
Pairwise Adjusted Mutual Information

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Abstract

1 A well-known metric for quantifying the similarity between two clusterings is
2 the adjusted mutual information. Compared to mutual information, a corrective
3 term based on random permutations of the labels is introduced, preventing two
4 clusterings being similar by chance. Unfortunately, this adjustment makes the
5 metric computationally expensive. In this paper, we propose a novel adjustment
6 based on pairwise label permutations instead of full label permutations. Specifically,
7 we consider permutations where only two samples, selected uniformly at random,
8 exchange their labels. We show that the corresponding adjusted metric, which
9 can be expressed explicitly, behaves similarly to the standard adjusted mutual
10 information for assessing the quality of a clustering, while having a much lower
11 time complexity. Both metrics are compared in terms of quality and performance
12 on experiments based on synthetic and real data.

13 1 Introduction

14 A well-known metric for quantifying the similarity between two clusterings of the same data is
15 the adjusted mutual information [Nguyen *et al.*, 2009; Vinh *et al.*, 2010]. Compared to mutual
16 information, this metric is *adjusted* against chance, meaning that the similarity cannot be due to
17 randomness but only to the structure of the dataset, appearing in both clusterings. This is the reason
18 why this metric is widely used in unsupervised learning, see [Zhang *et al.*, 2013; Thirion *et al.*, 2014;
19 Taha and Hanbury, 2015; Yang *et al.*, 2016; Wang *et al.*, 2017] for various applications.

20 The standard way of adjusting mutual information against chance is through random label permuta-
21 tions of one of the clusterings [Vinh *et al.*, 2010]. Unfortunately, this adjustment makes the metric
22 computationally expensive. Specifically, the time complexity of the metric is in $O(\max(k, l)n)$,
23 where k, l are the numbers of clusters in each clustering and n is the number of samples [Romano *et*
24 *al.*, 2014]. As a comparison, the time complexity of mutual information is equal to $O(kl)$ given the
25 contingency matrix of the clusterings, i.e., the matrix counting the number of samples in each pair of
26 clusters, one per clustering. The additional computational effort required by adjustment is significant
27 as the number of samples n is typically much larger than the numbers of clusters k, l .

28 In this paper, we propose a novel adjustment based on *pairwise* permutations. That is, we consider
29 permutations where only two samples, selected uniformly at random, exchange their labels. We
30 show that the corresponding adjusted metric, we refer to as *pairwise adjusted mutual information*,
31 is as efficient as adjusted mutual information for assessing the quality of a clustering, with a much
32 lower time complexity. In particular, the time complexity is the *same* as that of mutual information.
33 The gain in complexity is significant, as the computation time is now independent of the number of
34 samples n , given the contingency matrix.

35 The rest of the paper is organized as follows. We first provide the definition and key properties of
36 adjusted mutual information in the general setting of information theory. We then introduce mutual
37 information with pairwise adjustment and explain why the exact same properties are satisfied by

38 this new notion of adjusted mutual information. The application of both notions of adjustment to
 39 clustering, including the explicit expressions of the corresponding metrics, is presented in section 4.
 40 Experiments on both synthetic and real data are presented in section 5. Section 6 concludes the paper.

41 2 Adjusted mutual information

42 Let P be the uniform probability measure on $\Omega = \{1, \dots, n\}$, for some positive integer n . Let X, Y
 43 be random variables on the probability space (Ω, P) . Without any loss of generality, we assume that
 44 X and Y are mapping from Ω to sets consisting of consecutive integers, starting from 1. Denoting by
 45 H the entropy, the mutual information between X and Y is defined by [Cover and Thomas, 1991]:

$$I(X, Y) = H(X) + H(Y) - H(X, Y). \quad (1)$$

This is the information shared by X and Y , which is equal to 0 if X and Y are independent. A
 distance between X and Y can then be defined by:

$$d(X, Y) = H(X, Y) - I(X, Y) = H(X|Y) + H(Y|X).$$

46 This distance, known as the variation of information, is a metric in the quotient space of random
 47 variables under the equivalence relation $X \sim Y$ if and only if there is some bijection φ such that
 48 $X = \varphi(Y)$ [Meilä, 2003].

49 **Adjusted mutual information.** The adjusted mutual information between X and Y , corresponding
 50 to the mutual information between X and Y *adjusted* against chance, is defined by:

$$\Delta I(X, Y) = I(X, Y) - \mathbb{E}(I(X, Y_\sigma)), \quad (2)$$

51 where Y_σ is the random variable $Y \circ \sigma$, for any permutation σ of $\{1, \dots, n\}$, and the expectation is
 52 taken over all permutations σ , chosen uniformly at random.

53 **Remark 1** (Normalization). *It is frequent to also normalize adjusted mutual information, so as to*
 54 *get a score between 0 and 1 [Vinh et al., 2010; Romano et al., 2014]. In this paper, we only focus on*
 55 *the adjustment step. Note that normalization can be equally applied to both considered notions of*
 56 *adjustment and thus be studied separately.*

57 We have the equivalent definition:

$$\begin{aligned} \Delta I(X, Y) &= \mathbb{E}(H(X, Y_\sigma)) - H(X, Y), \\ &= \frac{1}{2}(\mathbb{E}(d(X, Y_\sigma)) - d(X, Y)). \end{aligned} \quad (3)$$

58 This equivalence follows from Proposition 1 and the fact that the definition is symmetric in X and Y .
 59 All proofs are available in the supplementary material.

60 **Proposition 1.** *We have for any random variables X and Y :*

$$\begin{aligned} H(X) &= \mathbb{E}(H(X_\sigma)), \\ \mathbb{E}(H(X, Y_\sigma)) &= \mathbb{E}(H(X_\sigma, Y)), \\ \mathbb{E}(I(X, Y_\sigma)) &= \mathbb{E}(I(X_\sigma, Y)). \end{aligned}$$

61 In view of (3), we expect $\Delta I(X, Y)$ to be positive if X and Y share information, as X is expected to
 62 be closer to Y (for the distance d) than to Y_σ , a randomized version of Y . There are specific cases
 63 where $\Delta I(X, Y) = 0$, as stated in Proposition 2; these cases will be interpreted in terms of clustering
 64 in section 4.

65 **Proposition 2.** *We have $\Delta I(X, Y) = 0$ whenever Y (or X , by symmetry) is constant or equal to*
 66 *some permutation of $\{1, \dots, n\}$.*

Adjusted entropy. Observing that $H(X) = I(X, X)$, we define similarly the adjusted entropy of
 X by:

$$\Delta H(X) = \Delta I(X, X) = H(X) - \mathbb{E}(I(X, X_\sigma)).$$

67 By (1), we get:

$$\Delta H(X) = \mathbb{E}(H(X, X_\sigma)) - H(X) = \frac{1}{2}\mathbb{E}(d(X, X_\sigma)). \quad (4)$$

68 Since d is a metric, this shows that the adjusted entropy of X is non-negative.

69 **Proposition 3.** We have $\Delta H(X) = 0$ if and only if X is constant or equal to some permutation of
70 $\{1, \dots, n\}$.

71 Proposition 3 characterizes random variables with zero adjusted entropy. Again, this result will be
72 interpreted in terms of clustering in section 4.

73 3 Pairwise adjustment

74 In this section, we introduce pairwise adjusted mutual information. The definition is the same as
75 adjusted mutual information, except that the permutation σ is now restricted to the set of pairwise
76 permutations. Specifically, we consider permutations σ for which there exists $i, j \in \{1, \dots, n\}$
77 such that $\sigma(i) = j$ and $\sigma(j) = i$, whereas $\sigma(t) = t$ for all $t \neq i, j$. We consider the set of such
78 permutations σ where the samples i, j are drawn uniformly at random in the set $\{1, \dots, n\}$. We
79 denote by σ_p such a random permutation. Observe that σ_p is the identity with probability $1/n$ (the
80 probability that $i = j$).

Pairwise adjusted mutual information. We define the *pairwise adjusted mutual information* as:

$$\Delta_p I(X, Y) = I(X, Y) - E(I(X, Y_{\sigma_p})).$$

81 This is exactly the same definition as the adjusted mutual information, except for the considered
82 permutations σ_p . It can be readily verified that the same properties apply, with the exact same proofs,
83 a key property being that the random permutations σ_p and σ_p^{-1} have the same distributions. In
84 particular, we have the analogue of (3):

$$\begin{aligned} \Delta_p I(X, Y) &= E(H(X, Y_{\sigma_p})) - H(X, Y), \\ &= \frac{1}{2}(E(d(X, Y_{\sigma_p})) - d(X, Y)). \end{aligned} \quad (5)$$

85 Moreover, $\Delta_p I(X, Y) = 0$ whenever X or Y is constant or equal to some permutation of $\{1, \dots, n\}$.

Pairwise adjusted entropy. We also define the *pairwise adjusted entropy* as:

$$\Delta_p H(X) = \Delta_p I(X, X) = H(X) - E(I(X, X_{\sigma_p})).$$

86 We have $\Delta_p H(X) \geq 0$, with equality if and only if X is constant or equal to some permutation of
87 $\{1, \dots, n\}$.

88 4 Application to clustering

89 Let $A = \{A_1, \dots, A_k\}$ and $B = \{B_1, \dots, B_l\}$ be two partitions of some finite set $\{1, \dots, n\}$ into k
90 and l clusters, respectively. Let $\Omega = \{1, \dots, n\}$ and P be the uniform probability measure over Ω .
91 Consider the random variables X and Y defined on (Ω, P) by $X^{-1}(i) = A_i$ for all $i = 1, \dots, k$ and
92 $Y^{-1}(j) = B_j$ for all $j = 1, \dots, l$. Note that $X(\omega)$ and $Y(\omega)$ can be interpreted as the *labels* i and j
93 of sample ω in clusterings A and B , for each $\omega \in \{1, \dots, n\}$.

94 We denote by $a_i = |A_i|$ the size of cluster A_i , by $b_j = |B_j|$ the size of cluster B_j , and by
95 $n_{ij} = |A_i \cap B_j|$ the number of samples both in cluster A_i and cluster B_j , for all $i = 1, \dots, k$ and
96 $j = 1, \dots, l$. The matrix $(n_{ij})_{1 \leq i \leq k, 1 \leq j \leq l}$ is known as the *contingency matrix*. Note that a_i and b_j
97 are the sums of row i and column j of the contingency matrix, respectively.

98 **Adjusted mutual information.** A well-known metric for assessing the similarity $s(A, B)$ between
99 clusterings A and B is the adjusted mutual information¹ $\Delta I(X, Y)$ between the corresponding
100 random variables X and Y . In words, this is the common information shared by clusterings A and B
101 not due to randomness.

102 By Proposition 2, we have $s(A, B) = 0$ whenever clustering A (or B , by symmetry) is trivial, that is,
103 it consists of a single cluster or of n clusters (one per sample). This is a key property, showing the
104 interest of the adjustment.

¹Recall that we don't normalize the metric, see Remark 1.

105 It is known that [Vinh *et al.*, 2010]:

$$\begin{aligned}
s(A, B) = & - \sum_{i=1}^k \sum_{j=1}^l \frac{n_{ij}}{n} \log \frac{n_{ij}}{n} \\
& + \sum_{i=1}^k \sum_{j=1}^l \sum_{c=(a_i+b_j-n)^+}^{\min(a_i, b_j)} \frac{a_i! b_j! (n-a_i)! (n-b_j)!}{n! c! (a_i-c)! (b_j-c)! (n-a_i-b_j+c)!} \frac{c}{n} \log \frac{c}{n},
\end{aligned} \tag{6}$$

106 with the notation $(\cdot)^+ = \max(\cdot, 0)$. The time complexity of this formula, which is dominated by the
107 second term, is in $O(\max(k, l)n)$ [Romano *et al.*, 2014]. In particular, it is linear in the number of
108 samples n .

109 Interestingly, we can similarly assess the quantity of information $q(A)$ contained in clustering
110 A through the adjusted entropy $\Delta H(X)$ of the corresponding random variable X . This is the
111 information contained in A not due to randomness. We have $q(A) \geq 0$ and, by Proposition 3,
112 $q(A) = 0$ if and only if clustering A is trivial, that is, it consists of a single cluster or of n clusters
113 (one per sample).

114 Since $q(A) = s(A, A)$, it follows from (6) that:

$$q(A) = - \sum_{i=1}^k \frac{a_i}{n} \log \frac{a_i}{n} + \sum_{i,j=1}^K \sum_{c=(a_i+a_j-n)^+}^{\min(a_i, a_j)} \frac{a_i! a_j! (n-a_i)! (n-a_j)!}{n! c! (a_i-c)! (a_j-c)! (n-a_i-a_j+k)!} \frac{c}{n} \log \frac{c}{n}.$$

115 The time complexity of this formula, also dominated by the second term, is in $O(kn)$. Again, this
116 complexity is linear in the number of samples n .

117 **Pairwise adjusted mutual information.** The main contribution of the paper is the following new
118 measure of similarity $s_p(A, B)$ between clusterings A and B , based on the pairwise adjusted mutual
119 information $\Delta_p I(X, Y)$ between the corresponding random variables X and Y . We have an explicit
120 expression for this similarity:

121 **Theorem 1.** *We have for any clusterings A, B :*

$$\begin{aligned}
s_p(A, B) = & 2 \sum_{i=1}^k \sum_{j=1}^l \frac{n_{ij}(n-a_i-b_j+n_{ij})}{n^2} \left(\frac{n_{ij}}{n} \log \frac{n_{ij}}{n} - \frac{n_{ij}-1}{n} \log \frac{n_{ij}-1}{n} \right) \\
& + 2 \sum_{i=1}^k \sum_{j=1}^l \frac{(a_i-n_{ij})(b_j-n_{ij})}{n^2} \left(\frac{n_{ij}}{n} \log \frac{n_{ij}}{n} - \frac{n_{ij}+1}{n} \log \frac{n_{ij}+1}{n} \right).
\end{aligned}$$

122 The time complexity of this formula is in $O(kl)$, like mutual information. It is independent of the
123 number of samples n , given the contingency matrix. Corollary 1 shows that the time complexity
124 reduces to $O(m)$, where m is the number of non-zero entries of the contingency matrix, provided the
125 latter is stored in sparse format.

126 **Corollary 1.** *We have for any clusterings A, B :*

$$\begin{aligned}
s_p(A, B) = & 2 \sum_{i,j:n_{ij}>0} \frac{n_{ij}(n-a_i-b_j+n_{ij})}{n^2} \left(\frac{n_{ij}}{n} \log \frac{n_{ij}}{n} - \frac{n_{ij}-1}{n} \log \frac{n_{ij}-1}{n} \right) \\
& + 2 \sum_{i,j:n_{ij}>0} \frac{(a_i-n_{ij})(b_j-n_{ij})}{n^2} \left(\frac{n_{ij}}{n} \log \frac{n_{ij}}{n} - \frac{n_{ij}+1}{n} \log \frac{n_{ij}+1}{n} + \frac{1}{n} \log \frac{1}{n} \right) \\
& - 2 \left(n^2 - \sum_{i=1}^k a_i^2 - \sum_{j=1}^l b_j^2 + \sum_{i,j:n_{ij}>0} n_{ij}^2 \right) \frac{1}{n} \log \frac{1}{n}.
\end{aligned}$$

127 Similarly, we can define the quantity of information $q_p(A)$ in clustering A through the pairwise
128 adjusted entropy $\Delta_p H(X)$ of the corresponding random variable X . Again, $q_p(A) \geq 0$, with
129 $q_p(A) = 0$ if and only if clustering A is trivial.

130 **Corollary 2.** *We have for any clustering A :*

$$q_p(A) = 2 \sum_{i=1}^k \frac{a_i(n - a_i)}{n^2} \left(\frac{a_i}{n} \log \frac{a_i}{n} - \frac{a_i - 1}{n} \log \frac{a_i - 1}{n} - \frac{1}{n} \log \frac{1}{n} \right).$$

131 Note that the time complexity of this formula is $O(k)$. It only depends on the number of clusters k ,
 132 and not on the number of samples n .

133 5 Experiments

134 In this section, we compare both notions of adjusted mutual information through experiments
 135 involving synthetic and real data. The experiments are run on a computer equipped with an AMD
 136 Ryzen Threadripper 1950X 16-Core Processor and 32 GB of RAM, with a Debian 10 OS. All codes
 137 and datasets used in the experiments are available in the supplementary material.

138 **Synthetic data.** We start with the simple case of $n = 100$ samples with clusters of even sizes,
 139 consisting of consecutive samples. Specifically, we consider the set of clusterings $A^{(s)}$, consisting of
 140 clusters of size s (except possibly the last one), for $s = 1, 2, \dots, 100$. In particular, both $A^{(1)}$ and
 141 $A^{(100)}$ are trivial clusterings while $A^{(5)}$ consists of 20 clusters of size 5.

142 Figure 1 gives the similarity between clusterings $A^{(10)}$ and $A^{(s)}$ with respect to s in terms of adjusted
 143 mutual information, for both notions of adjustment, i.e., $s(A^{(10)}, A^{(s)})$ and $s_p(A^{(10)}, A^{(s)})$. We
 144 observe very close behaviors, suggesting that both notions of adjustment tend to capture the same
 145 patterns in the clusterings. Note that the maximum similarity is attained for $s = 10$ in both cases, as
 146 expected. The similarity is equal to 0 for $s \in \{1, 100\}$ for both cases, in agreement with Proposition
 147 2. We also observe local peaks at $s = 20, 30, \dots, 90$, which can be interpreted by the fact that
 148 clustering $A^{(10)}$ is a refinement of clustering $A^{(s)}$ for these values of s ; similarly, the local peak at
 149 $s = 5$ may be interpreted by the fact that clustering $A^{(5)}$ is a refinement of clustering $A^{(10)}$. The
 Spearman correlation between both metrics over all values of s is equal to 0.99.

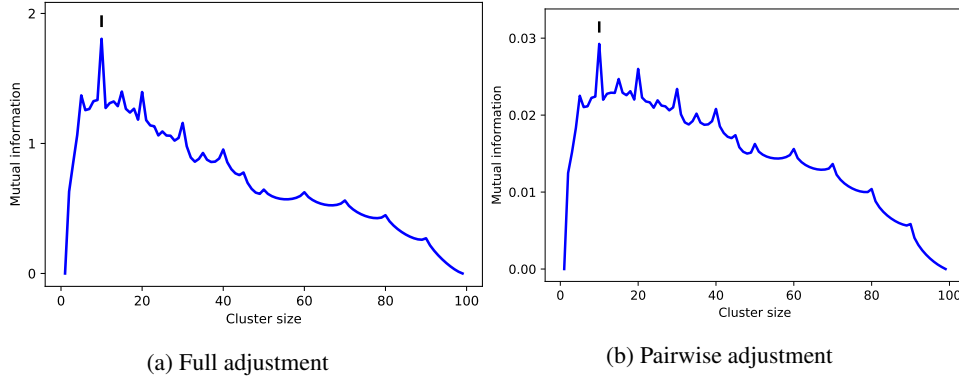


Figure 1: Comparison of metrics on synthetic data ($n = 100$).

150

151 We now consider random clusterings. Specifically, we assign n samples to k clusters independently
 152 at random, according to some probability distribution $p = (p_1, \dots, p_k)$, which is itself drawn at
 153 random². Consider three such random clusterings A, B, C (with the same parameters n and k , but
 154 different probability distributions p). We would like to know whether A is “closer” to B or to C . In
 155 particular, we are interested in testing whether both notions of adjusted mutual information give the
 156 same ordering in the sense that:

$$(s(A, B) - s(A, C))(s_p(A, B) - s_p(A, C)) \geq 0. \quad (7)$$

²Namely, $p \propto U$ where $U = (U_1, \dots, U_k)$ is a vector of k i.i.d. random variables uniformly distributed over $[0, 1]$.

157 We compute the average precision score (fraction of triplets A, B, C for which (7) is true) over 1 000
 158 independent samples of A, B, C , for different values of n and k . We repeat the experiment 100 times
 159 to get the mean and standard deviation. The results are given in Table 1. We observe a very high
 160 precision score, always higher than 93%, showing that both notions of adjusted mutual information
 161 tend to give the same ordering of these random clusterings.

n	k	Precision score
100	2	0.972 ± 0.004
100	5	0.952 ± 0.007
100	10	0.943 ± 0.006
100	20	0.955 ± 0.008
500	20	0.936 ± 0.007
1000	20	0.933 ± 0.006
1000	50	0.949 ± 0.008

Table 1: Precision score (mean \pm standard deviation)

162 For the performance gain, we compare the computation times of both versions of adjusted mutual
 163 information for the similarity between clusterings A and B , where A consists of $k = 10$ clusters
 164 of same size and B is a random clustering, drawn as in the previous experiment. Both versions of
 165 adjusted mutual information are coded in Python, with the standard version imported from scikit-learn.
 166 Figure 2 shows the computation time when the number of samples n grows from 10^2 to 10^7 . The
 167 performance gain brought by pairwise adjustment is significant. In particular, the computation time
 168 becomes independent of the number of samples.

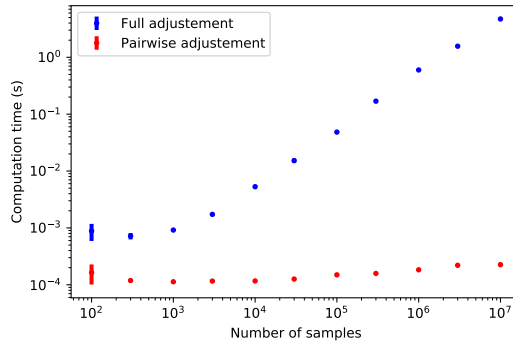


Figure 2: Computation time with respect to n (mean \pm standard deviation).

169 **Real data.** We first consider the 79 datasets of the benchmark suite [Gagolewski, 2020]³. We apply
 170 to each dataset each of the following clustering algorithms:

- 171 • k -means
- 172 • Affinity propagation
- 173 • Mean shift
- 174 • Spectral clustering
- 175 • Ward
- 176 • Agglomerative clustering
- 177 • DBSCAN
- 178 • OPTICS
- 179 • Birch
- 180 • Gaussian Mixture

³See https://github.com/gagolews/clustering_benchmarks_v1

181 We use the scikit-learn⁴ implementation of these algorithms, with the corresponding default param-
 182 eters⁵. We get 10 clusterings per dataset. The quality of each clustering is assessed through the
 183 similarity with the available ground-truth labels, using adjusted mutual information with either full
 184 adjustment or pairwise adjustment. We then compute the Spearman correlation of the corresponding
 185 similarities, a value of 1 meaning the exact same ordering of the 10 clusterings with full adjustment
 186 and pairwise adjustment. The results are shown in Figure 3, together with the speed-up in computation
 187 time due to pairwise adjustment. In both cases, the 79 datasets are ordered by the number of samples,
 188 ranging from 105 to 105 600 [Gagolewski, 2020].

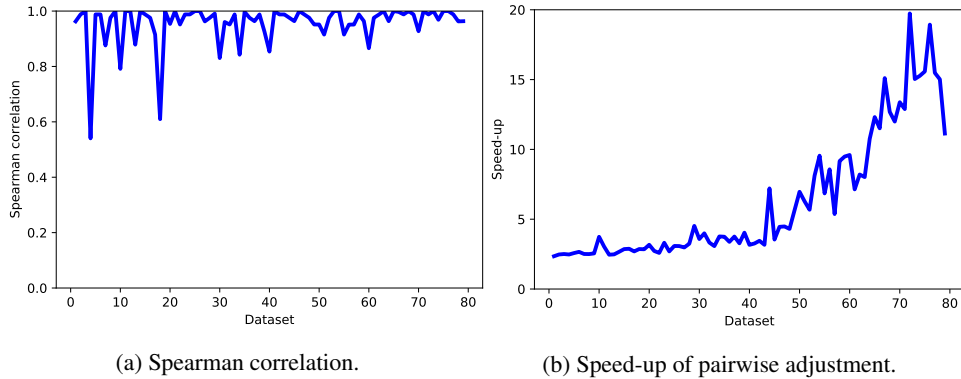


Figure 3: Comparison of metrics on the Gagolewski benchmark.

189 We first observe that the correlation is very high, suggesting again that both notions of adjusted mutual
 190 information tend to provide the same results. For 65 datasets among 79, the Spearman correlation is
 191 higher than 95%. As for the computation time, we observe a significant performance gain, by one
 192 order of magnitude for the largest datasets.

193 We have conducted the same experiments with OpenML [Vanschoren *et al.*, 2013]⁶. We selected all
 194 datasets with at least 1,000 but no more than 50,000 samples, at most 100 features (all numerical), no
 195 missing data and ground-truth labels forming clusters of at least 5 samples on average. The results
 196 are shown in Figure for the resulting 34 datasets. Again, the datasets are ordered by the number of
 197 samples, here ranging from 1,188 to 45,918. The conclusions are similar. In particular, the Spearman
 198 correlation is higher than 95% for 30 datasets among 34, and the performance gain exceeds 25 for the
 199 largest datasets.

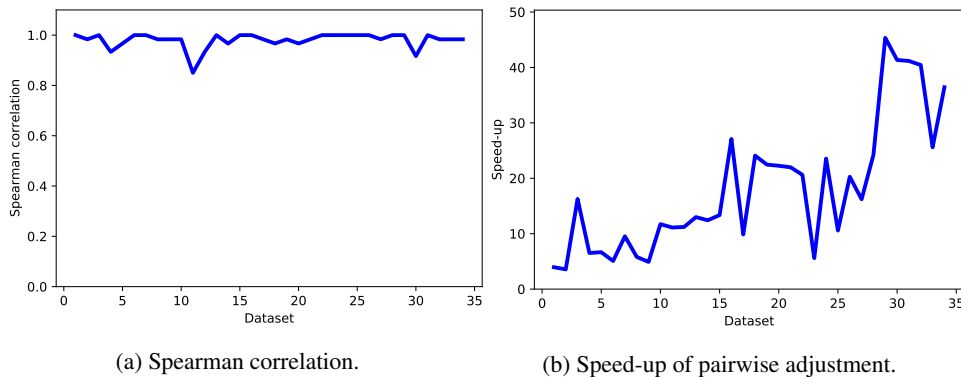


Figure 4: Comparison of metrics on OpenML datasets.

⁴<https://scikit-learn.org/>

⁵Dimension reduction is applied to the MNIST datasets, consisting of 70 000 images of size 28×28 each, see the supplementary material for details.

⁶<https://www.openml.org>

200 **6 Conclusion**

201 We have proposed another way of adjusting mutual information against chance, through pairwise
202 label permutations. The novel metric, whose explicit expression is given in Theorem 1, has a much
203 lower complexity than the usual adjusted mutual information. Interestingly, both metrics can also be
204 used to assess the quantity of information contained in a clustering, which the common property of
205 being equal to 0 if and only if the clustering is trivial, as stated in Proposition 3; again, the pairwise
206 adjusted entropy, given in Corollary 2, has a much lower complexity. Experiments on synthetic and
207 real data show that pairwise adjusted mutual information tends to provide the same results as the usual
208 adjusted mutual information for comparing clusterings, while involving much less computations.

209 For future work, we plan to extend this idea to other similarity metrics. While the practical interest
210 is less obvious for the Adjusted Rand Index [Hubert and Arabie, 1985], due to the fact that the
211 time complexity of this metric is already independent of the number of samples, it would be worth
212 considering other versions of information theoretic measures, as those studied in [Romano *et al.*,
213 2016].

214 **References**

- 215 Thomas M Cover and Joy A Thomas. *Elements of Information Theory*. Wiley, 1991.
- 216 Marek Gagolewski. Benchmark suite for clustering algorithms – version 1, 2020.
- 217 Lawrence Hubert and Phipps Arabie. Comparing partitions. *Journal of classification*, 2(1):193–218,
218 1985.
- 219 Marina Meilă. Comparing clusterings by the variation of information. In *Learning theory and kernel*
220 *machines*, pages 173–187. Springer, 2003.
- 221 Xuan Vinh Nguyen, Julien Epps, and James Bailey. Information theoretic measures for clusterings
222 comparison: is a correction for chance necessary? In *ICML*, 2009.
- 223 Simone Romano, James Bailey, Vinh Nguyen, and Karin Verspoor. Standardized mutual information
224 for clustering comparisons: one step further in adjustment for chance. In *International Conference*
225 *on Machine Learning*, pages 1143–1151, 2014.
- 226 Simone Romano, Nguyen Xuan Vinh, James Bailey, and Karin Verspoor. Adjusting for chance
227 clustering comparison measures. *The Journal of Machine Learning Research*, 17(1):4635–4666,
228 2016.
- 229 Abdel Aziz Taha and Allan Hanbury. Metrics for evaluating 3d medical image segmentation: analysis,
230 selection, and tool. *BMC medical imaging*, 15(1):29, 2015.
- 231 Bertrand Thirion, Gaël Varoquaux, Elvis Dohmatob, and Jean-Baptiste Poline. Which fmri clustering
232 gives good brain parcellations? *Frontiers in neuroscience*, 8:167, 2014.
- 233 Joaquin Vanschoren, Jan N. van Rijn, Bernd Bischl, and Luis Torgo. Openml: Networked science in
234 machine learning. *SIGKDD Explorations*, 15(2):49–60, 2013.
- 235 Nguyen Xuan Vinh, Julien Epps, and James Bailey. Information theoretic measures for clusterings
236 comparison: Variants, properties, normalization and correction for chance. *The Journal of Machine*
237 *Learning Research*, 11:2837–2854, 2010.
- 238 Bo Wang, Junjie Zhu, Emma Pierson, Daniele Ramazzotti, and Serafim Batzoglou. Visualization
239 and analysis of single-cell rna-seq data by kernel-based similarity learning. *Nature methods*,
240 14(4):414–416, 2017.
- 241 Zhao Yang, René Algesheimer, and Claudio J Tessone. A comparative analysis of community
242 detection algorithms on artificial networks. *Scientific reports*, 6:30750, 2016.
- 243 Jijie Zhang, Paschalia Kapli, Pavlos Pavlidis, and Alexandros Stamatakis. A general species
244 delimitation method with applications to phylogenetic placements. *Bioinformatics*, 29(22):2869–
245 2876, 2013.

246 **Checklist**

- 247 1. For all authors...
- 248 (a) Do the main claims made in the abstract and introduction accurately reflect the paper's
249 contributions and scope? [Yes] A variant of adjusted mutual information.
- 250 (b) Did you describe the limitations of your work? [Yes] Pairwise adjustment only applied
251 to mutual information in the present work, see Section 6.
- 252 (c) Did you discuss any potential negative societal impacts of your work? [N/A]
- 253 (d) Have you read the ethics review guidelines and ensured that your paper conforms to
254 them? [Yes]
- 255 2. If you are including theoretical results...
- 256 (a) Did you state the full set of assumptions of all theoretical results? [Yes] No specific
257 assumption is required. Theorem 1, Corollary 2 and 3 give explicit expressions using
258 notations defined at the beginning of Section 4.
- 259 (b) Did you include complete proofs of all theoretical results? [Yes] See the supplementary
260 material.
- 261 3. If you ran experiments...
- 262 (a) Did you include the code, data, and instructions needed to reproduce the main experi-
263 mental results (either in the supplemental material or as a URL)? [Yes] See the Jupyter
264 notebooks in the supplementary material.
- 265 (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they
266 were chosen)? [N/A] This is a metric for unsupervised learning. No data split required,
267 no hyperparameter.
- 268 (c) Did you report error bars (e.g., with respect to the random seed after running ex-
269 periments multiple times)? [Yes] See Table 1 and Figure 2 (not applicable to other
270 experiments).
- 271 (d) Did you include the total amount of compute and the type of resources used (e.g., type
272 of GPUs, internal cluster, or cloud provider)? [Yes] See the running times provided in
273 the Figures; the resources used are detailed at the beginning of section 5.
- 274 4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
- 275 (a) If your work uses existing assets, did you cite the creators? [Yes] See the references for
276 the datasets.
- 277 (b) Did you mention the license of the assets? [N/A]
- 278 (c) Did you include any new assets either in the supplemental material or as a URL? [N/A]
- 279
- 280 (d) Did you discuss whether and how consent was obtained from people whose data you're
281 using/curating? [N/A]
- 282 (e) Did you discuss whether the data you are using/curating contains personally identifiable
283 information or offensive content? [N/A]
- 284 5. If you used crowdsourcing or conducted research with human subjects...
- 285 (a) Did you include the full text of instructions given to participants and screenshots, if
286 applicable? [N/A]
- 287 (b) Did you describe any potential participant risks, with links to Institutional Review
288 Board (IRB) approvals, if applicable? [N/A]
- 289 (c) Did you include the estimated hourly wage paid to participants and the total amount
290 spent on participant compensation? [N/A]