Towards an information-theory for hierarchical partitions

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(Dated: March 9, 2020)

Complex systems often require descriptions covering a wide range of scales and organization levels, where a hierarchical decomposition of their description into components and sub-components is often convenient. To better understand the hierarchical decomposition of complex systems, in this work we prove a few essential results that contribute to the development of an information-theory for hierarchical-partitions.

I. INTRODUCTION

The decomposition of a system into its components and sub-components is the essence of reductionism. But the reductionist approach is not easily applicable for complex systems where different emergent patterns at several scales and organization levels are often observed [1, 2]. Nevertheless, the convenience of having a hierarchical-partitioning of the system representation is manifested in the various frameworks devised to hierarchically decompose the structure [3–9] and the behavior [10–12] of complex systems. In physics, these frameworks include the renormalization group theory of critical phenomena [13] and cluster expansion methods [14]. These methods are traditionally used with homogeneous hierarchies, but they have been also applied to heterogeneous cases where finding an appropriate decomposition is difficult [15–18] and where suitable methods for the comparison of hierarchical-partitions are helpful [19–21].

The development of methods for comparing hierarchies is generally non-trivial. Different proposals already exist, including tree-edit distance methods [22–27], ad-hoc methods [21, 28, 29], and even an information-theoretic method [30]. The ad-hoc methods could be useful for applications but often lack a well studied theoretical background. Methods based on tree-edit distances typically are of an algorithmic kind, hence they frequently rely on sub-optimal approximations or only work with fully labeled trees. Similarly, the existing information-theoretic methods cannot work with hierarchical-partitions either.

To fill the requirements of a comparison method for hierarchies that can be associated with a well defined theoretical background, we have recently introduced the Hierarchical Mutual Information (HMI) [19]. The HMI can be used to compare hierarchical-partitions in an analogous way in which the standard Mutual Information [31] is used to compare flat partitions [32]. The HMI has been proven to be a useful tool for the comparison of detected hierarchical community structures and related problems [20, 33]. Still, many of its theoretical properties remain to be understood.

In this work, we study the theoretical aspects of the HMI and how to exploit them to develop an information-theory for hierarchical-partitions. Specifically, in Sec. II we introduce some preliminary definitions and revisit the HMI. In Sec. III we present the main results. Firstly, we prove some fundamental properties of the HMI. Secondly, we use the HMI to introduce other information-theoretic quantities for hierarchical-partitions, emphasizing the study of the metric properties of the hierarchical generalization of the Variation of Information (VI) and the statistical properties of the hierarchical extension of the Adjusted Mutual Information (AMI). In Sec. IV we discuss some important consequences deriving from the presented results. Finally, in Sec. V we provide a summary of the contributions and corresponding opportunities for future works.

II. THEORY

A. Preliminary definitions

Let $T$ denote a directed rooted tree. We say that $t \in T$ when $t$ is a node of $T$. Let $T_t$ be the set of children of node $t \in T$. If $T_t = \emptyset$ then $t$ is a leaf of $T$. Otherwise, it is an internal node of $T$. Let $\ell_t$ denote the depth or topological distance between $t$ and the root of $T$. In particular, $\ell_t = 0$ if $t$ is the root. Let $T_{\ell}$ be the set of all nodes of $T$ at depth $\ell$. Clearly $T_{\ell+1} = \cup_{t \in T_{\ell}} T_t$. Let $T^t$ be the sub-tree obtained from $t$ and its descendants in $T$.

A hierarchical-partition $T := \{U_t : t \in T\}$ of the universe $U := \{1, ..., n\}$, the set of the first $n$ natural numbers, is defined in terms of a rooted tree $T$ and corresponding subsets $U_t \subset U$ satisfying

1) $\cup_{t \in T} U_t = U$ for all non-leaf $t$, and
2) $U_{t'} \cap U_{t''} = \emptyset$ for every pair of different $t', t'' \in T_t$.

For every non-leaf $t$, the set $T_t := \{U_{t'} : t' \in T_t\}$ represents a partition of $U_t$, and $T_t := \{U_t : t \in T_t\}$ is the ordinary partition of $U$ determined by $T$ at depth
of the universe

FIG. 1. Schematic representation of a hierarchical-partition $\mathcal{T}$ of the universe $U = \{1, 2, ..., 8\}$ with root $a$, 5 internal nodes including $a$, $b$ and $c$ and 6 leaves including $d$, $e$ and $f$. Some leaves may contain more than one element, e.g. $U_5 = \{1, 8\}$. Different leaves may exist at different depths $\ell$. For instance, leaf $d$ is at depth $\ell = 2$ while leaf $f$ is at depth $\ell = 3$. The subtree $T^b$ contains the nodes $c, d, e$ and $f$. The set $T_b$ contains the children $c$ and $d$ of $b$.

$\ell$. Furthermore, $\mathcal{T}^t := \{U_r : r \in T^t\}$ is the hierarchical-partition of the universe $U_t$ determined by the tree $T^t$ of root $t$. See Fig. 1 for a schematic representation of a hierarchical-partition of the universe $U = \{1, 2, ..., 8\}$.

B. The Hierarchical Mutual Information

The Hierarchical Mutual Information (HMI) [19] between two hierarchical-partitions $\mathcal{T}$ and $\mathcal{S}$ of the same universe $U$ reads

$$I(\mathcal{T}; \mathcal{S}) := I(\mathcal{T}^{t_0}; \mathcal{S}^{s_0})$$  \hspace{1cm} (1)

where $t_0$ and $s_0$ are the roots of trees $T$ and $S$, respectively,

$$I(\mathcal{T}^t; \mathcal{S}^s) := I(T_t; S_s) + \sum_{t' \in T_t, s' \in S_s} P(t' s'|ts) I(\mathcal{T}^{t'}; \mathcal{S}^{s'})$$  \hspace{1cm} (2)

is a recursively defined expression for every pair of nodes $t \in T$ and $s \in S$ with the same depth $\ell_t = \ell_s$. The probabilities in $P(t' s'|ts) = P(t' s'|ts)/P(ts)$ are ultimately defined from $P(t' s'|ts) := |U_t \cap U_s \cap U_t \cap U_s|/|U|$ and the convention $0/0 = 0$. The quantity

$$I(T_t; S_s) := H(T_t|ts) + H(S_s|ts) - H(T_t, S_s|ts)$$  \hspace{1cm} (3)

represents a mutual information between the standard partitions $U_t$ and $U_s$ restricted to the subset $U_t \cap U_s$ of the universe $U$, and is defined in terms of the three entropies

$$H(T_t|ts) := \sum_{t' \in T_t} -P(t'|ts) \ln P(t'|ts)$$  \hspace{1cm} (4)

and

$$H(T_t, S_s|ts) := \sum_{t' \in T_t, s' \in S_s} -P(t' s'|ts) \ln P(t' s'|ts)$$  \hspace{1cm} (5)

where the convention $0 \ln 0 = 0$ is adopted. For details on how to compute these quantities, please check our code [34].

III. RESULTS

For simplicity, we consider hierarchical-partitions $\mathcal{T}$ and $\mathcal{S}$ with all leaves at depths $\ell = L > 0$. The results can be easily generalized to trees with leaves at different depths at the expense of using more complicated notation.

A. Properties of the HMI

It is convenient to begin rewriting the hierarchical mutual information in the following alternative form, which is more convenient for our purposes (see App. A for a detailed derivation)

$$I(\mathcal{T}; \mathcal{S}) = I(\mathcal{T}^{t_0}; \mathcal{S}^{s_0})$$  \hspace{1cm} (7)

where $P(ts) := P(ts|t_0 s_0)$ and, in the last two lines we use flat—i.e. standard, non-hierarchical—conditional MIs and entropies of the stochastic variables $T_t$ and $S_s$ for $\ell = 0, 1, ..., L$. As the reader can see, then, we have rewritten the HMI as a level by level summatory of conditional MIs.

Starting from Eq. 7, we prove the following property of the HMI (see App. B for a detailed derivation)

$$I(\mathcal{T}; \mathcal{S}) \leq I(\mathcal{T}; \mathcal{T})$$  \hspace{1cm} (8)

In words, this result states that the HMI between two arbitrary hierarchical-partitions $\mathcal{T}$ and $\mathcal{S}$ of the same universe $U$ is smaller or equal to the mutual information between $\mathcal{T}$ and itself—or analogously between $\mathcal{S}$ and itself—mimicking in this way an analogous property that holds for the flat mutual information [31].
Now we exploit the result of Eq. 8 to show that the HMI can be properly normalized. Namely, if \( M(x, y) \) is any generalized mean—like the arithmetic-mean \( M(x, y) = (x + y)/2 \), the geometric-mean \( M(x, y) = \sqrt{xy} \), the max-mean \( M(x, y) = \max(x, y) \) or the min-mean \( M(x, y) = \min(x, y) \)—then the Normalized HMI (NHMI)

\[
i(T; S) := \frac{I(T; S)}{M(H(T), H(S))}
\]

satisfies \( 0 \leq i(T; S) \leq 1 \). The first inequality follows because \( I(T_{\ell + 1}; S_{\ell + 1}|T_\ell, S_\ell) \geq 0 \) for any \( \ell \). The second follows from Eq. 8.

### B. Deriving other information-theoretic quantities

Given the HMI, hierarchical versions of other information-theoretic quantities can be obtained by following the rules of the standard flat case. For example, the hierarchical entropy of a hierarchical-partition \( T \) can be defined as

\[
H(T) := I(T; T)
\]

\[
= \sum_{\ell=0}^{L-1} H(T_{\ell+1}|T_\ell)
\]

\[
= \sum_{\ell=0}^{L-1} H(T_{\ell+1}, T_\ell) - H(T_\ell)
\]

\[
= \sum_{\ell=0}^{L-1} H(T_{\ell+1}) - H(T_\ell)
\]

\[
= H(T_L)
\]

where we have used that \( H(T_{\ell+1}, T_\ell) = H(T_{\ell+1}) \) (see Eq. D6). Similarly, we can write down the hierarchical version of the joint entropy as

\[
H(T, S) := H(T) + H(S) - I(T; S)
\]

and the conditional entropy as

\[
H(T|S) := H(T) - H(T, S)
\]

Further, we can define a hierarchical version of the Variation of Information (VHI) as

\[
V(T; S) := H(T|S) + H(S|T) = H(T) + H(S) - 2I(T; S) = H(T, S) - I(T; S).
\]

Because of Eq. 8, the properties \( H(T, S) \geq 0, H(T|S) \geq 0 \) and \( V(T; S) \geq 0 \) follow, generalizing corresponding properties of the flat case. Unfortunately, we have found counter-examples violating the triangle inequality for the HVI, failing to generalize its flat counterpart in this particular sense [36]. For instance, for the hierarchical-partitions \( T = [[[1, 2], [3], [4]], S = [[2], [3], [1, 4]] \) and \( R = [[1], [2], [3], [4]] \), we find \( V(T; S) = V(S; R) \approx V(T; R) \approx 0.17 \), which is a negative quantity. It is important to remark, however, that the violation of the triangular inequality is relatively weak. For instance, for \( n = 4 \) the maximum difference is found to be \( 5.55 \) for \( T = [[[1, 2], [3], [4]], S = [[1], [3], [2], [4]] \) and \( R = [[[1], [2]], [3], [4]] \), which is significantly larger than 0.17. In fact, as shown in Fig. 2 where the complementary cumulative distribution of differences

\[
\Delta V(T, S, R) := V(T; S) + V(S; R) - V(T; R)
\]

is plotted for all \( T, S \) and \( R \) without repeating the symmetric cases \( \Delta V(T, S, R) \) and \( \Delta V(R, S, T) \), for different sizes \( n \), the overall contribution of the negative values is small, not only in magnitude but also in probability. Results for larger values of \( n \) are not included since the number of triples \( (T, S, R) \) grows quickly with \( n \), turning impractical their exhaustive computation. See App. C for how to generate all possible hierarchical-partitions for a given \( n \).

Although the HVI fails to satisfy the triangular inequality, the transformation

\[
d_n(T, R) = 1 - e^{-\frac{n}{2} V(T, R)}
\]

of \( V \) does it (see App. D for a detailed proof). In other words, \( d_n \) is a distance metric, so the geometrization of the set of hierarchical-partitions is possible. We confirm this in Fig. 3 by running computations analogous to those of Fig. 2 but for \( \Delta d_n \) instead of \( \Delta V \). Notice however that the distance metric \( d_n \) is non-universal, because it depends on \( n \). In fact, for \( n \to \infty \) it holds \( d_n(T; S) \to 1 - \delta_{T,S} \) which is a trivial distance metric—known as the discrete metric—that can only distinguish between equality and non-equality. These properties follow because, for fixed-size \( n \), the non-zero \( V \)'s are bounded from below by a finite positive quantity that tends to zero when \( n \to \infty \). We also remark that other concave growing functions besides that of Eq. 15 (or more specifically Eq. D11) can be used to obtain essentially the same result; a distance metric.

Although the flat VI is a distance metric—which is a desirable property for the quantitative comparison of entities—it also presents some limitations [37]. Hence, besides the HVI, the HMI, and the NHMI, it is convenient to consider other information-theoretic alternatives for the comparison of hierarchies. This is the case of the Adjusted Mutual Information (AMI) [38], which is devised to compensate for the biases that random coincidences produce on the NMI, and which we generalize into the hierarchical case by following the original definition recipe

\[
A(T; S) := \frac{I(T; S) - \langle I(T; S) \rangle}{M(H(T), H(S)) - \langle I(T; S) \rangle}.
\]

We called the generalization, the Adjusted HMI (AHMI). The definition of the AHMI requires the definition of a
In this way, Eq. 17 can be written as

\[
\langle I(T; S) \rangle := \sum_{\mathcal{R}, \mathcal{Q}} P(\mathcal{R}, \mathcal{Q}|T, S) I(\mathcal{R}; \mathcal{Q})
\]  

of the Expected Mutual Information (EMI) \[30\]. Here, the distribution \( P(\mathcal{R}, \mathcal{Q}|T, S) \) represents a reference null model for the randomization of a pair of hierarchical-partitions. Like in the original flat case \[30\], we define the distribution in terms of the well-known permutation model. It is important to remark, however, that other alternatives for the flat case have been recently proposed \[38\].

To describe the permutation model, let us first introduce some definitions. A permutation \( \tau \) is a bijection \( e \leftrightarrow \tau(e) \) over \( U \). We can define \( \tau T := \{ \tau U_t : t \in T \} \) as the hierarchical-partition of the permuted elements where \( \tau U_t := \{ \tau(e) : e \in U_t \} \) for all \( t \in T \). In this way, \( \tau T_\ell := \{ \tau U_r : r \in T_\ell \} \) becomes the partition emerging at depth \( \ell \) obtained from the permuted elements.

Now we are ready to define the permutation model for hierarchical-partitions. Consider a pair of permutations \( \tau \) and \( \sigma \) over \( U \) acting on corresponding hierarchical-partitions \( T \) and \( S \). The permutation model is defined as

\[
P(\mathcal{R}, \mathcal{Q}|T, S) := \frac{1}{(n!)^2} \sum_{\tau, \sigma} \delta_{\mathcal{R}, \tau T} \delta_{\mathcal{Q}, \sigma S}
\]

In this way, Eq. 17 can be written as

\[
\langle I(T; S) \rangle = \frac{1}{(n!)^2} \sum_{\tau, \sigma} I(\tau T; \sigma S)
\]

where the simplification \( \rho = \tau \sigma^{-1} \) can be used because the labeling of the elements in \( U \) is arbitrary.

The exact computation of Eq. 19 is expensive, even if the expressions are written in terms of contingency tables and corresponding generalized multivariate two-way hypergeometric distributions. This is because, at variance with the flat case, independence among random variables is compromised. Hence, we approximate the EMI by sampling permutations \( \rho \) until the relative error of the mean falls below 0.01.

In Fig. 4 we show results concerning how similarities occurring by chance result in non-negligible values of the EMI for randomly generated hierarchical-partitions. The cyan curve of crosses depicts the average of the HMI between pairs of randomly generated hierarchical-partitions of \( n \) elements. In App. E we describe the algorithm we use to randomly sample hierarchical-partitions of \( n \) elements. The previous curve overlaps with the black one of open circles corresponding to the average of the EHMI between the same pairs of randomly generated hierarchical-partitions. This result indicates that the permutation model is a good null model for the comparison of pairs of hierarchical-partitions without correlations. Moreover, these curves exhibit significant positive values, indicating that the HMI detects similarities occurring just by chance between the randomly generated hierarchical-partitions. To determine how significant these values are, the curve of magenta solid circles corresponds to the average of the hierarchical entropies of the generated hierarchical-partitions. As can be seen, the averaged hierarchical entropy lies significantly above the curve of the EMI. On the other hand, their ratio, which is a quantity in \([0, 1]\), is \( \approx 0.3 \) over the whole range.
Similarity by chance

I(T; S), A(T; S)

FIG. 4. (Color online) How similarity by chance affects the Hierarchical Mutual Information \( I \). In cyan crosses, values of \( I \) averaged by sampling pairs of randomly generated hierarchical-partitions \( T \) and \( S \) of the universe with \( n \) elements. In solid magenta circles, the average hierarchical entropy over the sampled \( T \). In open black circles, the Expected Hierarchical Mutual Information (EHMI) averaged over the same pairs of partitions. In open blue squares, the ratio between the first and the second curves. In solid green squares, the ratio is averaged by sampling 1000 pairs of randomly generated hierarchical-partitions. The EHMI is computed by sampling permutations \( \rho \) until the relative standard error of the mean falls below 0.01.

of studied sizes, as indicated by the green curve of solid squares. In other words, the similarities by chance affect non-negligibly the HMI. The curve of open blue squares depicts the averaged EHMI but for \( S = T \). The curve lies above but follows closely that of the EHMI between different hierarchical-partitions. This indicates that the effect of a randomized structure has a marginal impact besides that of the randomization of labels.

In Fig. 4 we show how the HMI between two hierarchical-partitions \( T \) and \( S \) decays with \( k \), when \( S \) is obtained from shuffling the identity of \( k \) of the elements in \( U \). Here, the HMI is averaged by sampling randomly generated hierarchical-partitions \( T \) at each \( n \) and \( k \). As expected, the EHMI decays as the imposed decorrelation increases. In fact, for \( k = n \) but \( S = T \), the obtained values match those of the blue curve of open squares in Fig. 4. In the figure, we also show the AHMI as a function of \( k \) for the different \( n \). Notice how, at difference with the HMI, the AHMI goes from \( A = 1 \) at \( k = 0 \) towards \( A = 0 \) at \( k = n \).

The previous results highlight the importance of the AHMI, in the sense that it conveys as a less biased measure of similarity as compared to the HMI.

FIG. 5. (Color online) Average Hierarchical Mutual Information \( I \) or HMI (solid) and Adjusted Hierarchical Mutual Information \( A \) or AHMI (dotted) between randomly generated hierarchical-partitions \( T \) and corresponding hierarchical-partitions \( S \) obtained from \( T \) by randomly shuffling the identity of \( k \) of the elements in \( U \). Different symbols represent hierarchical-partitions of different sizes \( n \). Each point is averaged over 10,000 samples of \( T \). The EHMI within the AHMI is computed as in Fig. 4.

IV. DISCUSSION

As we have shown, many similarities subsist between the corresponding flat and hierarchical information-theoretic quantities. Still, we remark that important differences also exist. For instance, according to Eq. (10), there is no unique hierarchical-partition maximizing the hierarchical entropy. This is because, in the hierarchical version of the entropy, only the standard partition defined at the last level \( L \) contributes. The contribution of the internal levels produces no effect. This result has important consequences. For example, a hierarchical generalization of the MaxEnt principle becomes ill-defined. This issue could be resolved by a slightly different reformulation of the principle. Namely, in the flat case, the standard MaxEnt can be replaced by the maximization of the MI between the distribution being maximized and the uniform distribution, or any other reference distribution that can be chosen depending on the purpose. This alternative reinterpretation of MaxEnt admits a hierarchical generalization through the HMI. Since the standard MaxEnt is broadly applied in physics, our work has the potential to stimulate analogous contributions for the hierarchical case.

Another important difference between the standard and the hierarchical cases is that, while the VI satisfies the triangular inequality, the hierarchical version HVI here presented does not. This may have important consequences for the geometrization of an information-theory
for hierarchies. On the other hand, we remember the reader that a transformation $d_n$ of the HVI is found to satisfy the triangular inequality, reason for which the geometrization of a hierarchical information-theory is still possible, although not in a universal way because the transformation is size-dependent.

V. CONCLUSIONS

In this work, we significantly push forward the formalization of an information-theory for hierarchical-partitions which we have previously introduced [19]. Specifically, we have shown analytically that the Hierarchical Mutual Information (HMI) generalizes well a well-known inequality of the traditional flat case. Then, we used this result to prove that the HVI admits an appropriate normalization like its flat counterpart, complementing our previous numerically supported conjecture about it. Later, we showed how to use the HMI to derive other information-theoretic quantities, such as the Hierarchical Entropy, the Hierarchical Conditional Entropy, the Hierarchical Variation of Information (HVI) and the Adjusted Hierarchical Mutual Information (AHMI). Finally, we studied the metric properties of the HVI, finding counter-examples violating the triangular inequality, and thus showing that the HVI fails to have the metric property of its flat analogous. On the other hand, we have found a transformation $d_n$ of the HVI that satisfies the metric properties, enabling a geometrization of the presented hierarchical generalization of the traditional information-theory.

Additionally, we have supported the analytical findings with corresponding numerical experiments. We offer open-source access to our code [31], including the code for the generation of hierarchical-partitions.

Our work opens new possibilities in the study of hierarchically organized physical systems, from the information-theoretic side, the statistical side, as well as from the applications point of view. For instance, it would be interesting to see if the HMI can be used to compute consensus trees out of a given ensemble; a well-known problem within the study of phylogenetic and taxonomic representations in computational biology [39–41].

VI. ACKNOWLEDGMENTS

JIP and NA acknowledge financial support from grants CONICET (PIP 112 20150 10028), FonCyT (PICT-2017-0973), SeCyTUNC (Argentina) and MinCyT Córdoba (PID PGC 2018). FS acknowledges support from the European Project SoBigData++ GA. 871042 and the PAl (Progetto di Attivitá Integrata) project funded by the IMT School Of Advanced Studies Lu. The authors thank CCAD – Universidad Nacional de Córdoba, http://ccad.unc.edu.ar/, which is part of SN~C-Ad – MinCyT, República Argentina, for the provided computational resources.

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Appendix A: Rewriting the HMI

It is convenient to begin rewriting the hierarchical mutual information in the following alternative form, which is more convenient for our purposes

\[
I(T;S) = I(T^{t_0};S^{s_0}) = I(T_{t_0};S_{s_0}|t_0s_0) \\
+ \sum_{t_1 \in T_{t_0}, s_1 \in S_{s_0}} P(t_1s_1|t_0s_0) \left( I(T_{t_1};S_{s_1}|t_1s_1) + \sum_{t_2 \in T_{t_1}, s_2 \in S_{s_1}} P(t_2s_2|t_1s_1)I(T_{t_2};S_{s_2}) \right) \\
= I(T_{t_0};S_{s_0}|t_0s_0) \\
+ \sum_{t_1 \in T_{t_1}, s_1 \in S_{s_1}} P(t_1s_1|t_0s_0)I(T_{t_1};S_{s_1}|t_1s_1) + \sum_{t_2 \in T_{t_2}, s_2 \in S_{s_2}} P(t_2s_2|t_0s_0)I(T_{t_2};S_{s_2}) \\
\vdots \\
= \sum_{t=0}^{L-1} \sum_{t \in T_t, s \in S_t} P(ts)I(T_t;S_t|ts).\]
Here, we have used the definition $P(ts) := P(ts|t_0s_0) = |U_t \cap U_s|/|U| = n_{ts}/n$. Similarly

$$\sum_{t \in T_t, s \in S_t} P(ts)H(T_t, S_t|ts) = \sum_{t \in T_t, s \in S_t} P(ts) \sum_{t' \in T_t, s' \in S_t} -P(t's'|ts)\ln P(t's'|ts)$$

$$(A2)$$

$$= \sum_{t \in T_t, s \in S_t} \sum_{t' \in T_{t+1}, s' \in S_{t+1}} -P(t's'ts)\ln P(t's'ts)$$

$$= \sum_{t \in T_t, s \in S_t} \sum_{t' \in T_{t+1}, s' \in S_{t+1}} -P(t's'ts)\ln P(t's'ts)$$

$$= \sum_{t \in T_t, s \in S_t} \sum_{t' \in T_{t+1}, s' \in S_{t+1}} -P(t's'ts)\ln P(t's'ts)$$

$$= H(T_{t+1}, S_{t+1}, T_t, S_t) - H(T_t, S_t)$$

$$= H(T_{t+1}, S_{t+1}|T_t, S_t).$$

where we have used that $\sum_{t \in T_t} \sum_{t' \in T_{t+1}} \equiv \sum_{t \in T_t}(\sum_{t' \in T_t} + \sum_{t' \in T_{t+1}/T_t}) \equiv \sum_{t \in T_t}(\sum_{t' \in T_t} + 0)$ because $P(t's'ts) = 0$ whenever $t'$ is not a child of $t$. The entropies in the last two lines are written in terms of the standard non-hierarchical or flat definition, for which

$$H(X', Y'|X, Y) = \sum_{x \in X, y \in Y} P(xy) \sum_{x' \in X', y' \in Y'} -P(x'y'|xy) \ln P(x'y'|xy)$$

$$(A3)$$

Finally, combining Eqs. (A1) and (A2) we arrive at

$$I(T; S) = \sum_{t=0}^{L-1} \sum_{t \in T_t, s \in S_t} P(ts)I(T_t; S_t|ts)$$

$$(A4)$$

$$= \sum_{t=0}^{L-1} \sum_{t \in T_t, s \in S_t} P(ts) \left[ H(T_t|ts) + H(S_t|ts) - H(T_t, S_t|ts) \right]$$

$$= \sum_{t=0}^{L-1} \left[ H(T_{t+1}|T_t, S_t) + H(S_{t+1}|T_t, S_t) - H(T_{t+1}, S_{t+1}|T_t, S_t) \right]$$

$$= \sum_{t=0}^{L-1} I(T_{t+1}; S_{t+1}|T_t, S_t).$$
Appendix B: HMI inequality

The inequality property for the HMI can be straightforwardly proven. Starting from Eq. (A1), we can write

\[ I(\mathcal{T}; S) = \sum_{\ell=0}^{L-1} \sum_{t \in T_\ell, s \in S_\ell} P(ts)I(T_\ell; S_s|ts) \]

\[ \leq \sum_{\ell=0}^{L-1} \sum_{t \in T_\ell, s \in S_\ell} P(ts)H(T_\ell|ts) \]

\[ = \sum_{\ell=0}^{L-1} \sum_{t \in T_\ell, s \in S_\ell} P(ts) \sum_{t' \in T_\ell} -P(t'|ts)\ln P(t'|ts) \]

\[ = \sum_{\ell=0}^{L-1} \sum_{t \in T_\ell} \sum_{t' \in T_\ell} -P(t'|s)\ln P(t'|ts) \]

\[ \leq \sum_{\ell=0}^{L-1} \sum_{t \in T_\ell} \sum_{t' \in T_\ell} - \left( \sum_{s \in S_\ell} P(t'|s) \right) \ln \left( \frac{\sum_{s \in S_\ell} P(t'|s)}{\sum_{s \in S_\ell} P(t'|ts)} \right) \]

\[ = \sum_{\ell=0}^{L-1} \sum_{t \in T_\ell} \sum_{t' \in T_\ell} -P(t'|t)\ln P(t'|t) \]

\[ \leq \sum_{\ell=0}^{L-1} H(T_{\ell+1}|T_\ell) \]

\[ = \sum_{\ell=0}^{L-1} \left[ H(T_{\ell+1}|T_\ell, T_\ell) + H(T_{\ell+1}|T_\ell, T_\ell) - H(T_{\ell+1}, T_{\ell+1}|T_\ell, T_\ell) \right] \]

\[ = \sum_{\ell=0}^{L-1} I(T_{\ell+1}; T_{\ell+1}|T_\ell, T_\ell) \]

\[ = I(\mathcal{T}; \mathcal{T}). \]

Here, in the first inequality, we have used a well-known property of the entropy, while in the second inequality, we have used the log-sum inequality [31].

Appendix C: Generating hierarchical-partitions

Before showing how to generate all hierarchical-partitions of a set, it is better to review first a way to generate all standard partitions (see Section 7.2.1.7 of [12]). Consider we have a way to generate all partitions of the set \( U_n := \{1, 2, ..., n\} \). Then, we can easily generate all the partitions of the set \( U_{n+1} := \{1, 2, ..., n, n+1\} \) as follows. For each partition of the set \( U_n \), generate all the partitions that can be obtained by adding the element \( n+1 \) to each part \( \mathcal{P} \) together with extending the partition with the part \( \{n+1\} \). For example, given the partition \( \{\{1,2\}, \{3\}\} \) of \( \{1,2,3\} \), then we generate the partitions \( \{\{1,2,4\}, \{3\}\} \), \( \{\{1,2\}, \{3,4\}\} \) and \( \{\{1,2\}, \{3\}, \{4\}\} \) of \( \{1,2,3,4\} \). In other words, this algorithm recursively implements induction.

To generate hierarchical-partitions, we follow a similar procedure to the one discussed for standard partitions. Consider we have an algorithm to generate all hierarchical-partitions of \( U_n \). Then, for each hierarchical-partition \( \mathcal{T} \) of \( U_n \), we generate the hierarchical-partitions \( \mathcal{T}' \) of \( U_{n+1} \) that can be obtained by applying the following operations to each of the nodes \( t \in \mathcal{T} \):

1. If \( t \) is a leaf, add \( n+1 \) to \( U_t \).
2. If \( t \) is not a leaf, add the child \( t' \) to \( t \) with \( U_{t'} = \{n+1\} \).
3. Replace \( t \) by a new node \( t'' \) with \( t \) and \( t' \) as children.
For example, the hierarchical-partitions of $U_2 = \{1, 2\}$ are $\{1, 2\}$ and $\{\{1\}, \{2\}\}$. Then: Operation 1 applied to the first hierarchical-partition results in $\{1, 2, 3\}$. Operation 1 applied to the second results in $\{\{1, 3\}, \{2\}\}$ and $\{\{1\}, \{2, 3\}\}$. Operation 2 on the second, results in the hierarchical-partitions $\{\{1\}, \{2, 3\}\}$. Operation 3 on the first, results in $\{\{1\}, \{2\}\}, \{\{1\}, \{3\}\}, \{\{1\}, \{3\}\}, \{\{2\}\}$ and $\{\{1\}, \{2, 3\}\}$. For more details, please check our code for an implementation of the algorithm [34].

Appendix D: Forcing triangular inequality for the Hierarchical Variation of Information

Let

$$d_{V_0}(\mathcal{T}; S) := 1 - e^{-V(\mathcal{T}; S)/V_0} \quad (D1)$$

be defined for some arbitrary $V_0 > 0$. Then, for an appropriate choice of $V_0$, $d_{V_0}$ becomes a distance metric satisfying the triangular inequality. The proof is as follows. First, $d_{V_0}$ is clearly a distance since: i) $d_{V_0}$ is a growing function of $V$, ii) $d_{V_0}(\mathcal{T}, S) = 0 \iff \mathcal{T} = S$ when $V_0 > 0$ and iii) $d_{V_0}$ is symmetric in its arguments. It remains to be shown that $d_{V_0}$ satisfies the triangular inequality for an appropriate choice of $V_0$. The triangular inequality for $d_{V_0}$ reads

$$\Delta d_{V_0}(\mathcal{T}; S; R) := d_{V_0}(\mathcal{T}; S) + d_{V_0}(S; R) - d_{V_0}(\mathcal{T}; R) \geq 1 - e^{-V(\mathcal{T}; S)/V_0} - e^{-V(S; R)/V_0} \geq 1 - 2e^{-\min(V(\mathcal{T}; S), V(S; R))/V_0} \quad (D2)$$

We can show that, for an appropriate choice of $V_0$, last line is always non-negative given that non-zero values of $V$ cannot be arbitrarily small. Thus, let us find a lower bound for the non-zero values of the Variation of Information between hierarchical-partitions. To do so, first, we notice that the Variation of Information between hierarchical-partitions can be decomposed into a summation of non-negative quantities over the different levels. Namely, following Eqs. 7, 10 and 13 we can write

$$V(\mathcal{T}; S) = \sum_{\ell=0}^{L-1} \left[ H(T_{\ell+1}|T_\ell) + H(S_{\ell+1}|S_\ell) - 2I(T_{\ell+1}; S_{\ell+1}|T_\ell, S_\ell) \right] \quad (D3)$$

with $V(T_{\ell+1}; S_{\ell+1}|T_\ell, S_\ell) \geq 0$ for every $\ell$ due to Eq. 8. Now, if the hierarchical-partitions $\mathcal{T}$ and $S$ are equal up to level $\ell'$ included—i.e., as stochastic variables, $T_\ell = S_\ell$ for all $\ell \leq \ell'$—then

$$I(\mathcal{T}; S) = \sum_{\ell=0}^{\ell'} I(T_{\ell+1}; S_{\ell+1}|T_\ell, S_\ell) + \sum_{\ell=\ell'+1}^{L-1} I(T_{\ell+1}; S_{\ell+1}|T_\ell, S_\ell) \quad (D4)$$

$$= I(T_{\ell'+1}; S_{\ell'+1}|T_0, S_0) + \sum_{\ell=\ell'+1}^{L-1} I(T_{\ell+1}; S_{\ell+1}|T_\ell, S_\ell)$$
because

\[ \sum_{\ell=0}^{\ell'} I(T_{\ell+1}; S_{\ell+1}|T_\ell, S_\ell) = I(T_{\ell'+1}; S_{\ell'+1}|T_\ell, S_\ell) + \sum_{\ell=0}^{\ell'-1} I(T_{\ell+1}; S_{\ell+1}|T_\ell, S_\ell) \]

\[ = I(T_{\ell'+1}; S_{\ell'+1}|T_\ell, S_\ell) + \sum_{\ell=0}^{\ell'-1} H(T_{\ell+1}|T_\ell) \]

\[ = H(T_{\ell'+1}|T_\ell) + H(S_{\ell'+1}|S_\ell) - H(T_{\ell'+1}, S_{\ell'+1}|S_\ell) + \sum_{\ell=0}^{\ell'-1} \left[ H(T_{\ell+1}, T_\ell) - H(T_\ell) \right] \]

\[ = H(T_{\ell'+1}, T_\ell) - H(T_\ell) + H(S_{\ell'+1}) - H(S_\ell) - H(T_{\ell'+1}, S_{\ell'+1}) + H(T_\ell, S_\ell) \]

\[ + \sum_{\ell=0}^{\ell'-1} \left[ H(T_{\ell+1}, T_\ell) - H(T_\ell) \right] \]

\[ = H(T_{\ell'+1}) - H(T_\ell) + H(S_{\ell'+1}) - H(S_\ell) - H(T_{\ell'+1}, S_{\ell'+1}) + H(T_\ell, S_\ell) - H(T_0) \]

\[ = H(T_{\ell'+1}) + H(S_{\ell'+1}) - H(T_{\ell'+1}, S_{\ell'+1}) - 0 \]

\[ = I(T_{\ell'+1}; S_{\ell'+1}|T_0, S_0). \]

Here, we have used identities such as

\[ H(T_{\ell+1}, T_\ell) = \sum_{t \in T_{\ell+1}} \sum_{t' \in T_\ell} -P(t'|t) \ln P(t'|t) \]

\[ = - \sum_{t \in T_\ell} \left( \sum_{t' \in T_{\ell+1}/T_\ell} P(t'|t) \ln P(t'|t) + \sum_{t' \in T_{\ell+1}/T_\ell} P(t'|t) \ln P(t'|t) \right) \]

\[ = - \sum_{t \in T_\ell} \left( \sum_{t' \in T_{\ell+1}/T_\ell} P(t'|t) \ln P(t'|t) + 0 \right), \quad \text{because if } t' \notin T_\ell \text{ then } P(t'|t) = 0, \]

\[ = - \sum_{t \in T_\ell} \sum_{t' \in T_{\ell+1}/T_\ell} P(t'|t) \ln P(t'|t) \]

\[ = - \sum_{t \in T_\ell} \sum_{t' \in T_{\ell+1}/T_\ell} P(t'|t') \ln P(t')', \quad \text{because } P(t'|t) = P(t') \text{ since } U_{\ell+1} \subseteq U_{\ell} \text{ whenever } t' \in T_\ell, \]

\[ = - \sum_{t' \in T_{\ell+1}/T_\ell} \ln P(t') \sum_{t \in T_\ell} P(t'|t) \]

\[ = - \sum_{t' \in T_{\ell+1}/T_\ell} P(t') \ln P(t') \]

\[ = H(T_{\ell+1}) \]

and \( H(T_\ell, S_\ell) = H(S_\ell). \) Combining Eqs. \[ \text{D5} \] and \[ \text{D5} \] we can write

\[ V(T; S) = V(T_{\ell'+1}; S_{\ell'+1}|T_0, S_0) + \sum_{\ell=\ell'+1}^{L-1} V(T_{\ell+1}; S_{\ell+1}|T_\ell, S_\ell). \]

Now, as shown in Ref. \[ \text{[43]} \], the Variation of Information between two different flat partitions cannot be smaller than \( 2/n \) when the size of the universe is \( n = |U|. \) In consequence, since \( T_0 = S_0 = U, \) then \( V(T; S) \geq V(T_{\ell'+1}; S_{\ell'+1}|T_0, S_0) \geq 2/n. \) Finally, from this lower bound and Eq. \[ \text{D2} \] we have \( \Delta d_V(T; S; \mathcal{R}) \geq 1 - 2e^{-2/(nV_0)} \) from where, by setting the r.h.s. to zero, we obtain \( V_0 = 2/(n \ln 2). \) In other words, we have shown that

\[ d_n(T; S) := 1 - e^{-n \ln 2 V(T; S)} \]

satisfies the triangular inequality and thus is a distance metric.
Appendix E: Generating random hierarchical-partitions

To generate or sample random hierarchical-partitions in a non-necessarily uniform manner we propose a recursive application of an algorithm to generate random flat partitions from a set of elements $U$. To generate random flat partitions of a set $U$ of $n$ elements, we first draw a number $z$ of "splitters" uniformly at random from the set $\{0, 1, 2, ..., n\}$. Then, we generate a sequence concatenating the $z$ splitters $|$ with the $n$ elements of $U$. Then, we randomly shuffle the sequence. Then, we split the sequence by removing the splitters and use the obtained non-empty parts to construct a partition. For example, if $U = \{1, 2, 3, 4, 5\}$ and $z = 3$, then we generate the sequence $||12345$ which after shuffling may result in $12|3||45$ from where the partition $\{\{1, 2\}, \{3\}, \{4, 5\}\}$ is obtained.

To generate random hierarchical-partitions, we recursively apply the previous algorithm, first to $U$, then to the obtained parts of $U$, then to the parts of the parts, and so on until non-divisible sets are obtained. For details please check our code [34].