Ranking the information content of distance measures

Aldo Glielmo^{1,*}, Claudio Zeni¹, Bingqing Cheng², Gábor Csányi³, Alessandro Laio¹

¹International School for Advanced Studies (SISSA), Via Bonomea 265, Trieste, Italy

²Department of Computer Science and Technology, University of Cambridge,

J. J. Thomson Avenue, Cambridge, CB3 0FD, United Kingdom

³Engineering Laboratory, University of Cambridge, Trumpington St,

Cambridge CB21PZ, United Kingdom

*aglielmo@sissa.it

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_{ij} 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 xy. The figure shows how a distance bound in the xy 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 xy 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_{ij} 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, $r_{ij}^A = 1$ if point jis 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 1b, depicting a cartoon of a dataset represented either in the two-dimensional space xy or in the less informative one-dimensional space x. Point j is the first neighbor of i in the space xy and it becomes the third neighbor in space x ($r_{ij}^x = 3$). Similarly, point k is the first neighbor of i in space x and it becomes fifth neighbor in space xy($r_{ik}^{xy} = 5$). In this case we find that $r_{ij}^x < r_{ik}^{xy}$ i.e., the rank in space x of first neighbors in space xy is smaller than the rank in space xy 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, $d_{xyz}^2 = (x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2$, or using a subset of these features (d_{xy} , d_{yz} and so on). Intuitively, d_{xyz} and d_{xy} are almost equivalent since the standard deviation along z is small, while there are information imbalances, say, between d_x and d_{xy} , which would allow saying that d_{xy} is more informative than d_x . In the first row of Figure 2, we plot the ranks computed using a second distance (for example the ranks in d_{xy} as a function of

those in d_{xyz} for panel a). In the second row of the figure we show the probability distribution $p(r^A \mid r^B = 1)$ of the ranks r_{ij}^A in space A restricted to those pairs for which $r_{ij}^B = 1$, 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_{xy} 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_{xy} 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 $p(r^B | r^A = 1)$. 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 $c_A = \int_0^{d_A} p_A(w \mid x) dw$, 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 $p(r^B \mid r^A = 1)$ shown in



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 $p(c_B | c_A)$ with c_A conditioned to be very small. This is important, since Sklar's theorem guarantees that the copula distribution $p(c_A, c_B)$ contains the entire correlation structure of the metric spaces A and B, independently of any details of the marginal distributions $p(d_A | x)$ and $p(d_B | x)$ [18–20].

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

$$\Delta(A \to B) = 2 \lim_{\epsilon \to 0} \langle c_B \mid c_A = \epsilon \rangle, \tag{1}$$

where we used the conditional expectation $\langle c_B | c_A = \epsilon \rangle = \int c_B p(c_B | c_A = \epsilon) dc_B$ to characterize the devi-

ation of $p(c_B | c_A = \epsilon)$ from a delta function. In the limit cases where the two spaces are equivalent or completely independent we have that $\langle c_B | c_A = \epsilon \rangle = \epsilon$ and $\langle c_B | c_A = \epsilon \rangle = 1/2$ respectively, so that the definition provided in Eq. (1) statistically confines Δ in the range (0,1). The information imbalance defined in Eq. (1) is estimated on a dataset with N data points as

$$\Delta(A \to B) \approx 2\langle r^B \mid r^A = 1 \rangle / N \tag{2}$$

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 $\Delta(A \to B)$ and $\Delta(B \to A)$, 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 2g. These relationships can be identified visually by plotting the two imbalances $\Delta(A \to B)$ 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 infor*mation imbalance planes.* In Figure 2h we present the information imbalance plane of the 3-dimensional Gaussian dataset discussed so far, and used for Figure 2a-f. Looking at this figure, one can immediately verify that the small variance along the z axis makes the two spaces xyz and xy practically equivalent. Similarly, one can verify that space x is correctly identified to be contained in xyz 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 $E_{t'}$ as a two-dimensional space composed of the number of weekly deaths $D_{t'}$ and the ratio $R_{t'} = C_{t'}/T_{t'}$ of confirmed cases $C_{t'}$ over total number of tests performed $T_{t'}$ per week at time t'. Here we use a time lag (t'-t) 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 $\Delta(P_t \to E_{t'})$ between the space of policy measures indicators P_t at time t and the space of epidemiological variables $E_{t'}$ at a later time t' > t? A low value of $\Delta(P_t \to E_t)$ means that P_t can predict $E_{t'}$. We first compute the information imbalances between all possible combinations of d policy variables among a total of ten. In Figure 3a we present the minimum information imbalance $\Delta(P_t \to E_{t'})$ achievable with any set of d policy measures.

For $d \leq 2$, $\Delta(P_t \rightarrow E_{t'})$ 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 con*tain* 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 $\Delta(E_{t+2} \to P_t)$ (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 500K (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 4.5Å 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 4a, 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 4d 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, ..., 4). c): Convergence of the "symmetric" information imbalance is defined as $\overline{\Delta}(A, B) = [\Delta(A \to B) + \Delta(B \to A)]/\sqrt{2}$; 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.

ACKNOWLEDGMENTS

AG, CZ, and AL gratefully acknowledge support from the European Union's Horizon 2020 research and innovation program (Grant No. 824143, MaX 'Materials design at the eXascale' Centre of Excellence). The authors would like to thank M. Carli, D. Doimo and I. Macocco (SISSA) for useful discussions and M. Caro (Aalto University) for precious help in using the TurboGap code.

- Yaqing Wang, Quanming Yao, James T. Kwok, and Lionel M. Ni. Generalizing from a few examples: A survey on few-shot learning. ACM Comput. Surv., 53(3), June 2020.
- [2] André Teixeira Lopes, Edilson de Aguiar, Alberto F. De Souza, and Thiago Oliveira-Santos. Facial expression recognition with convolutional neural networks: Coping with few data and the training sample order. *Pattern Recognition*, 61:610–628, 2017.
- [3] Alfredo Nazábal, Pablo M. Olmos, Zoubin Ghahramani, and Isabel Valera. Handling incomplete heterogeneous data using vaes. *Pattern Recognition*, 107:107501, 2020.
- [4] Cathie Sudlow, John Gallacher, Naomi Allen, Valerie Beral, Paul Burton, John Danesh, Paul Downey, Paul Elliott, Jane Green, Martin Landray, et al. Uk biobank: an open access resource for identifying the causes of a wide range of complex diseases of middle and old age. *Plos med*, 12(3):e1001779, 2015.
- [5] Han Altae-Tran, Bharath Ramsundar, Aneesh S. Pappu, and Vijay Pande. Low data drug discovery with oneshot learning. ACS Central Science, 3(4):283–293, 2017. PMID: 28470045.
- [6] Hironao Yamada, Chang Liu, Stephen Wu, Yukinori Koyama, Shenghong Ju, Junichiro Shiomi, Junko Morikawa, and Ryo Yoshida. Predicting materials properties with little data using shotgun transfer learning. ACS Central Science, 5(10):1717–1730, 2019.
- [7] Connor Shorten and Taghi M. Khoshgoftaar. A survey on image data augmentation for deep learning. *Journal* of Big Data, 6(1):60, Jul 2019.
- [8] Jie Cai, Jiawei Luo, Shulin Wang, and Sheng Yang. Feature selection in machine learning: A new perspective. *Neurocomputing*, 300:70–79, 2018.
- [9] A. Jović, K. Brkić, and N. Bogunović. A review of feature selection methods with applications. In 2015 38th International Convention on Information and Communication Technology, Electronics and Microelectronics (MIPRO), pages 1200–1205, 2015.
- [10] Xuelian Deng, Yuqing Li, Jian Weng, and Jilian Zhang. Feature selection for text classification: A review. *Mul*timedia Tools and Applications, 78(3):3797–3816, Feb 2019.
- [11] Laurens van der Maaten and Geoffrey Hinton. Visualizing Data using t-SNE. Journal of Machine Learning Research, 9:2579–2605, November 2008.
- [12] Leland McInnes, John Healy, and James Melville. Umap: Uniform manifold approximation and projection for dimension reduction. arXiv preprint arXiv:1802.03426, 2018.
- [13] Y Bengio, A Courville, and P Vincent. Representation Learning: A Review and New Perspectives. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 35(8):1798–1828, June 2013.
- [14] Kaya and Bilge. Deep Metric Learning: A Survey. Symmetry, 11(9):1066–26, September 2019.
- [15] Brian Kulis. Metric Learning: A Survey. Foundations and Trends® in Machine Learning, 5(4):287–364, 2013.
- [16] Trevor Hastie, Robert Tibshirani, and Jerome Friedman. *The Elements of Statistical Learning*. Springer Series in Statistics. Springer New York Inc., New York, NY, USA, 2001.

- [17] Michael Gashler, Dan Ventura, and Tony Martinez. Iterative non-linear dimensionality reduction with manifold sculpting. In J. Platt, D. Koller, Y. Singer, and S. Roweis, editors, Advances in Neural Information Processing Systems, volume 20. Curran Associates, Inc., 2008.
- [18] Roger B. Nelsen. An introduction to copulas. Springer, New York, 2006.
- [19] R. S. Calsaverini and R. Vicente. An informationtheoretic approach to statistical dependence: Copula information. *EPL (Europhysics Letters)*, 88(6):68003, dec 2009.
- [20] Houman Safaai, Arno Onken, Christopher D. Harvey, and Stefano Panzeri. Information estimation using nonparametric copulas. *Phys. Rev. E*, 98:053302, Nov 2018.
- [21] Emanuele Guidotti and David Ardia. COVID-19 Data Hub. Journal of Open Source Software, 5(51):2376, July 2020.
- [22] Thomas Hale, Anna Petherick, Toby Phillips, and Samuel Webster. Variation in government responses to covid-19. *Blavatnik school of government working paper*, 31:2020–11, 2020.
- [23] Nils Haug, Lukas Geyrhofer, Alessandro Londei, Elma Dervic, Amélie Desvars-Larrive, Vittorio Loreto, Beate Pinior, Stefan Thurner, and Peter Klimek. Ranking the effectiveness of worldwide covid-19 government interventions. *Nature Human Behaviour*, 4(12):1303–1312, Dec 2020.
- [24] Jan M. Brauner, Sören Mindermann, Mrinank Sharma, David Johnston, John Salvatier, Tomáš Gavenčiak, Anna B. Stephenson, Gavin Leech, George Altman, Vladimir Mikulik, Alexander John Norman, Joshua Teperowski Monrad, Tamay Besiroglu, Hong Ge, Meghan A. Hartwick, Yee Whye Teh, Leonid Chindelevitch, Yarin Gal, and Jan Kulveit. Inferring the effectiveness of government interventions against covid-19. Science, 371(6531), 2021.
- [25] Solomon Hsiang, Daniel Allen, Sébastien Annan-Phan, Kendon Bell, Ian Bolliger, Trinetta Chong, Hannah Druckenmiller, Luna Yue Huang, Andrew Hultgren, Emma Krasovich, Peiley Lau, Jaecheol Lee, Esther Rolf, Jeanette Tseng, and Tiffany Wu. The effect of large-scale anti-contagion policies on the covid-19 pandemic. *Nature*, 584(7820):262–267, Aug 2020.
- [26]Seth Flaxman, Swapnil Mishra, Axel Gandy, H. Juliette T. Unwin, Thomas A. Mellan, Helen Coupland, Charles Whittaker, Harrison Zhu, Tresnia Berah, Jeffrey W. Eaton, Mélodie Monod, Pablo N. Perez-Guzman, Nora Schmit, Lucia Cilloni, Kylie E. C. Ainslie, Marc Baguelin, Adhiratha Boonyasiri, Olivia Boyd, Lorenzo Cattarino, Laura V. Cooper, Zulma Cucunubá, Gina Cuomo-Dannenburg, Amy Dighe, Bimandra Djaafara, Ilaria Dorigatti, Sabine L. van Elsland, Richard G. FitzJohn, Katy A. M. Gaythorpe, Lily Geidelberg, Nicholas C. Grassly, William D. Green, Timothy Hallett, Arran Hamlet, Wes Hinsley, Ben Jeffrey, Edward Knock, Daniel J. Laydon, Gemma Nedjati-Gilani, Pierre Nouvellet, Kris V. Parag, Igor Siveroni, Hayley A. Thompson, Robert Verity, Erik Volz, Caroline E. Walters, Haowei Wang, Yuanrong Wang, Oliver J. Watson, Peter Winskill, Xiaoyue Xi, Patrick G. T. Walker, Azra C. Ghani, Christl A. Donnelly, Steven Riley, Michaela A. C.

Vollmer, Neil M. Ferguson, Lucy C. Okell, Samir Bhatt, and Imperial College COVID-19 Response Team. Estimating the effects of non-pharmaceutical interventions on covid-19 in europe. *Nature*, 584(7820):257–261, Aug 2020.

- [27] Kristian Soltesz, Fredrik Gustafsson, Toomas Timpka, Joakim Jaldén, Carl Jidling, Albin Heimerson, Thomas B Schön, Armin Spreco, Joakim Ekberg, Örjan Dahlström, Fredrik Bagge Carlson, Anna Jöud, and Bo Bernhardsson. The effect of interventions on COVID-19. *Nature*, pages 1–9, December 2020.
- [28] Lenka Zdeborová. Machine learning: New tool in the box. Nature Physics, 13(5):420–421, May 2017.
- [29] Kristof T Schütt, Stefan Chmiela, O A von Lilienfeld, Alexandre Tkatchenko, Koji Tsuda, and K R Müller. Machine Learning Meets Quantum Physics. Springer Nature, June 2020.
- [30] Giuseppe Carleo, Ignacio Cirac, Kyle Cranmer, Laurent Daudet, Maria Schuld, Naftali Tishby, Leslie Vogt-Maranto, and Lenka Zdeborová. Machine learning and the physical sciences. *Rev. Mod. Phys.*, 91:045002, Dec 2019.
- [31] Jonathan Schmidt, Mário R G Marques, Silvana Botti, and Miguel A L Marques. Recent advances and applications of machine learning in solid- state materials science. *npj Computational Materials*, pages 1–36, August 2019.
- [32] Keith T Butler, Daniel W Davies, Hugh Cartwright, Olexandr Isayev, and Aron Walsh. Machine learning for molecular and materials science. *Nature*, pages 1–9, July 2018.
- [33] Jörg Behler and Michele Parrinello. Generalized neuralnetwork representation of high-dimensional potentialenergy surfaces. *Physical review letters*, 98(14):146401, 2007.
- [34] Albert P Bartók, Mike C Payne, Risi Kondor, and Gábor Csányi. Gaussian approximation potentials: The accuracy of quantum mechanics, without the electrons. *Physical review letters*, 104(13):136403, 2010.
- [35] Kevin Ryan, Jeff Lengyel, and Michael Shatruk. Crystal Structure Prediction via Deep Learning. Journal of the American Chemical Society, 140(32):10158–10168, July 2018.
- [36] Zhenqin Wu, Bharath Ramsundar, Evan N Feinberg, Joseph Gomes, Caleb Geniesse, Aneesh S Pappu, Karl Leswing, and Vijay Pande. MoleculeNet: a benchmark for molecular machine learning. *Chemical Science*,

9(2):513-530, 2018.

- [37] Prasanna V Balachandran, Benjamin Kowalski, Alp Sehirlioglu, and Turab Lookman. Experimental search for high-temperature ferroelectric perovskites guided by twostep machine learning. *Nature Communications*, pages 1–9, April 2018.
- [38] A P Bartók, Sandip De, Carl Poelking, Noam Bernstein, J R Kermode, Gábor Csányi, and Michele Ceriotti. Machine learning unifies the modeling of materials and molecules. *Science Advances*, 3(12):e1701816, December 2017.
- [39] Bingqing Cheng, Ryan-Rhys Griffiths, Simon Wengert, Christian Kunkel, Tamas Stenczel, Bonan Zhu, Volker L Deringer, Noam Bernstein, Johannes T Margraf, Karsten Reuter, et al. Mapping materials and molecules. Accounts of Chemical Research, 53(9):1981–1991, 2020.
- [40] J Behler. Atom-centered symmetry functions for constructing high-dimensional neural network potentials. *The Journal of Chemical Physics*, 134(7):074106–14, February 2011.
- [41] A P Bartók, Risi Kondor, and Gábor Csányi. On representing chemical environments. *Physical Review B*, 87(18):184115–16, May 2013.
- [42] Miguel A. Caro. Optimizing many-body atomic descriptors for enhanced computational performance of machine learning based interatomic potentials. *Physical Review B*, 100:024112, Jul 2019.
- [43] A Glielmo, Claudio Zeni, and A De Vita. Efficient nonparametric n-body force fields from machine learning. *Physical Review B*, 97(18):1–12, May 2018.
- [44] Claudio Zeni, Kevin Rossi, A Glielmo, and Francesca Baletto. On machine learning force fields for metallic nanoparticles. Advances in Physics: X, 4(1):1–33, December 2019.
- [45] Volker L Deringer and Gábor Csányi. Machine learning based interatomic potential for amorphous carbon. *Physical Review B*, 95(9):094203, March 2017.
- [46] The quantum reference data are freely available at http://www.libatoms.org.
- [47] Mathieu Blondel, Olivier Teboul, Quentin Berthet, and Josip Djolonga. Fast differentiable sorting and ranking. In Hal Daumé III and Aarti Singh, editors, Proceedings of the 37th International Conference on Machine Learning, volume 119 of Proceedings of Machine Learning Research, pages 950–959. PMLR, 13–18 Jul 2020.