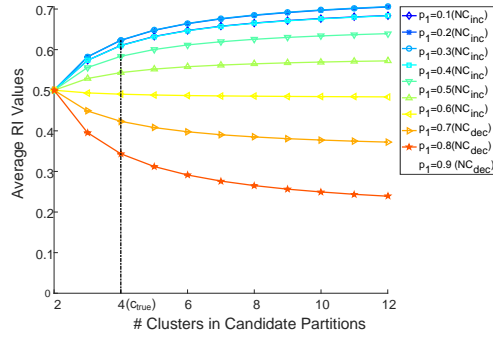


Figure 7: 100 trials average RI values with c in $\{2, \dots, 12\}$ for $c_{true} = 4$. $p_1 = |u_1|/N$, 9 steps 0.1 to 0.9, and the other 3 clusters uniformly distributed. When $p_1 > p^* = 0.683$, the RI decreases with c increasing (e.g., $p_1 = 0.7, 0.8, 0.9$). When $p_1 < p^* = 0.683$, the RI increases with c (e.g., $p_1 = 0.1, \dots, 0.6$).

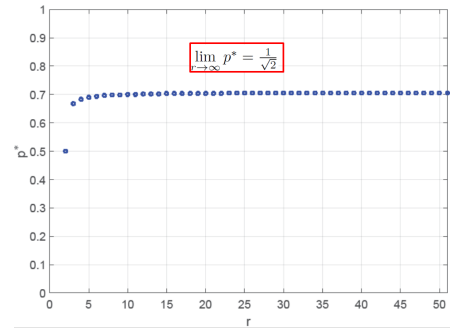


Figure 8: The relationship between p^* and r , for r in $\{2, \dots, 50\}$.

ample, in the GT2 bias testing (Section 5.3), $r = 5$, when $p_1 = 0.8 > \frac{1+\sqrt{3}}{4}$ ($\frac{1+\sqrt{3}}{4} \approx 0.683$), then the *RI* tends to decrease as c_i increases. Figure 7 illustrates GT2 bias on the *RI* graphically. The basis of this figure is the same experimental setting as Example 2 in Section 1.2 with $N = 1000$ and $c_{true} = 4$. We also show the relationship between r and p^* in Figure 8 (r takes integer values from 2 to 50). Actually, $\lim_{r \rightarrow \infty} p^* = \frac{1}{\sqrt{2}}$, where $\frac{1}{\sqrt{2}} \approx 0.7071$.

Next, we conclude our study by giving an experimental example to show that the *ARI* shows GT bias in certain scenarios.

7. Example of GT Bias for Adjusted Rand Index (*ARI*)

In this section we will illustrate that depending on the set of candidate partitions, *ARI* can show GT bias behavior in certain scenarios. Recall that the *ARI* in Figures 1 and 2 had NCflat bias for the method of partition generation used there. We will conduct experiments with a different set of candidates, and will discover that the *ARI* can be made to exhibit GT bias. We do two sets of experiments using the following protocols. We first generate ground truth U_{GT1} by randomly choosing 20% of the object labels from $N = 100,000$ objects to identify the first cluster. Then, we randomly choose 20% of the object labels from the remaining 80,000 objects as the second cluster, and finally, we randomly assign the rest of the cluster labels $[3, c_{true}]$ to the remaining objects, where $c_{true} \geq 3$. We generate a second ground truth U_{GT2} partition in the following way. We randomly choose 20% of the object labels from $N = 100,000$ objects as the first cluster. Then we randomly choose 50% of the object labels from the remaining 80,000 objects as the second cluster, and finally, we assign the rest of the cluster labels $[3, c_{true}]$ to the rest of objects, where $c_{true} \geq 3$. We set $c_{true} = 5$ for both U_{GT1} and U_{GT2} .

For these two sets of experiments, we generate 100 candidate partitions CP in this way. For each candidate $V_i \in CP$, we copy the first cluster from U_{GT1} or U_{GT2} as the first cluster in V_i . Then, we randomly assign the rest of cluster labels $[2, c_i]$ to the other 80,000 objects, where c_i ranges from $c = 2$ to $c = 15$.

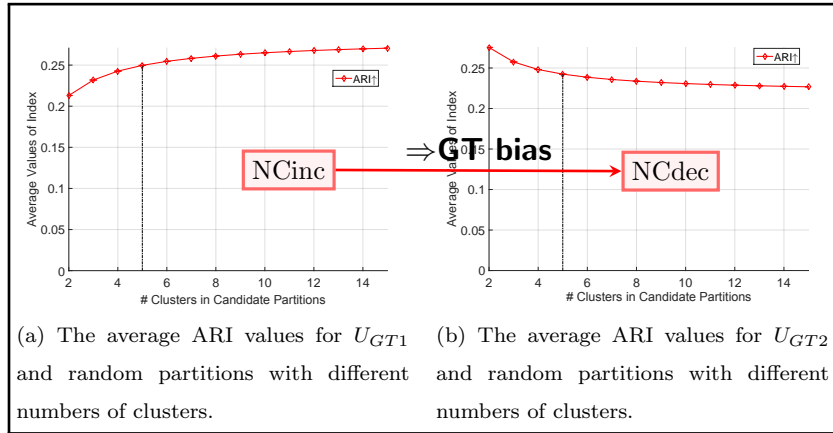


Figure 9: 100 trial average ARI values for two different ground truth and set of candidates with different numbers of clusters.

The results are shown in Figure 9. For these two experiments the ARI shows NCinc bias with U_{GT1} and shows NCdec bias with U_{GT} . Comparing Figures 9a and 9b shows that for these experiments, the ARI suffers from GT bias. For the exploration of this interesting phenomenon is beyond the scope of this paper, and is an interesting direction for future work.

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8. Conclusions

This paper examines several types of bias that may affect external cluster validity indices that are used to evaluate the quality of candidate partitions by comparison with a ground truth partition. They are: i) one of two types of NC bias (NCinc, NCdec), which arises when the mathematical model of the external CVI tends to be monotonic in the number of clusters in candidate partitions; ii) GT bias, which arises when the ground truth partitions alters the NC bias status of an external CVI; iii) GT1 bias, which arises when the numbers of clusters in the ground truth partitions alters the NC bias status of an external CVI; iv) GT2 bias, which arises when the distribution of the ground truth partitions alters the NC bias status of an external CVI.

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Numerical experiments with 26 pair-counting based external CVIs estab-

lished that for the method described in the examples, 5 of the 26 suffer from GT1bias and/or GT2bias, viz., the indices due to Rand (#1), Mirkin (#3),
555 Hubert (#5), Gower and Legendre (#24) and Rogers and Tanimoto (#25), the numbers referring to rows in Table 3. Actually, the 4 indices, Mirkin (#3), Hubert (#5), Gower and Legendre (#24) and Rogers and Tanimoto (#25), are all functions of RI. We point out that the observed bias behavior (NC bias, GT1 bias and GT2 bias) of the tested 26 indices was based on a particular way to
560 obtain candidate partitions. In our experiments the “clustering algorithm” used to generate the CPs was random draws from M_{hc_iN} . It is entirely possible that sets of CPs secured, for example, by running clustering clustering algorithms on a dataset will NOT exhibit the same bias tendencies. This is just another difficulty of external cluster validity indices, as was illustrated by the fact that
565 we could change the bias status of the ARI by changing the method of securing the candidate. The major point of this work is to draw attention to the fact that there can be a GT bias problem for external CVIs.

We then formulated an explanation for both types of GT bias with Rand Index based on the the Havrda-Charvat quadratic entropy. Our theory ex-
570 plained how RI’s NC bias behavior is influenced by the distribution of the ground truth partition and also the number of clusters in the ground truth. Our major results in Theorem 1, which provides a computable test that predicts the NC bias behavior of the Rand Index, and hence, all external CVIs related to it. Rand Index has been one of the most popular external CVIs due
575 to its simple, natural interpretation and has recently been applied in many research work [10, 11, 12, 14, 15, 16]. Thus, the identified GT bias behavior for RI with correponding explanation could be helpful for users who apply RI in their work. Finally, we gave an experimental example showing that the ARI can suffer from GT bias in certain scenarios.

580 We believe this to be the first systematic study of the effects of ground truth on the NC bias behavior of external cluster validity indices. We have termed this GT bias. There are many other external CVIs which have not been tested numerically or analyzed theoretically for GT bias. Our next undertaking

will be to study this phenomenon in the more general setting afforded by non
585 pair-counting based external CVIs.

Appendix A. Proofs

Proof of Lemma 1. As U and V are statistically independent, we can substitute Equation 10 into Equation 14, obtaining

$$\begin{aligned}
VI_2(U, V) &= 2H_2(U, V) - H_2(U) - H_2(V) \\
&= 2\left(H_2(U) + H_2(V) - \frac{1}{2}H_2(U)H_2(V)\right) - H_2(U) - H_2(V) \\
&= H_2(U) + (1 - H_2(U))H_2(V)
\end{aligned} \tag{A.1}$$

Proof of Theorem 1. According to lemma 1,

$$VI_2(U_{GT}, V) = H_2(U_{GT}) + (1 - H_2(U_{GT}))H_2(V) = a + bx \tag{A.2}$$

where $a = H_2(U_{GT})$ and $b = (1 - H_2(U_{GT})) = (1 - a)$ and $x = H_2(V)$. As any $V_i \in CP$ is uniformly distributed (balanced), then $H_2(V_i) = 2(1 - \sum_{i=1}^{c_i} (\frac{1}{c_i})^2)$ (refer to equation 8) and $H_2(V_i)$ increases as c_i increases. It is clear from
590 equation (A.2) that for fixed U_{GT} , VI_2 can be regarded as a straight line with y intercept $a = H_2(U_{GT})$ and slope $b = 1 - H_2(U_{GT}) = (1 - a)$, so the rate of growth (or decrease, or neither (flat)) of VI_2 depends on b . In other words, VI_2 could be increasing, decreasing or flat as c_i increases. More specifically, i) if $b > 0$, then $H_2(U_{GT}) < 1$, thus VI_2 increases as x (and c_i) increases; ii) if $b = 1$,
595 then $H_2(U_{GT}) = 1$, thus VI_2 is constant as x (and c_i) increases; iii) if $b < 0$, then $H_2(U_{GT}) > 1$, thus VI_2 decreases as x (and c_i) increases. According to Equation 16, we know that VI_2 and RI are inversely related. Thus, it is straightforward to prove the statements.

Proof of Corollary 1. According to Theorem 1, we know that depending on
600 the relationship between $H_2(U_{GT})$ and 1, i.e., the slope b in Equation A.2, that RI shows different NC bias status. As $H_2(U_{GT}) = 2(1 - \sum_{i=1}^r p_i^2)$ (Equation 8), then $b = 1 - H_2(U_{GT}) = 1 - 2(1 - \sum_{i=1}^r p_i^2) = 2(\sum_{i=1}^r p_i^2 - \frac{1}{2})$. Thus, we know

that the slope b , i.e., the relationship between $H_2(U_{GT})$ and 1, depends on the relationship between $\sum_{i=1}^r p_i^2$ and $\frac{1}{2}$. So, the three assertions of the corollary
605 follow by noting the relationship between $\sum_{i=1}^r p_i^2$ and $\frac{1}{2}$.

Proof of Theorem 2. According to Corollary 1, we know that the relationship between $\sum_{i=1}^r p_i^2$ and $\frac{1}{2}$ influences the NC bias status of RI. It is straightforward to see that p_i and r influence the relationship between $\sum_{i=1}^r p_i^2$ and $\frac{1}{2}$, thus p_i and r can potentially alter the NC bias status of RI. We have

$$\sum_{i=1}^r (p'_i)^2 - \frac{1}{2} = \sum_{i=1}^r (p'_i)^2 - \frac{1}{2} \sum_{i=1}^r p'_i = p'_1(p'_1 - \frac{1}{2}) + \sum_{i=2}^r p'_i(p'_i - \frac{1}{2}) \quad (\text{A.3})$$

Please note that p'_1 is the biggest cluster's density in the ground truth, based on which we discuss and summarize the influence of p_i and r on the NC bias status of RI. We can discuss the relationship between $p'_1(p'_1 - \frac{1}{2})$ and $\sum_{i=2}^r p'_i(p'_i - \frac{1}{2})$, which is equivalent to the relationship between $\sum_{i=1}^r p_i^2$ and $\frac{1}{2}$,
610 for the different NC bias status.

When $r > 2$: 1) if $p'_1 > \frac{1}{2}$, because $\sum_{i=1}^r p'_i = 1$, then $p'_2, \dots, p'_r < \frac{1}{2}$. Thus, with the help of Corollary 1, we have: i) if $p'_1(p'_1 - \frac{1}{2}) > \sum_{i=2}^r p'_i(\frac{1}{2} - p'_i)$, then $\sum_{i=1}^r (p'_i)^2 > \frac{1}{2}$, thus RI has NCdec bias; ii) if $p'_1(p'_1 - \frac{1}{2}) = \sum_{i=2}^r p'_i(\frac{1}{2} - p'_i)$, then $\sum_{i=1}^r (p'_i)^2 = \frac{1}{2}$, thus RI has NCflat bias; iii) if $p'_1(p'_1 - \frac{1}{2}) < \sum_{i=2}^r p'_i(\frac{1}{2} - p'_i)$,
615 then $\sum_{i=1}^r (p'_i)^2 < \frac{1}{2}$, thus RI has NCinc bias.

2) if $p'_1 = \frac{1}{2}$, then $p'_2, \dots, p'_r < \frac{1}{2}$ and $\sum_{i=1}^r (p'_i)^2 < \frac{1}{2}$, thus RI has NCinc bias;

3) if $p'_1 < \frac{1}{2}$, then $p'_2, \dots, p'_r < \frac{1}{2}$ and $\sum_{i=1}^r (p'_i)^2 < \frac{1}{2}$, thus RI has NCinc bias.

When $r = 2$: 1) if $p'_1 > \frac{1}{2}$, then $p'_1(p'_1 - \frac{1}{2}) > p'_2(\frac{1}{2} - p'_2)$ and $\sum_{i=1}^r (p'_i)^2 > \frac{1}{2}$, thus RI has NCdec bias; 2) if $p'_1 = \frac{1}{2}$, then $p'_2 = \frac{1}{2}$ and $\sum_{i=1}^r (p'_i)^2 = \frac{1}{2}$, thus RI
620 has NCflat bias. Thus, the RI suffers from GT bias according to the distribution of ground truth P and the number of clusters r in the ground truth.

Proof of Theorem 3. Corollary 1 shows that the NC bias of the RI depends on the relationship between $\sum_{i=1}^r (p_i)^2$ and $\frac{1}{2}$. Since $p_i = \frac{1}{r}$, then $\sum_{i=1}^r (p_i)^2 - \frac{1}{2} = \frac{1}{2}$

Then, according to Corollary 1, we have i) if $r = 2$, then RI has NCflat bias; ii) if $r > 2$, then RI has NCinc bias. By definition 3, different values for r
625

in U_{GT} , i.e., $r = 2$ or $r > 2$, result in different NC bias status for the RI, thus RI has GT1 bias.

Proof of Theorem 4. According to Corollary 1, we know that the relationship between $\sum_{i=1}^r (p_i)^2$ and $\frac{1}{2}$ determines the NC bias status of the RI. As $p_i = \frac{1-p_1}{r-1}$, $i = 2, \dots, r$, we have:

$$\begin{aligned} \sum_{i=1}^r p_i^2 - \frac{1}{2} &= p_1^2 + \sum_{i=2}^r p_i^2 - \frac{1}{2} \\ &= \frac{r}{r-1} p_1^2 - \frac{2}{r-1} p_1 + \frac{3-r}{2(r-1)} \end{aligned} \quad (\text{A.4})$$

Equation A.4 is quadratic in p_1 , and has one real positive root $p^* = \frac{2 + \sqrt{2(r-1)(r-2)}}{2r}$ in our case. Then:

630 **When $r > 2$:** i) if $p_1 > p^*$, then $\sum_{i=1}^r (p_i)^2 > \frac{1}{2}$, thus RI has NCdec bias; ii) if $p_1 = p^*$, then $\sum_{i=1}^r (p_i)^2 = \frac{1}{2}$, thus RI has NCflat bias; iii) if $p_1 < p^*$, then $\sum_{i=1}^r (p_i)^2 < \frac{1}{2}$, thus RI has NCinc bias.

When $r = 2$: i) if $p_1 = p^*$, then $\sum_{i=1}^r (p_i)^2 = \frac{1}{2}$, thus RI has NCflat bias; ii) if $p_1 \neq p^*$, then $\sum_{i=1}^r (p_i)^2 > \frac{1}{2}$, thus RI has NCdec bias.

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