A more efficient algorithm to compute the Rand Index for change-point problems

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ABSTRACT
In this paper we provide a more efficient algorithm to compute the Rand Index when the data cluster comes from change-point detection problems. Given $N$ data points and two clusters of size $r$ and $s$, the algorithm runs on $O(r + s)$ time complexity and $O(1)$ memory complexity. The traditional algorithm, in contrast, runs on $O(rs + N)$ time complexity and $O(rs)$ memory complexity.

KEYWORDS
Rand Index; Change-point detection; Segmentation; Machine Learning; Clustering

1. Introduction

The Rand Index is a classical evaluation metric in Statistics and Machine Learning. Originally proposed for clustering problems (Rand (1971)), it has found applications or adaptations to other tasks such as computer vision (Unnikrishnan, Pantofaru, and Hebert (2005), Unnikrishnan, Pantofaru, and Hebert (2007), coreference resolution (Recasens and Hovy (2011)), and change-point detection (Truong, Oudre, and Vayatis (2020)). When applied to the latter, the additional structure of the problem studied imposes that the clusters detected must be contiguous. For this scenario, we prove that the Rand Index can be computed in a more efficient manner.

2. Traditional Rand Index algorithm

Given two integers $r < s$, we will use the notation $r: s$ for $\{r, r+1, \ldots, s\}$. Let $A$ be a non-empty set, $N \in \mathbb{N}$, and $(x_i)_{i=1}^N$ a data set with $x_i \in A$ for all $i \in 1:N$. A cluster is defined as a partition $C = \{C_1, \ldots, C_r\}$ of $1:N$. This partition is usually learned by applying a machine learning algorithm, and the purpose group together data points that share feature similarities.

Denote by $I_C(i, j)$ the indicator function that sample $x_i$ and $x_j$ are on the same set for the cluster $C$. Given two clusters $C_1$ and $C_2$, define
\[ N_{11} = \left| \{(i, j) \in (1 : N) \times (1 : N) \mid i < j \text{ and } I_{C_1}(i, j) = 1 = I_{C_2}(i, j) \} \right| , \]
\[ N_{00} = \left| \{(i, j) \in (1 : N) \times (1 : N) \mid i < j \text{ and } I_{C_1}(i, j) = 0 = I_{C_2}(i, j) \} \right| . \]

The Rand Index is then defined as

\[ RI = \frac{N_{00} + N_{11}}{\binom{N}{2}} . \] (1)

The term \( N_{11} \) measures how many pairs of indices both clusters grouped together, and the term \( N_{00} \) how many pairs are put on different groups by both clusters. Therefore, \( N_{00} + N_{11} \) measures the total number of agreements between clusters. Finally, we scale by \( \binom{N}{2} \), the total number of pairs. The metric ranges on \([0, 1]\), attaining 1 if, and only if, the clusters are identical, and 0 if they are totally dissimilar.

Write \( C_1 = \{C_{11} \ldots C_{1r}\} \) and \( C_2 = \{C_{21} \ldots C_{2s}\} \). The traditional algorithm iterates through the data set to build a \( r \times s \) contingency table whose elements are \( n_{ij} = |C_{1i} \cap C_{2j}| \). The Rand Index is then computed by the equation

\[ RI = 1 - \frac{1}{2} \left( \sum_{i=1}^{r} \left( \sum_{j=1}^{s} n_{ij} \right)^2 + \sum_{j=1}^{s} \left( \sum_{i=1}^{r} n_{ij} \right)^2 \right) - \sum_{i=1}^{r} \sum_{j=1}^{s} (n_{ij})^2 \] . (2)

Therefore, the time complexity of the algorithm is \( O(rs + N) \), and its memory complexity is \( O(rs) \) since we need to store the contingency table.

3. Efficient Rand Index algorithm for CPD

Change-point detection is a multidisciplinary field of statistics which provides reliable methodologies to detect abrupt changes in time-series. Albeit its methods are not the focus of this work, we provide a simplified offline formulation of the problem. Consider a sequence \( \{X_i\}_{i=1}^{N} \) of independent random variables where \( X_i \) has cumulative distribution function \( F_i \) for all \( i \in 1 : N \). Assume that there exists a set \( C^* \) such that

\[ C^* = \{c^* \in 1 : (N - 1) \mid F_{c^*} \neq F_{c^*+1} \} . \]

We name \( C^* \) the true change-point set, and its elements are called change-points.

Whenever a change-point occurs, the distribution of the data changes, capturing the idea of abrupt change in the process behavior. The random variables between two consecutive change-points have the same distribution, so that they can be seen as belonging to the same group.

The main purpose of the change-point detection methods is to estimate the set \( C^* \) and the CDFs of each interval. For an introduction to change-point detection see Niu, Hao, and Zhang (2016) and Truong et al. (2020).
3.1. Rand Index CPD equation

Given $C = \{c_1, \ldots, c_k\}$, the sorted change-point set detected, there is a natural identification to a partition of $1 : N$. Defining $c_0 = 0$ and $c_{k+1} = N$, the set $C$ can be seen as the cluster

$$C = \{(c_{i+1})_{i=0}^k\}.$$  \hspace{1cm} (3)

Hence, a set with $k$ change-points has $k + 1$ contiguous clusters, each one ending on a change-point. To exemplify, assume $N = 10$ and $C = \{3, 8\}$. The equivalent cluster is $C = \{1, 2, 3\}, \{4, 5, 6, 7, 8\}, \{9, 10\}$.

When the clusters are contiguous, the Rand Index has a special form which depends only on the change-points.

**Theorem 3.1.** Let $C = \{c_1, c_2, \ldots c_r\}$ and $C^* = \{c^*_1, c^*_2, \ldots c^*_s\}$ be sorted change-point sets. Define $c_0 = c^*_0 = 0$ and $c_{r+1} = c^*_{s+1} = N$. Identifying the sets with clusters as in expression (3) the Rand Index is given by

$$RI = 1 - \frac{\sum_{i=0}^{r} \sum_{j=0}^{s} n_{ij} |c_{i+1} - c^*_{j+1}|}{\binom{N}{2}},$$

where

$$n_{ij} = \max \left(0, \min \left(c_{i+1}, c^*_{j+1}\right) - \max \left(c_i, c^*_j\right)\right).$$

**Proof.** Our strategy is to calculate the expression $a + b$ in the original formula by doing a partition of the pairs according to each element. For each $x$ in $1 : (N - 1)$ define $A_x$, the set of pairs $(x, y)$ where $x < y$ and which the partitions agree. Notice the partitions agree if they are in a single set in both partitions or in different sets in both partitions.

Since this pair is being counted in the sum $a + b$ and each pair of $a + b$ is in some $A_x$, we have that

$$a + b = \sum_{x=1}^{N-1} |A_x|.$$  

The restriction $x < y$ avoids a pair of being counted twice.

First, we know that there are a total of $N - x$ pairs $(x, y)$ of the form $x < y$. Let $i(x)$ and $j(x)$ be the indices of the smallest change-points in $C$ and $C^*$ that are greater or equal than $x$. Hence, $x \in (c_{i(x)} + 1) : c_{i(x)}$ and $x \in (c^*_{j(x)} + 1) : c^*_{j(x)}$. The partitions agree on all $(x, y)$ pairs where $y \in (x + 1) : \min(c_{i(x)}, c^*_{j(x)})$ since they place $x$ and $y$ on the same set. Additionally, they agree on the pairs $(x, z)$ for $z \in (\max(c_{i(x)}, c^*_{j(x)}) + 1) : N$ since they place $x$ and $z$ on different sets.

From this reasoning, there are a total of $|c_{i(x)} - c^*_{j(x)}|$ disagreements, so that
\[ |A_x| = (N - x) - |c_i(x) - c_j^*(x)|. \]

We can now substitute in the original equation

\[ RI = \sum_{x=1}^{N-1} \frac{|A_x|}{\binom{N}{2}} = 1 - \frac{\sum_{x=1}^{N-1} |c_i(x) - c_j^*(x)|}{\binom{N}{2}}. \]

Let \( I_{ij} = ((c_i + 1) : c_{i+1}) \cap ((c_j^* + 1) : c_{j+1}^*). \) It is easy to show that \((I_{ij})_{i=1,j=1}^{r,s}\) forms a partition for \(1 : N.\) For every element \(x\) of \(I_{ij}\), we have \(i(x) = i + 1\) and \(j(x) = j + 1\), so that \(|A_x| = |c_{i+1} - c_{j+1}^*|\). Hence

\[
\sum_{x=1}^{N-1} |c_i(x) - c_j^*(x)| = \sum_{i=0}^{r} \sum_{j=0}^{s} \sum_{x \in I_{ij}} |A_x|
= \sum_{i=0}^{r} \sum_{j=0}^{s} n_{ij} |c_{j+1}^* - c_{i+1}|,
\]

where \(n_{ij} = \#I_{ij}\). It is straightforward to show that

\[ n_{ij} = \max \left(0, \min \left(c_{i+1}, c_{j+1}^*\right) - \max \left(c_i, c_j^*\right)\right), \]

which finishes the proof.

\[ \square \]

### 3.2. Rand Index CPD algorithm

Considering that the change-point sets are sorted, 0 at the first entry and \(N\) at the last entry, it is easy to provide an algorithm to compute the expression above. However, most terms \(n_{ij}\) evaluate 0. With a bit of effort, we can avoid unnecessary computations.

On one hand, if at the end of iteration \(i\)-th iteration for the first summation and \(j\)-th iteration for the second summation we have \(c_{i+1} < c_{j+1}^*\), then we must have that \(n_{ik}\) will be 0 for all \(k \geq j+1\). This happens because the \(\min \left(c_{i+1}, c_k^*\right) - \max (c_i, c_k^*) = c_{i+1} - c_k^* < 0\).

On the other hand, if \(c_{i+1} \geq c_{j+1}^*\), then we know that \(n_{ik}\) evaluates 0 for all \(k \leq j\). Therefore, on the value of the index \(i\), we can skip all values of \(j\) below \(k\). The pseudocode below provides an implementation taking these observations into account.
Algorithm 1 Compute Rand Index CPD

```plaintext
procedure RICPD(C1, C2)
    r ← size(C1)  ▷ Note C1[1] = 0; C1[r] = N
    s ← size(C2)  ▷ Note C2[1] = 0; C2[s] = N
    d ← 0         ▷ Dissimilarity
    begj ← 0      ▷ Skipping unnecessary iterations

    for i ∈ 1 : (r - 1) do
        for j ∈ begj : (s - 1) do
            M ← min(C1[i + 1], C2[j + 1]) − max(C1[i], C2[j])
            M ← max(0, M)
            d ← d + M|C1[i + 1] − C2[j + 1]|
            if C1[i + 1] < C2[j + 1] then
                break
            else
                begj ← j + 1
            end if
        end for
    end for
    N ← C1[r]
    RI ← 1 − \frac{d}{\binom{s}{2}}

    return RI
end procedure
```

It is straightforward that the algorithm runs on $O(1)$ in memory complexity. For the time complexity, given $i ∈ 0 : r$, let $J(i) = \max\{j ∈ 0 : s|c^i_{j+1} ≤ c_{i+1}\}$. The $i$-th iteration does not perform any computations on the indices smaller than $J(i - 1)$ since we update the starting location of $j$. Moreover, it breaks on $j = J(i) + 1$. Since the number of operations is constant, the time complexity $T(r, s)$ satisfies

\[
T(r, s) \leq \beta + \sum_{i=1}^{r} \alpha(J(i) + 1 - J(i - 1)) \\
\leq \beta + r\alpha + \alpha \sum_{i=1}^{r} (J(i) - J(i - 1)) ,
\]

for some constants $\alpha, \beta > 0$. Observing that we have a telescopic sum and that $J(r) = s$, we get

\[
T(r, s) \leq \beta + \alpha(r + s) = O(r + s) .
\]
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References

Niu, Y. S., Hao, N., & Zhang, H. (2016, 11). Multiple change-point detection: A selective overview. *Statist. Sci., 31*(4), 611–623. Retrieved from https://doi.org/10.1214/16-STS587

Rand, W. M. (1971). Objective criteria for the evaluation of clustering methods. *Journal of the American Statistical Association, 66*, 846-850.

Recasens, M., & Hovy, E. (2011). Blanc: Implementing the rand index for coreference evaluation. *Natural Language Engineering, 17*(4), 485–510.

Truong, C., Oudre, L., & Vayatis, N. (2020, Feb). Selective review of offline change point detection methods. *Signal Processing, 167*, 107299. Retrieved from http://dx.doi.org/10.1016/j.sigpro.2019.107299

Unnikrishnan, R., Pantofaru, C., & Hebert, M. (2005). A measure for objective evaluation of image segmentation algorithms. 2005 IEEE Computer Society Conference on Computer Vision and Pattern Recognition (CVPR’05) - Workshops, 34-34.

Unnikrishnan, R., Pantofaru, C., & Hebert, M. (2007). Toward objective evaluation of image segmentation algorithms. *IEEE Transactions on Pattern Analysis and Machine Intelligence, 29*(6), 929-944.

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