PARTIAL INFORMATION DECOMPOSITION REVEALS THE STRUCTURE OF NEURAL REPRESENTATIONS

David A. Ehrlich\textsuperscript{1,*}, Andreas C. Schneider\textsuperscript{2,*}, Michael Wibral\textsuperscript{1}, Viola Priesemann\textsuperscript{2}, and Abdullah Makkeh\textsuperscript{1}

\textsuperscript{1}Goettingen Campus Institute for Dynamics of Biological Networks, Georg-August University Goettingen, Goettingen
\textsuperscript{2}Max Planck Institute for Dynamics and Self-Organization, Goettingen

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ABSTRACT

In neural networks, task-relevant information is represented jointly by groups of neurons. However, the specific way in which the information is distributed among the individual neurons is not well understood: While parts of it may only be obtainable from specific single neurons, other parts are carried redundantly or synergistically by multiple neurons. We show how Partial Information Decomposition (PID), a recent extension of information theory, can disentangle these contributions. From this, we introduce the measure of "Representational Complexity", which quantifies the difficulty of accessing information spread across multiple neurons. We show how this complexity is directly computable for smaller layers. For larger layers, we propose subsampling and coarse-graining procedures and prove corresponding bounds on the latter. Empirically, for quantized deep neural networks solving the MNIST task, we observe that representational complexity decreases both through successive hidden layers and over training. Overall, we propose representational complexity as a principled and interpretable summary statistic for analyzing the structure of neural representations.

1 Introduction

Despite their tremendous success, the inner workings of artificial neural networks remain mostly elusive to this date \cite{1,2,3}. It is known that, since all of the information a network can use to solve a task must already be contained in the model’s inputs, the purpose of hidden internal components remains to distill the pertinent features and make them available to later computational steps. However, the way in which the features are represented among multiple neurons and how this representation changes throughout the training phase is not well understood \cite{4,5}. This lack of understanding continues to pose a major obstacle to the adoption of machine learning techniques in critical settings, such as medical image analysis or self-driving cars, but also hinders principled development of better machine learning algorithms \cite{3,6,7}.

The difficulty of extracting information from internal representations in hidden layers is a key factor for interpretability and network performance alike. As a first step towards these objectives, one needs to rigorously define and quantify this difficulty, which originates from complex higher-order interrelations between neurons. These relations – if present – make it necessary to consider large groups of neurons at a time to be able to discriminate between different target values. The number of neurons minimally needed to obtain a piece of target-discriminatory information is conceptually related to the classical question of how many neurons are active in the representation of an input item, and may thus be viewed as an information-theoretic equivalent of a sparsity measure. We propose to quantify this information sparsity in a principled way by answering an intuitive question: On average, how many neurons do I need to observe simultaneously in order to gain access to a piece of information?

\textsuperscript{*}These authors contributed equally to this work.
\textsuperscript{†}davidalexander.ehrlich@uni-goettingen.de
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Figure 1: Mereological diagram symbolizing how the PID atoms \( \Pi(T : S_\alpha) \) constitute all classical mutual information quantities involving three source variables, as introduced by Williams and Beer [13]. Classical mutual information terms are represented by black ovals with general redundancies given by their overlaps. The PID atoms correspond to the contiguous areas of the overlaps and are labelled by their corresponding antichains \( \alpha \). The green shading indicates the degree of synergy \( m \) of the respective atoms.

From the perspective of Information Theory (IT, [8]), neural networks are information channels that forward the task-relevant part of the input to the output layer while shedding task-irrelevant parts [9]. However, the idea of using IT to quantify the information in the activations of deep neural network hidden layers has been met with fierce debate after methodological flaws surfaced [10, 11] in the influential early works by Tishby et al. [9, 12]. We address these issues in this work and show how information theory can be applied to quantized networks in a theoretically sound way.

However, the question posed above on how features are represented cannot be answered using classic IT alone due to its inability to disentangle redundant and synergistic contributions between multiple neurons [13], leading to inevitable double- or under-counting of information contributions. Non-overlapping information contributions can be obtained by decomposing the mutual information between a target random variable \( T \) and several source variables \( S = (S_1, \ldots, S_n) \) into information atoms \( \Pi(T : S_\alpha) \) such that

\[
I(T : S) = \sum_\alpha \Pi(T : S_\alpha),
\]

which has been made possible by the introduction of a recent extension to IT known as Partial Information Decomposition (PID) [13]. The atoms are the smallest set of quantities from which the mutual information between \( T \) and all possible subsets of \( S \) can be combined (Figure 1) [14]. Each information atom is referred to by its corresponding ‘antichain’ \( \alpha \), which will be explained in Section 3.1.

From the PID atoms, we can answer the question of how many neurons are needed to access an average piece of information in a principled way by introducing the summary statistic we term “Representational Complexity”. A representational complexity of \( C = 1 \) means that all information can be obtained from single neurons, while a representational complexity \( C \) that is equal to the number of neurons in a layer means that no information can be obtained about the target unless one has access to all neurons. By tracking the representational complexity \( C \) of the hidden layers over training we shed light upon a key aspect of how the internal representations of the target variable evolve during the training phase. This understanding may subsequently be employed to improve network designs by providing a tool to compare the dynamics in different network architectures.

The main contributions of this work are (i) describing a principled approach for applying PID to analyze the representations in Deep Neural Networks (DNNs), (ii) the introduction of representational complexity as a measure of information sparsity, (iii) discussing subsampling and coarse-graining procedures for the estimation of representational complexity and proofs of bounds on the latter and (iv) empirical results in quantized DNNs showing a decrease in representational complexity over training and through successive hidden layers.
2 Related works

Tishby and Zaslavsky [9] were among the first to attempt to analyze deep neural networks from an information-theoretic perspective. Information theory, which was developed for the analysis of noisy information channels [8], allows to quantify information in an observer-independent way and helps to form a clear criterion of relevancy of information in hidden representations by distinguishing between the mutual information of layer activations with the network’s target variable (i.e., labels) and with the input variables. Viewing the networks as a sequence of such channels, Shwartz-Ziv and Tishby [12] computed mutual information from binned activations of the individual hidden layers, and plotted the resulting trajectory in what they termed the information plane.

However, their claim to estimate actual mutual information quantities of the network variables with their binning approach was later shown to be unfounded [10][11]. Because of the continuous nature of the activation values and the deterministic, almost always injective mapping from inputs to activation values given by the network itself, the true mutual information between the network’s inputs or label and a hidden layer is either infinite, in the case of continuous features, or constant and equal to the finite entropy of the discrete inputs or labels [10][11][15]. For this reason, the results shown by Shwartz-Ziv and Tishby [12] do not constitute estimates of actual information-theoretic quantities and may at best be reinterpreted as measures for geometric clustering [11][15].

Building on this realization, Goldfeld et al. [11] showed that a meaningful information-theoretic analysis can be performed by disrupting the injectivity and limiting the channel capacity of the network forward function. While they achieve this by explicitly adding Gaussian noise to each activation value, we achieve the same goal by training and analyzing quantized very-low precision activation values in this work. This approach is in line with recent trends towards low [16] and very-low precision [17] computing for reasons of efficiency and scalability. The crucial difference to Shwartz-Ziv and Tishby [12]’s binning approach lies in the fact that the quantization we employ is intrinsic to the network itself, making mutual information quantities well-defined and meaningful as well as ensuring the data processing inequality holds for the Markov chain of successive hidden layers.

The picture of artificial neural networks as mere information channels needs to be refined following the insight that network layers need not only to pass on all relevant information, but also to transform it in such a way that it becomes accessible for subsequent processing. To understand this representation of information within each layer, one needs to go beyond analyzing hidden layers as a whole and look at the structure of information representation across the neurons within those layers instead, which can be done in a principled way by employing partial information decomposition.

Previous works on PID in artificial neural networks have used PID to motivate and interpret classical mutual information quantities and used it to analyze filters in convolutional neural networks [18]. Furthermore, Tax et al. [19] used PID to analyze pairs of neurons in generative neural networks and find that the networks move towards more unique representations of the target in later stages of training. We expand upon this approach by being the first to analyze all neurons of a layer as individual PID sources, which allows also to uncover higher-order interactions between them.

Closely connected to our approach, Reing et al. [20] derived scalable measures for quantifying higher-order interactions between neurons using information theory. By focusing more on scalability, however, the authors trade in some of the interpretability and expressivity of an approach based on PID. Furthermore, Reing et al. [20] cover mostly the analysis of representations without reference to a target variable, while we focus on analyzing only task-relevant information contributions.

In the context of representation learning, information-theoretic approaches focus mostly on quantifying the degree of entanglement of latent dimensions in Variational Autoencoders, often with respect to the information about some underlying generative factor. This is done by measuring the total correlation [21] as a summary statistic or the difference between two classical mutual information quantities [22][23]. These works are related to ours, but analyze only a specific layer, do not use the label information as target and stay within the realm of classical IT.

Other works on representations in deep neural networks have attempted to define notions of usable information based on the idea of restricting the ability of an observer to perfectly decode the presented information [24][25]. A related approach is the probing of representations using simple linear readouts, for example Alain and Bengio [26], who find empirical evidence hinting at less complex representations in deeper layers. Additionally, several other summary statistics of representations have been suggested based on dimensionality analysis [27] or canonical correlation analysis [28][29].

Several other complexity measures were compared by Jiang et al. [30], who analyzed them in terms of their ability to predict the networks’ capacity for out-of-sample generalization. This idea is founded on the intuitive notion that less complex representations should be more robust to minor changes in the inputs. As our paper is focused on interpretability and theoretical soundness of the novel measure of representational complexity, potential ties to generalization ability have not been studied as of yet.
3 Deriving an interpretable measure for the complexity of a representation from partial information decomposition

3.1 Partial information decomposition

The mutual information \( I(T : S) = I(T : S_1, \ldots, S_n) \) that several source random variables \( S = \{ S_1, \ldots, S_n \} \) carry about a target \( T \) can be distributed amongst the sources in very different ways. While some pieces of information are unique to certain sources, others are encoded redundantly by different sources, while yet others are only accessible synergistically from several sources taken together. With three or more sources, even more complex contributions, in general describing redundancies between synergies, emerge. For example, some information about \( T \) might be accessible either from source \( S_3 \) alone, or – redundantly to this – from a synergistic combination of sources \( S_1 \) and \( S_2 \), but from nowhere else; this information would constitute one of the information atoms \( \Pi \).

As mentioned before, these information atoms can be combined to form all classical mutual information quantities \( I(T : S_a) \) between \( T \) and subsets of sources \( S_a = \{ S_i | i \in a \} \) with indices \( a \subseteq \{ 1, \ldots, n \} \). Conversely, the information atoms can be uniquely identified by which classical mutual information quantities they contribute to. Mathematically, this notion is captured by their corresponding parthood distribution \( \Phi : \mathcal{P}(\{ 1, \ldots, n \}) \rightarrow \{ 0, 1 \} \) – a binary function defined on the powerset \( \mathcal{P} \) of source indices that is equal to “1” for exactly those sets \( a \) of source indices for which the atom \( \Pi(T : S_a) \) is part of the mutual information \( I(T : S_a) \) \[14\]. Thus, the mutual information of any set of sources \( S_a \) and \( T \) can be written as

\[
I(T : S_a) = \sum_{\{ \Phi | \Phi(a) = 1 \}} \Pi(T : S_\Phi).
\] (2)

Instead of labelling the atoms by their parthood distribution \( \Phi \), the atoms can equivalently be referenced as \( \Pi(T : S_a) \) using certain sets of source indices \( \alpha \in \mathcal{P}(\{ 1, \ldots, n \}) \), which can be mapped one-to-one to parthood distributions \[13\] and are referred to as antichains \[13\] (see Appendix A.1). The antichains make apparent the connection between atoms and their meaning as redundancies between synergies: For example, the atom from before capturing the information that can be obtained either from \( S_3 \) alone or synergistically from \( S_1 \) and \( S_2 \) together is referred to by the antichain \( \{ 1, 2 \}, \{ 3 \} \).

The number of atoms scales super-exponentially with the number of sources \( n \) – increasing from 7579 for \( n = 5 \) sources to over 7.8 million for \( n = 6 \) \[13\] – while there are only \( 2^n - 1 \) classical mutual information quantities providing constraints. Note, however, that this increase in the number of atoms should not be mistaken for a shortcoming of PID but rather as an acknowledgement of the vast number of configurations information can be encoded in in multiple variables. One way to resolve this underdeterminedness is through the introduction of a measure for redundancy \( I_r(T : S_a) = I_r(T : \{ S_{a_1}, \ldots, S_{a_\beta} \}) \) between collections of sources indexed by \( a_\beta \subseteq \{ 1, \ldots, n \} \). Noting that mutual information can be interpreted as a “self-redundancy” such that \( I(T : S_a) = I_r(T : \{ S_a \}) \), these redundancies can be constructed from the information atoms in an analogous and consistent way to Equation (1) as

\[
I_r(T : S_a) = \sum_{\beta \leq a} \Pi(T : S_\beta),
\] (3)

where \( \leq \) refers to the partial order of antichains on the redundancy lattice (see Appendix A.2) \[13\]. Since now the number of defining equations is equal to the number of atoms, these can be computed by inverting Equation (3), which is known as a Moebius-Inversion \[13\].

Over recent years, a number of different measures have been suggested which fulfill a multitude of different additional desiderata \[52\], e.g., from decision theory \[53\], game theory \[54\] or Kelly gambling \[55\]. In this paper, we utilize the SxPID measure introduced by Makkeh et al. \[56\], where ‘Sx’ stands for shared exclusions of probability mass. In essence, the measure defines redundancy by the regions of probability space which are jointly excluded by the realizations of multiple collections of random variables. As the measure draws only on notions from probability theory, and is the only known differentiable PID measure to date, it is the most canonical choice for our purpose of analyzing neural networks. The concept of representational complexity, however, can readily be generalized to any other redundancy-based multivariate PIDs.

3.2 Representational complexity

In order to understand the representation of task-relevant information in multiple equivalent source variables, we introduce in the following a principled way to evaluate the question of how much of the system needs to be observed
simultaneously to access a particular piece of information. We propose that this difficulty of retrieving information may be quantified by computing the minimum number of sources that are needed jointly in order to reveal the information.

Note, however, that this question cannot be answered by classical information theory due to its inability to disentangle synergistic and redundant contributions: For two source variables $S_1$ and $S_2$, their joint mutual information $I(T : S_1, S_2)$ about the target variable $T$ differs from the sum $I(T : S_1) + I(T : S_2)$, because synergy between the source variables drives up the joint mutual information while redundancy can simultaneously diminish it. Since redundant information can be obtained from single neurons while synergy requires both neurons to be accessible, classical IT is insufficient to answer how many neurons are needed to access an average piece of information.

The PID atoms, on the other hand, can be uniquely assigned a “Degree of Synergy” $m$ given by

$$ m(\alpha) := \min_{\mathbf{a} \in \alpha} |\mathbf{a}|, $$

which quantifies how many sources are minimally needed to gain access to that atom’s information (Figure 1).

Finally, the average degree of synergy, weighted by the relative information contributions of the respective atoms, defines the “Representational Complexity” $C$ as

$$ C := \frac{1}{I(T : \mathbf{S})} \sum_{\alpha} \Pi(T : \mathbf{S}_\alpha) m(\alpha). $$

A representational complexity of $C = 1$ means that all information can be obtained from single sources, while $C$ is equal to the number of sources if the information is spread purely synergistically between all of them.

The concept of representational complexity is linked to the idea of sparse coding in neuroscience $^{[37]}$, in that both approaches aim to capture the relevance of higher-order relations between neurons. While sparsity measures quantify the spread of activity tied to individual realizations across the neuron population, e.g., by measuring the momentary average of non-zero neurons, representational complexity measures the spread of information, i.e., how distributed the ability to distinguish between realizations of the target variable (e.g. the label in classification tasks) is. Note further that representational complexity is computed on the mutual information with the networks target variable, thus relating to only task-relevant components of the activation patterns, while sparsity measures are generally not selective about the task-relevancy of the activations.

**Example applications of representational complexity** To become familiar with the intuitive interpretation of representational complexity, we demonstrate its use with simple information encodings in small toy examples. Consider a categorical random variable with a finite number of distinct classes, which are labelled by integers and occur with the same probability. How does representational complexity differ between different representations of this information in multiple binary neurons?

Firstly, imagine four distinct values are represented sparsely across four neurons (Figure 2A). As for all one-hot encodings, the representational complexity of this encoding is equal to one (Appendix A.4). This is intuitively clear: For each realization, you only need access to the one neuron that is equal to 1 to fully determine the correct label.

Using the same task and neurons, we can also encode the same information in a more complex way. For instance, take pairs of neurons that redundantly represent digits of a binary representation of the label index (Figure 2B). In this case, there is no longer a single neuron that contains the full information about the target, which is reflected by an increase of the representational complexity to $C = 1.21$.

Using all of the neurons’ capacity by encoding 16 distinct states in the four neurons in a binary code (Figure 2C), the representational complexity increases further: $C$ reaches a value of 1.67 as more information has to be encoded synergistically between the four neurons. The reason why $C$ is not equal to 4, despite the fact that the correct label can only be isolated with access to all four neurons, is that parts of the information, e.g., the parity of the label number, can be extracted from fewer than all sources. Conversely, if we now again expand the 16 realizations to 16 neurons in a one-hot encoding (Figure 2D), we revert back to a representational complexity of just $C = 1$. From this, we gain the intuitive realization that the closer one gets to the channel capacity, the more one is forced to encode some of the information in more complex, higher-synergy terms.

However, even small amounts of information can be encoded in a highly synergistic manner. Consider the more realistic case of two discrete neurons with eight activation levels each, with the target value being the exclusive disjunction (XOR) of the thresholded neurons’ activations (Figure 2E). Despite encoding just a single bit of information, the representational complexity assumes a value of $C = 1.89$. This value is close to the theoretical maximum value of $C = n = 2$, with the small difference being due to the nature of the SxPID redundancy measure. Extending this task to the parity of three thresholded neurons (Figure 2F), the representational complexity attains a value of $C = 2.83$, similarly close to its maximum.
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Figure 2: Demonstration of representational complexity with simple examples. Subfigures A-D show different label encoding schemes in binary neurons $S_1, \ldots, S_n$ (circles). Subfigure E shows an encoding of two labels (red and blue) in two eight-level neurons, while F shows the three-dimensional extension. The corresponding representational complexities $C$ are denoted in the bottom left corner.

Figure 3: Representational complexity of hidden layers with respect to the label decreases over training and throughout successive hidden layers. A The MNIST classifier network consists of seven fully-connected layers with tanh activation functions for all but the last layer, which is equipped a softmax activation function. B The representational complexity of the three small hidden layers $L_3$, $L_4$ and $L_5$ are computed from their PID atoms on the train data set. The solid lines show the average of 20 randomly initialized runs, the shaded areas contain 95% of the data points. The inset shows train and test set accuracy.

4 Application to deep neural networks

To exemplify the utility of our measure, we show how it can be applied to analyze the hidden layer representations of a deep neural network classifier solving the well-established MNIST handwritten digit recognition task [38]. The small network consists of seven fully-connected layers, starting with a vector of the 784 grayscale pixel values of the image input, tapering down to only five neurons in layers $L_3$, $L_4$ and $L_5$ and culminating in a ten neuron one-hot output vector, in which each neuron represents one of the ten possible digits (Figure 3A). The structure has been chosen such
that the three successive five-neuron layers can be analyzed in full, as it is practically infeasible at present to compute the full PID for more than five sources because of the fast-growing number of PID atoms.

In order to limit the channel capacity to be able to observe non-trivial information dynamics [11], all layers are discretized to eight or four quantization levels (3 or 2 bits) during both training and analysis (Appendix A.5). The networks are trained using stochastic gradient descent for $10^5$ training epochs and reach, with eight quantization levels, an average accuracy of $99.9(1)\%$ on the train and $96.1(4)\%$ on the test set for 20 runs with unique random weight initializations. Details about quantization schemes and forward-stochastic backprop algorithm used in training can be found in Appendix A.5.

4.1 Representational complexity in small layers

The quintivariate, i.e., five-source-variable, PID of the hidden layers $L_2$, $L_3$, and $L_4$ with the ground-truth label can be computed in full on the network with eight quantization levels, which allows to track the representational complexity both over training and through the successive layers (Figure 3B). We find that both with increasing training epoch and layer index, the representational complexity $C$ decreases.

This decrease in representational complexity appears to be a robust trend observable in networks independent of the encoding enforced on the output layer. While a neural network seems to approach the output complexity in the case of a one-hot output representation, for which $C_{\text{one-hot}} = 1$ (proven in Appendix A.4), the representational complexity of the hidden layers decreases below that of the targeted output representation in the case of a binary label encoding (Appendix A.6).

4.2 Representational complexity in larger layers

Typical production neural networks have layers which are much wider than five neurons (e.g. [39, 40]). Since the compute required for a full PID for six or more source variables is prohibitive because of the rapidly increasing number of atoms, in order to be able to apply the tool of PID in general and representational complexity in particular to wider layers, one needs to devise procedures to reduce the number of random variables to analyze. In this section, we present two complementary approaches to make representational complexity applicable to moderately larger networks, namely subsampling and coarse-graining, and show the latter to be the more theoretically sound approach.

Subsampling A straightforward approach for reducing the number of random variables, which has been employed in previous works (i.e., [19]), is to subsample only $\hat{n}$ neurons from a layer to use as PID sources. By randomly selecting five neurons from the second layer of the network with four quantization levels, we again observe a decrease of the representational complexity of the hidden layer with respect to the label over the training phase (Figure 4A, B), albeit with a larger amount of variability.

However, this approach suffers from fundamental conceptual flaws. By dissecting the mutual mutual information terms $I(T : S_a)$ of the target with only a subset of neurons $S_a$, only atoms with a degree of synergy of less than or equal to $\hat{n}$ can be quantified, resulting in a potential underestimation of representational complexity. At the same time, pieces of information that appear to only be obtainable synergistically within one subset $S_a$ of sources may very well be redundant with a single source $S_i \not\in S_a$, thus leading to potential overestimation of representational complexity. For these reasons, we find subsampling to be an unsuitable approach for overcoming the scaling difficulties of PID.

Coarse-graining A complementary, more theoretically sound approach to reduce the number of variables is to combine multiple neurons, forming fewer higher-dimensional random variables; this procedure will be referred to as coarse-graining. In Appendix A.3 we prove that if $d$ neurons $S_j$ each are combined to random variables $\hat{S}_j$, the true representational complexity of the layer is bounded from below by the coarse-grained representational complexity computed from $\hat{S} = \{\hat{S}_1, \ldots, \hat{S}_{n/d}\}$, while being simultaneously bounded from above by $d$ times this value, i.e.,

$$C(T : \hat{S}) \leq C(T : S) \leq dC(T : \hat{S}).$$

In our example network with four quantization levels, the representational complexity computed from randomly assigned neuron pairs in the second hidden layer consisting of ten neurons, exhibits a decreasing pattern over training that is highly similar to that of the representational complexity computed with individual neurons as sources in layers $L_3$ to $L_5$ (Figure 4C, D).
5 Discussion

In this work, we introduced representational complexity as a measure of sparsity of task-relevant information in neural networks. We first explained how a principled and meaningful application of information theory in neural networks is possible by using quantized activation values in both training and evaluation. Subsequently, we derived representational complexity from partial information decomposition and show it to be the theoretically sound answer to the question of how many neurons need to be observed simultaneously in order to access an average piece of information. To go beyond the limitations PID gives for the number of source variables, we presented subsampling and coarse-graining procedures. We discussed issues with the former approach, while proving bounds on the latter approach.

In small quantized deep neural networks, we find representational complexity to decrease both over training and through successive layers. We empirically find the reduction to be a robust result which can not only be observed when analyzing small layers neuron-wise, but also when using subsampling or coarse-graining on larger layers. Furthermore, we provide first evidence that the final values the representational complexity converges to do not depend on the representational complexity of the chosen output representation.

These results indicate problems with previous approaches that apply PID by subsampling only pairs of sources (e.g. [19]). Since the representational complexity is high in the early stages of training, high-order interactions between neurons appear to play a major role. These, however, go unnoticed in pairwise approaches.

Limitations Scaling our approach to larger networks remains a challenge. To mitigate this problem, we introduced subsampling and coarse-graining procedures, which allow the application of representational complexity to moderately large networks. However, while subsampling suffers from conceptual flaws, the proven attainable bounds on coarse graining become impractically loose for large networks. For typical production networks we suggest two approaches: Firstly, results found on small toy networks may be generalizable to larger networks, e.g., by inductive proofs, and secondly, estimation of representational complexity could become feasible by finding a way to compute it without computing all PID atoms beforehand. The latter can be achieved by employing a PID based on synergy instead of redundancy, for example by extending on ideas of Rosas et al. [41].

Furthermore, our analysis methods are currently restricted to intrinsically discrete systems, as SxPID was originally defined for discrete variables only [36]. However, in the meantime, a continuous generalization of SxPID has been proven to exist and to be measure-theoretically well-defined [42]. Once an efficient estimator for this generalized measure is available, this will make it possible to analyze also continuous systems in which the total mutual information is inherently restricted to a finite value, e.g., by some form of noise in the system.

Outlook We have here shown how to use the representational complexity to understand the structure of the internal representations as an average across all source and target realizations. Due to the local nature of SxPID, this analysis
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can also be further broken down into the representational complexity for individual target realizations, i.e., class labels. Such an analysis may reveal for example that some classes are linked to representations of high complexity while others are not, or that some classes are represented with low complexity earlier than others during training, while yet others fail to reach a low complexity.

Some theoretical properties of representational complexity have yet to be uncovered. For instance, a lower bound to $C$ might be derived from the notion that closer to channel capacity, one is forced to represent some information in higher synergy terms.

Given the PID atoms, a whole suite of other interesting and easily interpretable measures can be devised. One enticing candidate is the average multiplicity of information, defined as $M = (1/I(T : S)) \sum_\alpha \Pi(\alpha) |\alpha|$. The quantity reflects the average number of times a piece of information is represented redundantly and thus appears to be a promising candidate to serve as a complementary summary statistic to representational complexity, which relates to the synergy of the information encoding.

More generally, we promote representational complexity as a principled novel tool for general complex systems in which a group of equivalent variables jointly holds information about a target variable. New possible applications include both other artificial network architectures such as recurrent or convolutional networks, but also biological or ecological systems. Being derived from first principles in information theory and partial information decomposition, representational complexity provides a clear and intuitive interpretation and the suggested subsampling and coarse-graining procedures make it applicable to a wide variety of questions.

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A Appendix

A.1 Equivalence between parthood distributions and antichains

An information atom $\Pi$ can be equivalently referenced by either its parthood distribution $\Phi$ as $\Pi(T : S_{\phi})$ or its corresponding antichain $\alpha$ as $\Pi(T : S_{\alpha})$. This equivalence is given by the facts that (i) the parthood distributions $\Phi : \mathcal{P} \rightarrow \{0, 1\}$ are monotonic, i.e., they fulfill the relation $a \subseteq b \Rightarrow \Phi(a) \leq \Phi(b)$, and (ii) antichains are succinct representations of such monotonic boolean functions. To gain a deeper insight into the equivalent descriptions of the atoms, we will thus address these two points one by one in the following.

First, note that the monotonicity of the parthood distributions necessarily follows from the properties of mutual information: The mutual information $I(T : S_{\alpha})$ between the target $T$ and a subset of sources $S_{\alpha}$ is contained in the mutual information $I(T : S_{b})$ whenever $b$ is a superset of $a$. This fact is a result of the chain rule of mutual information and the non-negativity of (conditional) mutual information \[ I(T : S_{\alpha}) = I(T : S_{\alpha}, S_{b/\alpha}) = I(T : S_{\alpha}) + I(T : S_{b/\alpha}) \geq I(T : S_{\alpha}) \] and formalizes the intuitive fact that the predictability of the target can only increase when additional source variables are observed. This means that if an atom $\Pi$ is part of the mutual information $I(T : S_{\alpha})$, i.e., $\Phi(a) = 1$, it also has to be part of $I(T : S_{b})$, i.e., $\Phi(b) = 1$ whenever $a \subseteq b$, which is exactly the property of monotonicity: $a \subseteq b \Rightarrow \Phi(a) \leq \Phi(b)$.

Second, note that any boolean function is uniquely defined by the set of inputs $f^{-1}[\{1\}] := \{a \in \mathcal{P} | f(a) = 1\}$ that are mapped to “1”. Given the constraint of monotonicity, this representation can be compressed even further: Any sets which are supersets of others need not be recorded, as these are forced to map to “1” by monotonicity. Thus, a monotonic boolean function can be represented by $\alpha \subseteq f^{-1}[\{1\}]$, constructed by removing all sets in $f^{-1}[\{1\}]$ which are supersets of others. The resulting set of sets $\alpha$ then contains only sets which are incomparable given the partial order of set inclusion, which are referred to in the literature as “antichains” \[13\].

Therefore, each PID $I(T : S_{\phi})$ atom identified with a parthood distribution $\Phi$ can be represented by the antichain representation of $\Phi$, which provides an equivalent labelling of the atom as $I(T : S_{\alpha})$.

A.2 The lattice structure of PID

Similar to the ordering of the mutual information terms described before, the general redundancies $I_{\gamma}(T : S_{\phi})$ also have a canonical ordering. Here, the intuitive idea is that a redundancy $I_{\gamma}(T : S_{\phi})$ is contained in another redundancy $I_{\gamma}(T : S_{\phi'})$ if the latter is part of all the mutual information terms $I(T : S_{\alpha})$ that the first is part of, which makes any part of information contained in $I_{\gamma}(T : S_{\phi})$ also contained in $I_{\gamma}(T : S_{\phi'})$. In terms of parthood distributions, this condition is given by \[14\]

\[
\Phi \sqsubseteq \Psi \Leftrightarrow (\Psi(a) = 1 \Rightarrow \Phi(a) = 1 \text{ for any } a \subseteq \{1, \ldots, n\}).
\]

Using the equivalence established in Appendix A.1 this partial order can be expressed in terms of antichains as \[13\]

\[
\alpha \preceq \beta \Leftrightarrow \forall b \in \beta \exists a \in \alpha : a \subseteq b.
\]

This partial ordering defines the algebraic structure of the “Redundancy Lattice”. Interpreting the redundancies $I_{\gamma}$ as partial sums on this lattice, as described in Equation 3, the atoms can be computed from the redundancies by means of a Moebius Inversion \[13\].

A.3 Proof of bounds on representational complexity by coarse-graining

To make representational complexity applicable to settings with more source random variables, we propose coarse-graining, i.e., combining source variables to form fewer, but higher dimensional, “super variables”, as a suitable procedure. As a first step, we clarify how the new coarse-grained variables are constructed from the original variables using a coarse-grain mapping.

Definition A.1 (Coarse-Grain mapping). For $n, \bar{n} \in \mathbb{N}_{\geq 0}$ and $\bar{n} < n$, an $n$-to-$\bar{n}$ coarse-graining $f : \{1, \ldots, n\} \rightarrow \{1, \ldots, \bar{n}\}$ is a surjective function that maps variable indices to fewer coarse-grained variable indices.

We write the pre-image of the coarse-grain mapping for subsets of coarse-grained source indices $\bar{\alpha} \subseteq \{1, \ldots, \bar{n}\}$ as $f^{-1}[\bar{\alpha}] = \{i \in \{1, \ldots, n\} | f(i) \in \bar{\alpha}\}$. 


Furthermore, we write sets of random variables indexed by the set of indices $\alpha \in \mathcal{P} (\{1, \ldots, n\})$ as $S_\alpha = \{S_i | i \in \alpha \}$ and finally sets of sets of random variables indexed by sets of indices $\alpha \in \mathcal{P}(\mathcal{P}(\{1, \ldots, n\}))$ as $S_\alpha = \{S_{\alpha'} | \alpha' \in \alpha \}$.

Using this notion of a coarse-grain mapping, we can define what a coarse-grained random variables is.

**Definition A.2** (Coarse-Grained Random Variable). Given a vector-valued random variable $S = (S_1, \ldots, S_n)$ and an $n$-to-$\hat{n}$ coarse-grain mapping $f$, the coarse-grained vector-valued random variable $\tilde{S}$ is defined as $\tilde{S} = (\tilde{S}_1, \ldots, \tilde{S}_{\hat{n}})$, where the elements $\tilde{S}_i = S_{f^{-1}(\{i\})} = \{S_k | f(k) = i\}$ are themselves vector-valued random variables, called coarse-grained variables, partitioning the $n$ original variables into $\hat{n}$ variables.

**Example A.1.** Given four source variables $S = (S_1, S_2, S_3, S_4)$, the mapping

$$f : \{1, 2, 3, 4\} \to \{1, 2\}, \ i \mapsto \begin{cases} 1, & i \in \{1, 2\} \\ 2, & i \in \{3, 4\} \end{cases}$$

defines the two coarse-grained random variables $\tilde{S}_1 = (S_1, S_2)$ and $\tilde{S}_2 = (S_3, S_4)$.

In general, a coarse-grain mapping can produce coarse-grained variables consisting of different numbers of original variables. An important special case, however, is that of the uniform coarse-grain mapping, which always maps $d$ source variables to one $d$-dimensional “super-variable”.

**Definition A.3** (Uniform coarse-grain mapping). A uniform coarse-grain mapping of order $d \in \mathbb{N}_{>0}$ such that $d/n$ is given by $f : \{1, \ldots, n\} \to \{1, \ldots, n/d\}$, $i \mapsto \lfloor (i - 1)/d \rfloor + 1$, where $\lfloor \cdot \rfloor$ refers to rounding down to the nearest integer.

Having defined the coarse-grained variables $\tilde{S}$, the next question that arises is how the PID atoms of the original variables can be combined to form the coarse-grained PID atoms of $\tilde{S}$.

**Theorem A.1** (Coarsening of PID atoms). The PID atoms $\Pi(T : \tilde{S}_\hat{\beta})$ of the coarse-grained source variable $\tilde{S}$ are composed of the PID atoms $\Pi(T : S_\beta)$ of the original sources $S$ as

$$\Pi \left( T : \tilde{S}_\hat{\beta} \right) = \sum_{\Phi : \Phi \circ f^{-1} = \hat{\Phi}} \Pi \left( T : S_\beta \right).$$  \hfill (9)

**Proof.** A PID atom $\Pi(T : S_\beta)$ is a part of the coarse-grained PID atom $\Pi(T : \tilde{S}_{\hat{\beta}})$ exactly if it contributes to the same mutual information terms $I \left( T : \tilde{S}_\hat{\beta} \right)$ with the coarse-grained variables $\tilde{S}_\hat{\beta}$. Since the identity

$$I \left( T : \tilde{S}_\hat{\beta} \right) = I \left( T : S_{f^{-1}[\hat{\beta}]} \right)$$

follows readily from the definition of the coarse-grained variables, we find that if $\Pi(T : S_\beta)$ is part of $I \left( T : S_{f^{-1}[\hat{\beta}]} \right)$, i.e., $\Phi(f^{-1}[\hat{\beta}]) = 1$, it is also part of $I \left( T : \tilde{S}_\hat{\beta} \right)$ in the coarse-grained picture, and vice-versa. Thus, the parthood relations of $\Pi(T : S_\beta)$ with regards to the coarse-grained variables are captured by the parthood distribution $\hat{\Phi} = \Phi \circ f^{-1}$, which leads to the conclusion that it must be part of the coarse-grained atom $\Pi \left( T : \tilde{S}_\hat{\beta} \right)$. The coarse-grained atoms must now be the sums of all original atoms which contribute to the same coarse-grained mutual information terms; thus the theorem follows.

This coarse-grained PID naturally gives rise to both a lower and an upper bound on the representational complexity of the original variables. As a first step, we show how representational complexity can be equally computed from the parthood distribution $\Phi$ of an atom.

**Lemma A.1** (Computing the degree of synergy from a parthood distribution). The degree of synergy of the atom indexed by the parthood distribution $\Phi$ is given by $m(\Phi) = \min_{\Phi(\alpha) = 1} |\alpha|$. \hfill (10)

**Proof.** The parthood distribution $\Phi$ corresponding to an antichain $\alpha$ is the boolean function that maps all $\alpha \in \alpha$ and all supersets thereof to one. This means, in addition to all sets $\alpha \in \alpha$, that $\Phi^{-1}[\{1\}]$, the fibre of 1 under $\Phi$, contains only sets $\alpha' \supset \alpha$, for which $|\alpha'| > |\alpha|$ and which thus have no influence on the minimum cardinality of sets:

$$m(\alpha) := \min_{\alpha \in \alpha} |\alpha| = \min_{\alpha \in \Phi^{-1}[\{1\}]} |\alpha| = \min_{\Phi(\alpha) = 1} |\alpha| =: m(\Phi).$$
The next step in our quest to prove bounds on the representational complexity is to prove bounds on the degree of synergy $m$.

**Lemma A.2.** Let $\Phi$ and $\tilde{\Phi}$ refer to the parthood distributions of an atom and a coarse-grained atom, respectively. If $\Pi(T : S_\Phi)$ is part of $\Pi(T : \tilde{S}_\tilde{\Phi})$, then the degree of synergy $m(\Phi)$ is constrained by the degree of synergy $m(\tilde{\Phi})$ as $m(\tilde{\Phi}) \leq m(\Phi) \leq dm(\tilde{\Phi})$, where the upper bound holds for a uniform coarse-graining of order $d$.

**Proof.** Let the atom $\Pi(T : S_\Phi)$ be part of the coarse-grained atom $\Pi(T : \tilde{S}_\tilde{\Phi})$. It follows from Equation (9) that $\tilde{\Phi} = \Phi \circ f^{-1}$ and therefore

$$m(\tilde{\Phi}) = \min_{\Phi(\tilde{a})=1} |\tilde{a}| = \min_{\Phi \circ f^{-1}(a)=1} |a| = \min_{\Phi(a)=1} |f(a)| \leq \min_{\Phi(a)=1} |a| = m(\Phi),$$

where the fact that $|f(a)| \leq |a|$ has been used. Note similarly that for a uniform coarse-graining of order $d$, $d|f(a)| \geq |a|$ holds, hence one finds a lower bound to $m(\tilde{\Phi})$ as

$$m(\tilde{\Phi}) = \min_{\Phi(a)=1} |f(a)| \geq \frac{1}{d} \min_{\Phi(a)=1} |a| = \frac{1}{d} m(\Phi).$$

From the bounds on the synergistic degree, the bounds on the representational complexity - which is a weighted average of synergistic degrees - are straightforward to derive.

**Theorem A.2.** The representational complexity of a vector of sources $S = (S_1, \ldots, S_n)$ with respect to some target $T$ is bounded from below by the representational complexity of any coarse-graining $\tilde{S}$

$$C(T : \tilde{S}) \leq C(T : S). \quad (11)$$

**Proof.**

$$C(T : \tilde{S}) = \frac{1}{I(T : S)} \sum_{\Phi} \Pi(T : \tilde{S}_\tilde{\Phi}) m(\tilde{\Phi})$$

$$= \frac{1}{I(T : S)} \sum_{\tilde{\Phi}} \left( \sum_{\Phi} \Pi(T : S_\Phi) \right) m(\tilde{\Phi}) \quad \text{(Theorem A.1)}$$

$$\leq \frac{1}{I(T : S)} \sum_{\tilde{\Phi}} \sum_{\Phi} \Pi(T : S_\Phi) m(\Phi) \quad \text{(Lemma A.2)}$$

$$= \frac{1}{I(T : S)} \sum_{\Phi} \Pi(T : S_\Phi) m(\Phi)$$

$$= C(T : S).$$

**Theorem A.3.** The representational complexity of a vector of sources $S = (S_1, \ldots, S_n)$ with respect to some target $T$ is bounded from above by $d$ times the representational complexity of a uniform coarse-graining of order $d$

$$C(T : S) \leq d C(T : \tilde{S}). \quad (12)$$
Proof.

\[
C(T : \tilde{S}) = \frac{1}{I(T : S)} \sum_{\Phi} \Pi(T : \tilde{S}_\Phi) m(\Phi) \\
= \frac{1}{I(T : S)} \sum_{\Phi} \left( \sum_{\Phi : \Phi \circ f^{-1} = \tilde{\Phi}} \Pi(T : S_\Phi) \right) m(\Phi) \quad \text{(Theorem A.1)} \\
\geq \frac{1}{I(T : S)} \sum_{\Phi} \sum_{\Phi : \Phi \circ f^{-1} = \tilde{\Phi}} \Pi(T : S_\Phi) m(\Phi) / d \quad \text{(Lemma A.2)} \\
= \frac{1}{d I(T : S)} \sum_{\Phi} \Pi(T : S_\Phi) m(\Phi) \\
= \frac{1}{d} C(T : S).
\]

\[\square\]

### A.4 Proof of representational complexity of one-hot encoding

In DNNs solving a classification task, the output labels are typically encoded in a “One-Hot Encoding”, in which there are as many neurons as classes with only the neuron corresponding to the correct class being one while all others are zero. Here we prove that all such encodings have a representational complexity of $C = 1$.

**Definition A.4** (One-hot encoding). The one-hot encoding $\tilde{Y}$ of a categorical variable $Y$ with finite ordered alphabet $A_Y = \{y_1, y_2, \ldots, y_n\}$ is the image of the bijective mapping

\[
\tau : A_Y \to A_{Y'} \subset \{0, 1\}^n, \quad y \mapsto \tilde{y} = (\delta_{y,y_j})_j = (0, \ldots, 0, 1, 0, \ldots, 0),
\]

where $\delta_{y,y_j}$ is the Kronecker Delta.

In what follows, we recall the concepts of local mutual information $i$, local SxPID redundancy $i_{(\tau)}^{sx+}$, and its additive decomposition into local informative redundancy $i_{(\tau)}^{sx+}$ and local misinformative redundancy $i_{(\tau)}^{sx-}$. These information functionals are needed in proving that any one-hot encoding has a representational complexity equals to one.

**Definition A.5** (Local information and their informative and misinformative parts). Let $T$ be the target variable and $S$ be the set of sources. Then, we have the following:

- The mutual information $I(T : S)$ is, in fact, the expected value of the local mutual information $i(t : s)$ as follows:

\[
I(T : S) := \sum_{t, s} \mathbb{P}(t \cap s) \log_2 \frac{\mathbb{P}(t \cap s)}{\mathbb{P}(t) \mathbb{P}(s)} = \mathbb{E}_{t, s}[i(t : s)].
\]

- The local mutual information $i(t : s)$ can take negative values and so it is decomposed into non-negative informative $i^+(t : s)$ and misinformative $i^-(t : s)$ parts as follows:

\[
i^+(t : s) := \log_2 \frac{1}{\mathbb{P}(s)} = \log_2 \frac{1}{\mathbb{P}(s)}, \\
i^-(t : s) := \log_2 \frac{\mathbb{P}(t \cap s)}{\mathbb{P}(t) \mathbb{P}(s)} = \log_2 \frac{1}{\mathbb{P}(s|T(t|t))}.
\]

- The SxPID redundancy $I_{(\tau)}^{sx}(T : S_\alpha)$ is in its turn the expected value of the local redundant information $i_{(\tau)}^{sx}(t : s_\alpha)$ as follows:

\[
I_{(\tau)}^{sx}(T : S_\alpha) = \sum_{t, s} \mathbb{P}(t \cap s) \log_2 \frac{\mathbb{P}(t) - \mathbb{P}(t \cap \bigcup_{\alpha \in \alpha} s_\alpha)}{\mathbb{P}(t) \left[1 - \mathbb{P}\left(\bigcup_{\alpha \in \alpha} s_\alpha\right)\right]} = \mathbb{E}_{t, s}[i_{(\tau)}^{sx}(t : s_\alpha)].
\]
• The local SxPID redundancy \( i_{\alpha}^\Sigma (t : s_\alpha) \) can also take negative values and so it is decomposed into nonnegative informative \( i_{\alpha}^{\Sigma^+} (t : s_\alpha) \) and misinformative \( i_{\alpha}^{\Sigma^-} (t : s_\alpha) \) parts as follows:

\[
\begin{align*}
  i_{\alpha}^{\Sigma^+} (t : s_\alpha) &:= \log_2 \frac{1}{1 - P(\bigcap_{a \in \alpha} \bar{s}_a)} = \log_2 \frac{1}{p_{s_\alpha}(s_\alpha)}, \\
  i_{\alpha}^{\Sigma^-} (t : s_\alpha) &:= \log_2 \frac{P(t)}{P(t) - P(t \cap \bigcap_{a \in \alpha} \bar{s}_a)} = \log_2 \frac{1}{p_{s_\alpha \mid \mathcal{S}}(s_\alpha \mid t)}.
\end{align*}
\]

**Lemma A.3.** The misinformative part of the redundancy \( I_{\alpha}^{\Sigma^-} (T : s_\alpha) \) vanishes if there exists a mapping \( f : T \to S \) from the target to the sources.

**Proof.** If there exists a function \( f : T \to S \), all conditional probabilities of the form \( p_{s_\alpha \mid \mathcal{T}}(s_\alpha \mid t) = p_{S_\alpha \mid \mathcal{T}}((s_{\alpha,1} \cap s_{\alpha,2} \cap \ldots) \cup \ldots \mid t) \) are equal to one or zero. Thus, \( I_{\alpha}^{\Sigma^-} (T : s_\alpha) = - \sum_{s,t} p_{S_\alpha,T}(s,t) \log_2 p_{S_\alpha \mid \mathcal{T}}(s_\alpha \mid t) = 0 \) for any \( \alpha \).

To uniquely determine the label from a one-hot representation, it is sufficient to observe the one neuron that is equal to one. One, however, needs the same information by observing all neurons which are equal to zero, since, by exclusion, the last one then has to be one. Let \( \alpha_j := \{j, j-1, j+1, \ldots, n\} \) be the antichain describing the redundant information between the \( j \)-th source and the rest of the sources taken together. Further, let \( I(Y : \bar{Y}) \) describe the mutual information between a random variable \( Y \) and its one-hot representation, which is trivially equal to its entropy \( H(Y) \) due to the construction of \( \bar{Y} \).

**Lemma A.4.** The size of the local SxPID redundancy \( i_{\alpha}^\Sigma (y_j : \bar{y}_{\alpha_j}) \) is \(- \log_2 p_Y(y)\).

**Proof.** Since the one-hot representation is a bijective function of the variable, Lemma A.3 implies that the misinformative part of the redundancy vanishes. The local SxPID redundancy in question then amounts to \( i_{\alpha}^\Sigma (y_j : \bar{y}_{\alpha_j}) = i_{\alpha}^{\Sigma^+} (y_j : \bar{y}_{\alpha_j}) = - \log_2 p_Y(y_j \cup (y_1 \cap \cdots \cap y_{j-1} \cap y_{j+1} \cap \cdots \cap y_n)) = - \log_2 p_Y(y_j \cup y) = - \log_2 p_Y(y). \)

The atoms are ordered on a lattice by the partial ordering relation between atoms with antichains \( \alpha \) and \( \beta \) being given by \( \alpha \preceq \beta \iff \forall b \in \beta \exists a \in \alpha \) such that \( a \subseteq b \). \( (13) \)

The atoms are, then, computed as the Mobius inversion of the corresponding redundancies on the lattice, which is referred to throughout the literature as the Redundancy Lattice.

**Lemma A.5.** The degree of synergy \( m \in \mathbb{N} \) increases monotonically on the redundancy lattice, i.e., \( \alpha \preceq \beta \Rightarrow m(\alpha) \leq m(\beta) \).

**Proof.** Let \( \alpha, \beta \in \mathcal{P}(\mathcal{P}\{1, \ldots, n\}) \) be two antichains on the \( n \) redundancy lattice such that \( \alpha \preceq \beta \). By definition of the degree of synergy (Equation \( (4) \)), there exists a set \( b \in \beta \) such that \( m(\beta) = |b| \). For this \( b \), it follows from the definition of the partial order of the antichains that there must then also exist a set \( a \in \alpha \) for which \( a \subseteq b \). Thus, \( \alpha \preceq \beta \Rightarrow m(\alpha) \leq |a| \leq |b| = m(\beta) \).

**Theorem A.4.** The representational complexity of a categorical random variable \( Y \) and its one-hot representation is equal to one.

**Proof.** The local mutual information of the event \( (T = t, S = s) \) amounts to \( i(y : \bar{y}) = - \log_2 (p_Y(y)) \) and is thus equal to the local redundancy \( i_{\alpha}^\Sigma (y_j : \bar{y}_{\alpha_j}) \) (Lemma A.4). Because all local atoms are non-negative (Lemma A.3), all local atoms \( \pi \) with antichains \( \beta \) succeeding \( \alpha_j \) must be zero. Since \( m(\alpha_j) = 1 \) and \( m(\beta) = 1 \) for all \( \beta \preceq \alpha \) (Lemma A.5), the representational complexity of the one-hot encoding is \( C = 1 \).

### A.5 DNN implementation

The networks analyzed in this paper are fully-connected feed-forward deep neural networks with quantized activation values, but float-precision weights. These networks are trained on the 60000 28x28 grayscale pictures of handwritten digits of the training set of the well-established MNIST dataset [38]. To get better statistics for the test error, the 60000 test samples of the QMNIST dataset have been utilized [44]. The networks use \texttt{tanh} activation functions on the hidden layers, while on the output layer employing a \texttt{softmax} (for one-hot output layer) or \texttt{sigmoid} (for binary output layer).
A total of three different networks have been trained with 20 different random weight initializations each: Figures A.5.1 B and C have been computed on networks trained and evaluated with eight quantization levels per neuron but with different output layer representations: While the networks represented in Figure A.5.1 B have a ten-neuron one-hot output layer, the networks whose results are depicted in Figure A.5.1 C have only four output neurons of which each represents one bit of the binary representation of the numeric label. While the networks shown in Figures A.5.1 B and D share the same network architecture as the ones in Figure A.5.1, they have been trained and evaluated with only four quantization levels to make the computation of the coarse-grained PID more efficient.

For all networks, we used stochastic gradient descent with a batch size of 64, learning rate of 0.01 and Xavier weight initialization. The networks with one-hot output representation employ a cross-entropy loss, while for the binary representation, a mean square error loss was chosen. Parameters and accuracies of the networks are summarized in Table A.1.

To analyze artificial neural networks using information-theoretic tools, we developed the nninfo python package. The package will be published on GitHub after the review process has concluded to preserve the authors’ anonymity.

| Network | #runs | #quantization levels | Output rep. (#neurons) | train acc. | test acc. |
|---------|-------|----------------------|------------------------|------------|-----------|
| Default | 20    | 8                    | one-hot (10)           | 99.96(2)   | 95.0(4)   |
| Binary  | 20    | 8                    | binary (4)             | 99.59(4)   | 95.4(2)   |
| Reduced | 20    | 4                    | one-hot (10)           | 99.80(8)   | 94.7(4)   |
|         |       |                      |                        |            |           |

Table A.1: Network parameters and final accuracies for the three DNNs referenced in this paper.

### A.5.1 Quantization schemes

In order to limit the information capacity of the networks, the activation values have been quantized to very few discrete values. For evaluation, the quantized activations \( \ell \) are computed from the continuous values \( \hat{\ell} \) as

\[
\ell = \epsilon \left\lfloor \frac{\hat{\ell} - \sigma_{\text{min}}}{\epsilon} \right\rfloor + \sigma_{\text{min}},
\]

where \( \lfloor \cdot \rfloor \) denotes rounding to the closest integer, the bin size \( \epsilon \) is given by \( \epsilon = (\sigma_{\text{max}} - \sigma_{\text{min}})/(n_{\text{bins}} - 1) \) and \( \sigma_{\text{min}} \) and \( \sigma_{\text{max}} \) are the bounds of the activation function. This quantization scheme has been chosen as it reproduces the bounds exactly, i.e., \( \hat{\ell} = \sigma_{\text{min}}/\sigma_{\text{max}} \rightarrow \ell = \sigma_{\text{min}}/\sigma_{\text{max}} \), and limits the rounding error to \( \epsilon/2 \).

For the training phase, the activation values of the forward pass are stochastically to make the training more robust. The stochastic scheme builds on the deterministic scheme presented before in that it rounds the values to the same value. However, whether values are rounded up or down to the nearest rounding point is no longer deterministic but given by a probability scaling linearly with the distance from the next two rounding points, giving

\[
\ell = \epsilon \lambda + \sigma_{\text{min}} \quad \text{where} \quad \lambda = \begin{cases} 
\left\lfloor \frac{\hat{\ell} - \sigma_{\text{min}}}{\epsilon} \right\rfloor & r > \left( \frac{\hat{\ell} - \sigma_{\text{min}}}{\epsilon} \right) \mod 1 \\
\left\lceil \frac{\hat{\ell} - \sigma_{\text{min}}}{\epsilon} \right\rceil & r \leq \left( \frac{\hat{\ell} - \sigma_{\text{min}}}{\epsilon} \right) \mod 1 
\end{cases}
\]

and \( r \in [0, 1] \) is drawn i.i.d. from a uniform distribution for each neuron and each evaluation.

### A.6 Effect of choosing a different output encoding

In order to analyze the effect that the output encoding has on the representational complexity of earlier layers, we implemented a network with the same architecture and task as the previous one but differing in the way the labels are represented in the output layer. For this, we chose a 4-bit binary representation of the 10 MNIST labels. The representational complexity of the binary output layer for 10 equiprobable classes has been numerically determined to be \( C = 1.46 \).

The representational complexity of the three five-neuron layers of the network with binary output encoding show a very similar convergence behaviour as the networks with one-hot output representation (Figure A.5.1). The initial increase in representational complexity to a maximum at circa epoch 12 is likely due to a early restructuring of the representation made necessary by this more complex encoding.
Figure 5: **Representational complexity in neural networks with binary output encoding shows similar convergence as networks with one-hot output encoding.** The representational complexity of the binary output encoding has been indicated by a dotted line.