Minimum adjusted Rand index for two clusterings of a given size

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Abstract

In an unpublished presentation, Steinley reported that the minimum adjusted Rand index for the comparison of two clusterings of size \( r \) is \(-1/r\). However, in a subsequent paper Chacón noted that this apparent bound can be lowered. Here, it is shown that the lower bound proposed by Chacón is indeed the minimum possible one. The result is even more general, since it is valid for two clusterings of possibly different sizes.

Keywords: adjusted Rand index, external clustering evaluation, minimum agreement

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1 Introduction

The adjusted Rand index is one of the most commonly used similarity measures to compare two clusterings of a given set of objects. Indeed, it is the recommended criterion for external clustering evaluation in the seminal study of Milligan and Cooper (1986). Nevertheless, many other measures for external clustering evaluation were recently surveyed in Meilă (2016).

Initially, Rand (1971) considered a similarity index between two clusterings (the Rand index) defined as the proportion of object pairs that are either assigned to the same cluster in both clusterings or to different clusters in both clusterings. However, Morey and Agresti (1984) noted that such an index does not take into account the possible agreement by chance, and Hubert and Arabie (1985) introduced a corrected-for-chance version of the Rand index, which is usually known as the adjusted Rand index (ARI).

Exploring the situations of extremal agreement, as measured by the ARI, has been a subject of interest since the very inception of this index. Indeed, Hubert and Arabie (1985) posed the problem of finding the maximum ARI subject to given clustering marginals; i.e., when constrained to have fixed, given cluster sizes in each of the clusterings. Numerical algorithms to tackle this problem were developed initially by Messatfa (1992), and later by Brusco and Steinley (2008) and Steinley, Hendrickson and Brusco (2015), and an explicit solution for clusterings of size 2 has been recently shown in Chacón (2020).

A related but different problem was considered in an unpublished presentation by Steinley (2015). There, it was reported that the minimum ARI for two clusterings with $r$ clusters is $-1/r$. However, Chacón (2019) noted that it is possible to find clustering pairs with even lower agreement in terms of the ARI, and conjectured a different lower bound, valid for the more general case where the two clustering sizes are not necessarily equal. The main contribution of this paper is to show that the latter bound is indeed the smallest possible one. More precise notation is introduced in Section 2, where in addition the main result is rigorously stated. Its proof and another auxiliary lemma of independent interest are given in Section 3.

2 Notation and main result

A clustering of a set $\mathcal{X}$ of $n$ objects is a partition of $\mathcal{X}$ into non-empty, disjoint and exhaustive classes, called clusters. The number of such classes is known as the size of the clustering. Given two clusterings $\mathcal{C} = \{C_1, \ldots, C_r\}$ and $\mathcal{D} = \{D_1, \ldots, D_s\}$, of sizes $r$ and $s$, respectively, all the information regarding their concordance is registered in the $r \times s$ matrix $\mathbf{N}$ whose $(i, j)$th element $n_{ij}$ records the cardinality of $C_i \cap D_j$. This matrix is usually known as confusion matrix or contingency table. Its row-wise and column-wise totals, $(n_{1+}, \ldots, n_{r+})$ and $(n_{+1}, \ldots, n_{+s})$, with $n_{i+} = \sum_{j=1}^s n_{ij}$ and $n_{+j} = \sum_{i=1}^r n_{ij}$, give an account of the cluster
sizes in \( C \) and \( D \), respectively, and are commonly referred to as the marginals, or marginal clustering distributions. Note that all cluster sizes must be strictly greater than zero in order to respect the assumptions on the clustering sizes.

The Rand index is a summary statistic for \( N \), based on inspecting the behaviour of object pairs across the two clusterings. There are four possible types of object pairs, formed by taking into account if: a) both objects belong to the same cluster in both clusterings, b) they belong to the same cluster in \( C \) but to different clusters in \( D \), c) they belong to different clusters in \( C \) but to the same cluster in \( D \), and d) they belong to different clusters in both clusterings. The cardinalities of each of these categories will be denoted \( a \), \( b \), \( c \) and \( d \), respectively. They can be easily expressed in terms of the entries of \( N \) and its marginals; for instance, Hubert and Arabie (1985) noted that

\[
\begin{align*}
  a &= \frac{1}{2} \left( \sum_{i=1}^r \sum_{j=1}^s n_{ij}^2 \right) - n, \\
  b &= \frac{1}{2} \left( \sum_{i=1}^r n_{ii}^2 - \sum_{i=1}^r \sum_{j=1}^s n_{ij}^2 \right), \\
  c &= \frac{1}{2} \left( \sum_{j=1}^s n_{jj}^2 - \sum_{j=1}^s \sum_{i=1}^r n_{ij}^2 \right), \\
  d &= \left( \sum_{i=1}^r \sum_{j=1}^s n_{ij}^2 \right) + n^2 - \sum_{i=1}^r n_{ii}^2 - \sum_{j=1}^s n_{jj}^2.
\end{align*}
\]

With this notation, the Rand index is defined as

\[ RI = \frac{(a + d)}{(a + b + c + d)} = \frac{(a + d)}{N} \]

where \( N = a + b + c + d = \binom{n}{2} = n(n - 1)/2 \) is the total number of pairs of objects from \( X \). It takes the values in \([0, 1]\), with 1 corresponding to perfect agreement between the clusterings and 0 attained for the comparison of the two so-called trivial clusterings: one with all the \( n \) objects in a single cluster, and the other one with \( n \) clusters with a single object in each of them (see Albatineh, Niewiadomska-Bugaj and Mihalko, 2006).

One of the drawbacks of the Rand index is that it does not take into account the possibility of agreement by chance between the two clusterings (Morey and Agresti, 1984). Hence, Hubert and Arabie (1985) obtained \( E[RI] \), the expected value of this index when the partitions are made at random, but keeping the same marginal clustering distributions, and suggested to alternatively use the ARI, a corrected-for-chance version of the Rand index defined by

\[ ARI = \frac{(RI - E[RI])}{(1 - E[RI])}. \]

Steinley (2004) provided a concise formula for the ARI, which reads as follows:

\[ ARI = \frac{N(a + d) - ((a + b)(a + c) + (c + d)(b + d))}{N^2 - ((a + b)(a + c) + (c + d)(b + d))}. \]

Note that the ARI is undefined if \( r = s = 1 \), so it will be assumed henceforth that at least one of the clusterings has more than one cluster, i.e., that \( \max\{r, s\} > 1 \).

These preliminaries allow us to formulate the main result of this paper, which is the following.
Theorem 1. The minimum ARI for two clusterings of sizes \( r \) and \( s \), respectively, is attained for a comparison of \( n = r + s - 1 \) objects, in which the \( r \times s \) contingency table \( N \) has exactly one row of ones, exactly one column of ones and all the remaining entries are zeroes. Such a minimum value can be explicitly written as

\[
\min ARI = \left[ 1 - \frac{1}{2} \left( \frac{r + s - 1}{2} \right) \left( \binom{r}{2}^{-1} + \binom{s}{2}^{-1} \right) \right]^{-1}
\]  

(1)

if \( \min \{ r, s \} \geq 2 \) and \( \min ARI = 0 \) if \( \min \{ r, s \} = 1 \).

The expression for the minimum ARI given in Theorem 1 is equivalent to, but notably simpler than, the one announced in Chacón (2019). For \( r = s \geq 2 \), Equation (1) simplifies to \(-r / (3r - 2)\), and this value is strictly lower than the conjectured \(-1/r\) in Steinley (2015) for all \( r > 2 \).

In order to get insight on the behaviour of the minimum ARI as \( r \) and \( s \) increase, it is useful to note that, by means of the simple first order approximation \( \binom{r}{2} \sim \frac{r^2}{2} \), it follows that

\[
\min ARI \approx -2 \frac{r^2 s^2}{r^4 + 2r^3 s + 2r s^3 + s^4}
\]

for large values of \( r \) and \( s \).

3 Proofs

The proof of Theorem 1 makes use of the following result, which is of independent interest. Intuitively, it shows that if a certain amount is to be distributed among several parts, the configuration that yields the maximum sum of the part squares is that which accumulates the highest possible quantity in one of the parts and keeps the remaining ones to their minimum.

Lemma 1. Let \( a_1 \geq a_2 \geq \cdots \geq a_p \) and \( t \geq \sum_{i=1}^p a_i \) be real numbers and consider the region

\[
A \equiv A(t; a_1, \ldots, a_p) = \{(x_1, \ldots, x_p) \in \mathbb{R}^p: \sum_{i=1}^p x_i = t \text{ and } x_i \geq a_i \text{ for all } i = 1, \ldots, p\}.
\]

The maximum of \( \sum_{i=1}^p x_i^2 \) over \( A \) is attained for \( x_1 = t - \sum_{i=2}^p a_i, x_2 = a_2, \ldots, x_p = a_p \). Hence, \( \max \{ \sum_{i=1}^p x_i^2: (x_1, \ldots, x_p) \in A \} = \left( t - \sum_{i=2}^p a_i \right)^2 + \sum_{i=2}^p a_i^2 \).

Proof. The result follows by noting that if \( a \leq b \) then

\[
a^2 + b^2 \leq (a - c)^2 + (b + c)^2
\]

for any \( c \geq 0 \).

Now we are ready to prove the main result of the paper.

Proof of Theorem 1. First note that minimizing the ARI is equivalent to maximizing the semimetric \( ARD = 1 - ARI \) introduced in Chacón (2019), where it is also shown that it can
be readily expressed as

\[
\text{ARD} \equiv \text{ARD}(a, b, c, d) = \frac{N(b + c)}{(a + b)(b + d) + (a + c)(c + d)}.
\] (2)

It is clear that the roles of \(b\) and \(c\) in (2) are interchangeable, in the sense that \(\text{ARD}(a, b, c, d) = \text{ARD}(a, c, b, d)\). The same is true for the roles of \(a\) and \(d\). Moreover, \(\text{ARD}\) is clearly a decreasing function of \(a\) and \(d\), so its maximum value is attained for the lowest possible values of \(a\) and \(d\).

Albatineh, Niewiadomska-Bugaj and Mihalko (2006) noted that \(a = 0\) if and only if \(n_{ij} \in \{0, 1\}\) for all \(i = 1, \ldots, r\) and \(j = 1, \ldots, s\) and \(d = 0\) if and only if \(\min\{r, s\} = 1\). Hence, when one of the clusterings consists of a single cluster, the contingency table with maximum \(\text{ARD}\) is a row or column vector of ones, with resulting \(\text{ARD} = 1\), so minimum \(\text{ARI} = 0\).

On the other hand, if \(\min\{r, s\} \geq 2\) then necessarily \(d > 0\), but it is equally possible to have \(a = 0\) if all the entries of \(N\) are just zeroes or ones, so this will be imposed henceforth. Notice that this yields \(n \leq rs\), which means that the highest values of the \(\text{ARD}\) are achieved when the number of objects is small. For \(a = 0\) we have \(d = N - (b + c)\), and the \(\text{ARD}\) simplifies to

\[
\text{ARD} = \frac{N(b + c)}{b^2 + c^2 + \{(N - (b + c))(b + c)\}} = \frac{N}{N - 2bc/(b + c)},
\] (3)

which is an increasing function of \(b\) and \(c\). So, to maximize it, we must find the maximum possible values for \(b\) and \(c\).

Since \(a = 0\), it follows that \(b = \left(\sum_{i=1}^{r} n_{i+}^2 - n\right)/2\) and \(c = \left(\sum_{j=1}^{s} n_{+j}^2 - n\right)/2\). Hence, maximizing \(b\) is equivalent to maximizing the sum of the squared sizes of the clusters of \(\mathcal{C}\), constrained to the facts that the total size is \(n\) and each cluster has size greater than or equal to one (because degenerate, empty clusters are not allowed). This is exactly the setting of Lemma 1 for \(p = r, a_1 = \cdots = a_r = 1\) and \(t = n\). So for \(n \geq r\) (which is necessary to have \(r\) non-empty clusters in \(\mathcal{C}\)), the maximum value of \(b\) is attained when there is a cluster in \(\mathcal{C}\) with \(n - (r - 1)\) objects and the remaining \(r - 1\) clusters have one object each, so that \(\sum_{i=1}^{r} n_{i+}^2 = \{n - (r - 1)\}^2 + r - 1\).

Moreover, the fact that all \(n_{ij} \in \{0, 1\}\) also implies that the maximum size of any cluster in \(\mathcal{C}\) is \(s\), which for the configuration maximizing \(b\) yields \(n - (r - 1) \leq s\). And, in view of the maximum value of \(\sum_{i=1}^{r} n_{i+}^2\), among all the sample sizes \(n\) that satisfy the latter constraint, the one for which \(b\) is maximum corresponds precisely to \(n - (r - 1) = s\), that is, to \(n = r + s - 1\). Hence, the confusion matrix that maximizes \(b\) must have one row with all its entries equal to one, and each of the remaining rows having exactly one entry equal to one and all the rest equal to zero. In principle, the nonzero entries of the latter rows could be arbitrarily placed but, mimicking the above reasoning regarding \(b\), the value of \(c\) is maximized when there is a column with all its entries equal to one, so the contingency...
table configuration that maximizes the ARD must be precisely the one announced in the statement of the theorem.

In addition, it is straightforward to check that the configuration that maximizes the ARD has \( a = 0, b = \binom{s}{2}, c = \binom{r}{2} \) and \( d = \binom{n}{2} - \binom{r}{2} - \binom{s}{2} = (r-1)(s-1) \) since \( n = r + s - 1 \). Hence, from [3] it follows that the maximum ARD is given by

\[
1 - 2 \left( \frac{r + s - 1}{2} \right)^{-1} \left( \frac{r}{2} \frac{s}{2} \right) \left\{ \frac{r}{2} + \frac{s}{2} \right\}^{-1}
\]

so that the minimum ARI is as stated in the theorem.

\[\square\]

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