# Ranking the information content of distance measures 

Aldo Glielmo ${ }^{1, *}$, Claudio Zeni ${ }^{1}$, Bingqing Cheng ${ }^{2}$, Gábor Csányi ${ }^{3}$, Alessandro Laio ${ }^{1}$<br>${ }^{1}$ International School for Advanced Studies (SISSA), Via Bonomea 265, Trieste, Italy<br>${ }^{2}$ Department of Computer Science and Technology, University of Cambridge, J. J. Thomson Avenue, Cambridge, CB3 0FD, United Kingdom<br>${ }^{3}$ Engineering Laboratory, University of Cambridge, Trumpington St, Cambridge CB21PZ, United Kingdom<br>*aglielmo@sissa.it


#### Abstract

Real-world data typically contain a large number of features that are often heterogeneous in nature, relevance, and also units of measure. When assessing the similarity between data points, one can build various distance measures using subsets of these features. Using the fewest features but still retaining sufficient information about the system is crucial in many statistical learning approaches, particularly when data are sparse. We introduce a statistical test that can assess the relative information retained when using two different distance measures, and determine if they are equivalent, independent, or if one is more informative than the other. This in turn allows finding the most informative distance measure out of a pool of candidates. The approach is applied to find the most relevant policy variables for controlling the Covid-19 epidemic and to find compact yet informative representations of atomic structures, but its potential applications are wide ranging in many branches of science.


## Introduction

An open challenge in machine learning is to extract useful information from a database with relatively few data points, but with a large number of features available for each point $1-3$. For example, clinical databases typically include data for a few hundreds patients with a similar clinical history, but an enormous amount of information for each patient: the results of clinical exams, imaging data, and a record of part of their genome 4]. In cheminformatics and materials science, molecules and materials can be described by a large number of features, but databases are limited in size by the great cost of the calculations or the experiments required to predict quantum properties [5, 6. In short, real-world data are often "big data", but in the wrong direction: instead of millions of data points, there are often too many features for a few samples. As such, training accurate learning models is challenging, and even more so when using deep neural networks, which typically require a large amount of independent samples 7.

One way to circumvent this problem is to perform preliminary feature selection, and discard features that appear irrelevant or redundant [2, 8-10]. Alternatively, one can perform a dimensional reduction aimed at finding a representation of the data with few variables built as functions of the original features $11-13$.

In some cases, explicit features are not available, as in the case of raw text documents or genome sequences. What one can always define, even in these cases, are distances between data points whose definition, however, can be rather arbitrary [14, 15]. How can one select, among an enormous amount of possible choices, the most appropriate distance measure for a given task? Finding the correct distance is of course as difficult as performing feature selection or dimensionality reduction. In fact,
these tasks can be considered equivalent if explicit features are available, since in this case a particular choice of features naturally gives rise to a different distance function computed through the Euclidean norm.

In this work, we approach feature/distance learning through a novel statistical and information theoretic concept. We pose the question: given two distance measures $A$ and $B$, can we identify whether one is more informative than the other? If distance $A$ is more informative than distance $B$, even partial information on the distance $A$ can be predictive about $B$, while the reverse will not necessarily be true. If this happens, and if the two distances have the same complexity e.g, they are built using the same number of features, $A$ should be generally preferred with respect to $B$ in any learning model.

We introduce the concept of "information imbalance", a measure able to quantify the relative information content of one distance measure with respect to another. We show how this tool can be used for feature learning in different branches of science. For example, by optimizing the information content of a distance measure we are able to select from a set of more than 300 material descriptors, a subset of around 10 which is sufficient to define the state of a material system, and predict its energy. Moreover, we find the combinations of national policy measures which are most effective in containing the Covid-19 epidemic. In this case, the information imbalance also provides striking evidence on the causality relationship between these policies and the severity of the epidemic.

## The information imbalance

Inspired by the widespread idea of using local neighborhoods to perform dimensional reduction [16] and clas-


FIG. 1. a): Illustration of the distance rank of two points in different feature spaces $A$ and $B$. The rank $r_{i j}$ of point $j$ relative to $i$ is equal to 1 in space $A$, meaning that $j$ is the first neighbor of $i$. This is not the case in space $B$, where point $j$ is the third neighbor of point $i$. b): Illustration of how ranks can be used to verify that space $x$ is less informative than space $x y$. The figure shows how a distance bound in the $x y$ space automatically implies a distance bound in the less informative $x$ space. The opposite is not necessarily true and, in principle, the first neighbor of a point in the $x$ space can be at any distance from the point in the $x y$ space.
sification 17 we quantify the relative quality of two distance measures by analyzing the ranks of the first neighbors of each point. For each pair of points $i$ and $j$, the rank $r_{i j}$ of point $j$ relative to point $i$, is obtained by sorting the pairwise distances between $i$ and rest of the points from smallest to largest. For example, $r_{i j}^{A}=1$ if point $j$ is the first neighbor of point $i$ according to the distance $d_{A}$. The rank of two points will be, in general, different when computed using a different distance measures $B$, as illustrated in Figure 1a.

The key idea of our approach is that distance ranks can be used to identify whether one metric is more informative than the other. Take the example given in Figure 11b, depicting a cartoon of a dataset represented either in the two-dimensional space $x y$ or in the less informative one-dimensional space $x$. Point $j$ is the first neighbor of $i$ in the space $x y$ and it becomes the third neighbor in space $x\left(r_{i j}^{x}=3\right)$. Similarly, point $k$ is the first neighbor of $i$ in space $x$ and it becomes fifth neighbor in space $x y$ $\left(r_{i k}^{x y}=5\right)$. In this case we find that $r_{i j}^{x}<r_{i k}^{x y}$ i.e., the rank in space $x$ of first neighbors in space $x y$ is smaller than the rank in space $x y$ of first neighbors in space $x$.

To give a more quantitative example, let's consider a dataset of points harvested from a 3-dimensional Gaussian whose standard deviation along the $z$ direction is a tenth of those along $x$ and $y$. In this case, one can define a Cartesian distance between data points either using all the three features, $d_{x y z}^{2}=\left(x_{i}-x_{j}\right)^{2}+\left(y_{i}-y_{j}\right)^{2}+\left(z_{i}-z_{j}\right)^{2}$, or using a subset of these features ( $d_{x y}, d_{y z}$ and so on). Intuitively, $d_{x y z}$ and $d_{x y}$ are almost equivalent since the standard deviation along $z$ is small, while there are information imbalances, say, between $d_{x}$ and $d_{x y}$, which would allow saying that $d_{x y}$ is more informative than $d_{x}$. In the first row of Figure 2, we plot the ranks computed using one distance against the ranks computed using a second distance (for example the ranks in $d_{x y}$ as a function of
those in $d_{x y z}$ for panel a). In the second row of the figure we show the probability distribution $p\left(r^{A} \mid r^{B}=1\right)$ of the ranks $r_{i j}^{A}$ in space $A$ restricted to those pairs for which $r_{i j}^{B}=1$, namely to the nearest neighbors according to distance $B$. In panels a and b , we compare the most informative distance containing all three coordinates to the one containing only $x$ and $y$ coordinates. Given the small variance along the $z$ direction, these two distance measures are practically equivalent, and this results in rank distributions strongly peaked around one. In panels c and d, we compare the two metrics $d_{x y}$ and $d_{x}$. In this case, the former is clearly more informative than the latter, and we find that the distribution of ranks when passing from $d_{x y}$ to $d_{x}$ is more peaked around small values than when going in the opposite direction. Finally, for two metrics built using independent coordinates $(x$ and $y$, in panels c and f ) the rank distributions are completely uniform.

We hence propose to assess the relationship between any two distance measures $d_{A}$ and $d_{B}$ by using the properties of the conditional rank distribution $p\left(r^{B} \mid r^{A}=1\right)$. The closer this distribution is to a delta function peaked at one, the more information about space $B$ is contained within space $A$.

This intuition can be made more rigorous through the statistical theory of copula variables. We can define a copula variable $c_{A}$ as the cumulative distribution $c_{A}=\int_{0}^{d_{A}} p_{A}(w \mid x) d w$, where $p_{A}(w \mid x)$ is the of probability of sampling a data point within distance $w$ from $x$ in the $A$ space. The value of $c_{A}$ can be estimated from a finite dataset by counting the fraction of points that fall within distance $d_{A}$ of point $x, c_{A} \approx r_{A} / N$. Copula variables and distance ranks can be considered continuous-discrete analogues of each other. As a consequence, the distributions $p\left(r^{B} \mid r^{A}=1\right)$ shown in







g
h

| Relationship | Imbalances |
| :--- | :--- |
| $A$ and $B$ are equivalent: they carry <br> identical information. | $\Delta(A \rightarrow B) \approx 0$ <br> $\Delta(B \rightarrow A) \approx 0$ |
| $A$ and $B$ are orthogonal: they carry |  |
| completely independent information. |  | | $\Delta(B \rightarrow B) \approx 1$ |
| :--- |
| $\Delta(B \rightarrow A) \approx 1$ |
| $A$ is more informative than $B$ : the |
| information of $B$ is contained in $A$. | | $\Delta(A \rightarrow B) \approx 0$ |
| :--- |
| $\Delta(B \rightarrow A) \approx 1$ |
| $A$ and $B$ share symmetric |



FIG. 2. Illustration of the information imbalance calculation and usage on a 3D Gaussian dataset with a small variance along $z$. a), c), e): scatter plot of the rank between ordered pairs of points. The highlighted regions indicate the points considered for generating the bottom plots. b), d), f): Probability of that two points have a given rank in one representation given that they are first neighbors in the other. The three columns represent different pairs of representations. g): The four different types of relationships that can characterize the relative information content of two metric spaces $A$ and $B$. h): Information imbalance plane for the 3D Gaussian dataset discussed. The different colors roughly mark the regions corresponding to the four types of relationships listed in g .

Figure 2 are nothing else but estimates of the copula distributions $p\left(c_{B} \mid c_{A}\right)$ with $c_{A}$ conditioned to be very small. This is important, since Sklar's theorem guarantees that the copula distribution $p\left(c_{A}, c_{B}\right)$ contains the entire correlation structure of the metric spaces $A$ and $B$, independently of any details of the marginal distributions $p\left(d_{A} \mid x\right)$ and $p\left(d_{B} \mid x\right)$ [18-20].

Using the copula variables, we define the "information imbalance" from space $A$ to space $B$ as

$$
\begin{equation*}
\Delta(A \rightarrow B)=2 \lim _{\epsilon \rightarrow 0}\left\langle c_{B} \mid c_{A}=\epsilon\right\rangle \tag{1}
\end{equation*}
$$

where we used the conditional expectation $\left\langle c_{B}\right| c_{A}=$ $\epsilon\rangle=\int c_{B} p\left(c_{B} \mid c_{A}=\epsilon\right) d c_{B}$ to characterize the devi-
ation of $p\left(c_{B} \mid c_{A}=\epsilon\right)$ from a delta function. In the limit cases where the two spaces are equivalent or completely independent we have that $\left\langle c_{B} \mid c_{A}=\epsilon\right\rangle=\epsilon$ and $\left\langle c_{B} \mid c_{A}=\epsilon\right\rangle=1 / 2$ respectively, so that the definition provided in Eq. (1) statistically confines $\Delta$ in the range $(0,1)$. The information imbalance defined in Eq. (1) is estimated on a dataset with $N$ data points as

$$
\begin{equation*}
\Delta(A \rightarrow B) \approx 2\left\langle r^{B} \mid r^{A}=1\right\rangle / N \tag{2}
\end{equation*}
$$

We remark that the conditional expectation used in Eq. (1) is only one of the possible quantities that can be used to characterize the deviation of the conditional copula distribution from a delta function. Another attractive
option is the entropy of the distribution. In the Supplementary Information (SI) (S1.3), we show how these two quantities are related and we demonstrate that the specific choice does not substantially affect the results. In the SI (S1.2), we also show how copula variables can be used to connect the information imbalance to the standard information theoretic concept of mutual information.

By measuring the information imbalances $\Delta(A \rightarrow B)$ and $\Delta(B \rightarrow A)$, we can identify four classes of relationships between the two spaces $A$ and $B$. We can find whether $A$ and $B$ are equivalent or independent, whether they symmetrically share both independent and equivalent information, or whether one space contains the information of the other. These relationships are presented in Figure 2p. These relationships can be identified visually by plotting the two imbalances $\Delta(A \rightarrow B)$ and $\Delta(B \rightarrow A)$ against each other in a graph as done in Figure 2h. We will refer to this kind of graphs as information imbalance planes. In Figure 2 h we present the information imbalance plane of the 3-dimensional Gaussian dataset discussed so far, and used for Figure $2 \mathrm{a}-\mathrm{f}$. Looking at this figure, one can immediately verify that the small variance along the $z$ axis makes the two spaces $x y z$ and $x y$ practically equivalent. Similarly, one can verify that space $x$ is correctly identified to be contained in $x y z$ and that the two spaces $x$ and $y$ are classified as orthogonal. The figure also includes a point corresponding to a different dataset sampled from a 4-dimensional isotropic Gaussian with dimensions $\tilde{x}, \tilde{y}, \tilde{z}$ and $\tilde{w}$. This point (black star) shows that the spaces $\tilde{x} \tilde{y} \tilde{z}$ and $\tilde{y} \tilde{z} \tilde{q}$ are correctly identified as sharing symmetric information.

Importantly, the information imbalance only depends on the local neighborhood of each point and, for this reason, it is naturally suited to analyze data manifolds which are arbitrarily nonlinear. In the SI (section 2.1), we show that our approach is able to correctly identify the best feature for describing a spiral of points wrapping around one axis, and a sinusoidal function.

## Identifying causal relationships in the spreading of the Covid-19 epidemic

We now use the information imbalance measure to verify whether national policy measures have been useful in containing the Covid-19 epidemic, and to identify which measures have been the most effective. The "Covid-19 Data Hub" provides comprehensive and up to date information on the Covid-19 epidemic [21, including epidemiological indicators such as the number of confirmed infections and the number of Covid-19 related deaths for nations where this is available, as well as the policy indicators that quantify the severity of the governmental measures such as school and workplace closing, restrictions on gatherings and movements of people, testing and contact tracing 22. More details on the dataset are available in the SI (S2.2.1).

We define the space of policy measures $P_{t}$ as the set of policy indicators at week $t$, and the state of the epidemic $E_{t^{\prime}}$ as a two-dimensional space composed of the number of weekly deaths $D_{t^{\prime}}$ and the ratio $R_{t^{\prime}}=C_{t^{\prime}} / T_{t^{\prime}}$ of confirmed cases $C_{t^{\prime}}$ over total number of tests performed $T_{t^{\prime}}$ per week at time $t^{\prime}$. Here we use a time lag $\left(t^{\prime}-t\right)$ of two weeks, but the analysis is similar for time lags of one and three weeks; these results are reported in the SI (S2.2.2).

What is the information imbalance $\Delta\left(P_{t} \rightarrow E_{t^{\prime}}\right)$ between the space of policy measures indicators $P_{t}$ at time $t$ and the space of epidemiological variables $E_{t^{\prime}}$ at a later time $t^{\prime}>t$ ? A low value of $\Delta\left(P_{t} \rightarrow E_{t}\right)$ means that $P_{t}$ can predict $E_{t^{\prime}}$. We first compute the information imbalances between all possible combinations of $d$ policy variables among a total of ten. In Figure $\sqrt{3} a$ we present the minimum information imbalance $\Delta\left(P_{t} \rightarrow E_{t^{\prime}}\right)$ achievable with any set of $d$ policy measures.

For $d \leq 2, \Delta\left(P_{t} \rightarrow E_{t^{\prime}}\right)$ is close to one, indicating that no single or couple of policy measure is predictive about the state of the epidemic, consistently with [23]. When three or more policy measures are considered, the information imbalance decreases rapidly reaching a value of about 0.28 when almost all policy measures are considered. This sharp decrease and the low information imbalance clearly indicate that policy measures do contain information on the future state of the epidemic. As a sanity check, a dummy policy variable was introduced for this test (blue hexagon). This variable is never selected by the algorithm, and its addition deteriorates the information content of the policy space. We finally note that the information imbalance $\Delta\left(E_{t+2} \rightarrow P_{t}\right)$ (shown in Figure 3b) remains considerably high for any number of policy variables. This is a clear indication of the asymmetry in the relationship between policy measures and state of the epidemic, and of the sensitivity of the information imbalance to causality and to the arrow of time.

Our analysis show that policy interventions have been effective in containing the spreading of the Covid-19 epidemic, a result which has been already verified in a number of studies [23-26]. In accordance with these studies, we also find that multiple measures are necessary to effectively contain the epidemic, with no single policy being sufficient on its own [27], and that the impact of policy measures increases monotonically with the number of measures put in place. We find that a small yet effective set of policy measures has been the combination of testing, stay home restrictions and restrictions on international movement and gatherings. While our results are computed as averages over all nations considered, further analysis carried out in the SM (S2.2.3) on disjointed subsets of nations give results which are consistent with our main findings. In the SM (S2.2.4), we also show that when building a model for predicting future Covid-19 related deaths, one can optimally choose the relative scale of heterogeneous epidemiological variables using the information imbalance. This is important in real-world applications, where features are often characterized by different units of measure and different scales


FIG. 3. Information imbalances between sets of policy variables $P_{t}$ and the state of the epidemic after two weeks $E_{t+2}$. a): Minimum information imbalances from $P_{t}$ to $E_{t+2}$ achievable with a given number of policy measures. b): The corresponding information imbalance plane with the number of policy variables going from 1 to 10 reported in the gray circles. Point 10 is not visible as it lies below point 9 . The figure shows that the policy measures space $P_{t}$ can predict the state of the epidemic $E_{t+2}$, while $E_{t+2}$ cannot predict $P_{t}$.
of variations.

## Selection and compression of descriptors for atomistic systems

We now show that the information imbalance criterion can be used to assess the information content of commonly used numerical descriptors of the geometric arrangement of atoms in materials and molecules, as well as to compress the dimension (number of features) of a given descriptor with minimal loss of information. Such atomistic descriptors are needed for applying any statistical learning algorithm to problems in physics and chemistry [28-32]. Example applications include the interpolation of potential energy surfaces [33, 34, the prediction of a variety of molecular and materials properties [35-37], and visualization and exploration of atomistic databases 38, 39.

We first consider a database consisting of an atomic trajectory of amorphous silicon generated from a molecular dynamics simulation at 500 K (see S2.3.1 of the SM for details). At each time step of this trajectory we select a single local environment by including all the neighboring atoms within the cutoff radius of $4.5 \AA$ from a given central atom. In this simple system, which does not undergo any significant atomic rearrangement, one can define a fully informative distance measure as the minimum over all rigid rotations of the root mean square deviation (rmsd) of two local environments (details in S2.3.2 of the SM).

In Figure 4 a , this ground truth distance measure is compared with some of the descriptors most commonly used for materials modeling: the "Atom-centered Symmetry Functions" (ACSF) [33, 40, the "Smooth Overlap of Atomic Positions" (SOAP) [41, 42] and the 2 and 3 -body kernels [43, 44]. Unsurprisingly, all descriptors are contained in the ground truth distance measure. For ACSF and SOAP representations, one can increase the
resolution by increasing the size of the descriptor in a systematic way, and we found that doing this allows both representations to converge to the ground truth.

A SOAP descriptor typically involves a few hundred components. Following a procedure similar to the one used in the last section to select policy measures, we use the information imbalance to efficiently compress this high-dimensional vector with minimal loss of information (more details are given in S2.3.3 of the SM). We perform this compression for a complex database of local atomic environments sampled from different phases of carbon [45] [46. As illustrated in Figure 4b and c, the selection leads to a rapid decrease of the information imbalance, and converge much more quickly than other strategies such as random selection (blue squares) and standard sequential selection (green triangles). Figure 4 d depicts the test error of a potential energy model constructed using a a state-of-the-art Gaussian process regression model 34] (see S2.3.5 of the SM) on the compressed descriptors, as a function of the size of the descriptors and for the different compression strategies considered. Remarkably, the graph shows that a very accurate model can be obtained using only 16 out of the 324 original components of the SOAP vector considered here 42. In the SM (S2.3.6), we present more details on the components selected by our procedure, and show that they appear in an order that can be understood considering the fundamental structure of the SOAP descriptor.

## Conclusions

In this work we introduce the information imbalance, a new method to assess the relative information content between two distance measures. The key property which makes the information imbalance useful is its asymmetry: it is different when computed using a distance $A$ as a reference and a distance $B$ as a target, and when the two distances are swapped. This allows distinguishing


FIG. 4. Use of the information imbalance for the selection and compression atomistic descriptors. a): Information imbalances between ground truth "rmsd" distance metric and standard atomistic descriptors. b): Information imbalances between a full description and the most informative $d$-plet of components $(d=1, \ldots, 4)$.c): Convergence of the "symmetric" information imbalance with the number of components for three different compression strategies. The symmetric information imbalance is defined as $\bar{\Delta}(A, B)=[\Delta(A \rightarrow B)+\Delta(B \rightarrow A)] / \sqrt{2}$; more details can be found in the SM (S2.3.3). d): Force error on a validation set of a machine learning potential energy model built on the compressed descriptors.
three classes of similarity between two distance measures: a full equivalence, a partial but symmetric equivalence, and an asymmetric equivalence, in which one of the two distances is observed to contain the information of the other.

The potential applications of the information imbalance criterion are multifaceted. The most important one is probably the long-standing and crucial problem of feature selection 11-13. Low-dimensional models typically allow for more robust predictions in supervised learning tasks [2, 8]. Moreover, they are generally easier to interpret and can be used for direct data visualization if sufficiently low dimensional. We design feature selection algorithm by selecting the subset of features which minimizes the information imbalance with respect to a target property, or to the original feature space.

As we have showcased, such algorithms can be "exact" if the distances to be compared are relatively few (as done for the Covid-19 database) or approximate, if one has to compare a very large number of distances (as done for the atomistic database). Such algorithms work well even when in the presence of strong nonlinearities and correlations within the feature space. This is exemplified by the analysis of the Covid-19 dataset, where 4 policy measures which appear similarly irrelevant when taken singularly, were instead identified as maximally informative when taken together with regards to the future state of the epidemic.
Other applications include dimensionality reduction, as the information imbalance could be used directly as an objective function. Admittedly such function will in general be non differentiable and highly non-linear but, in spite of this, efficient optimization algorithms could be
developed exploiting recent results on the computation of approximate derivatives for sorting and ranking operations 47.
Another potentially fruitful line of research would be exploiting the information imbalance to optimize the performance of deep neural networks. For example, in SM (S2.3.7), we show that one can reduce the size of the input layer of a neural network that predicts the energy of a material, yielding more computationally efficient and robust predictions. However, one can imagine to go much further, and compare distance measures built using the representations in different hidden layers, or in different architectures. This could allow for designing maximally informative and maximally compact neural network architectures. We finally envision potential applications of the proposed method in the study of causal relationships: we have seen that in the Covid-19 database the use of information imbalance makes it possible to distinguish the future from the past, as the former contains information about the latter, but not vice-versa. We believe that this empirical observation can be made robust by dedicated theoretical investigations, and used in practical applications in other branches of science.

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