Reconciling emergences: An information-theoretic approach to identify causal emergence in multivariate data

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The broad concept of emergence is instrumental in various of the most challenging open scientific questions – yet, few quantitative theories of what constitutes emergent phenomena have been proposed. This article introduces a formal theory of causal emergence in multivariate systems, which studies the relationship between the dynamics of parts of a system and macroscopic features of interest. Our theory provides a quantitative definition of downward causation, and introduces a complementary modality of emergent behaviour – which we refer to as causal decoupling. Moreover, the theory allows practical criteria that can be efficiently calculated in large systems, making our framework applicable in a range of scenarios of practical interest. We illustrate our findings in a number of case studies, including Conway’s Game of Life, Reynolds’ flocking model, and neural activity as measured by electrocorticography.

While most of our representations of the physical world are hierarchical, there is still no agreement on how the co-existing “layers” of this hierarchy interact. On the one hand, reductionism claims that all levels can always be explained based on sufficient knowledge of the lowest scale and, consequently – taking an intentionally extreme example – that a sufficiently accurate theory of elementary particles should be able to predict the existence of social phenomena like communism. On the other hand, emergentism argues that there can be autonomy between layers, i.e. that some phenomena at macroscopic layers might only be accountable in terms of other macroscopic phenomena. While emergentism might seem to better serve our intuition, it is not entirely clear how a rigorous theory of emergence could be formulated within our modern scientific worldview, which tends to be dominated by reductionist principles.

Emergent phenomena are usually characterised as either strong or weak [1]. Strong emergence corresponds to the somewhat paradoxical case of supervenient properties with irreducible causal power [2]; i.e. properties that are fully determined by microscopic levels but can nevertheless exert causal influences that are not entirely accountable from microscopic considerations [3]. Strong emergence has been as much a cause of wonder as a perennial source of philosophical headaches, being described as “uncomfortably like magic” while accused of being logically inconsistent [2] and sustained on illegitimate metaphysics [4]. Weak emergence has been proposed as a more docile alternative to strong emergence, where macroscopic features have irreducible causal power in practice but not in principle. A popular formulation of weak emergence is due to Bedau [4], and corresponds to properties generated by elements at microscopic levels in such complicated ways that they cannot be derived via explanatory shortcuts, but only by exhaustive simulation. While this formulation is usually accepted by the scientific community, it is not well-suited to address mereological questions about emergence in scenarios where parts-whole relationships are the primary interest.

Part of the difficulty in building a deeper understanding of strong emergence is the absence of simple but clear analytical models that can serve the community to guide discussions and mature theories. Efforts have been made to introduce quantitative metrics of weak emergence [5], which enable fine-grained data-driven alternatives to traditional all-or-none classifications. In this vein, an attractive alternative comes from the work on causal emergence introduced in Ref. [6] and later developed in Refs. [7, 8], which showed that macroscopic observables can sometimes exhibit more causal power (as understood within the framework of Pearl’s do-calculus [9]) than microscopic variables. However, this framework relies on strong assumptions that are rarely satisfied in practice, which severely hinders its applicability [10].

Inspired by Refs. [5, 6], here we introduce a practically useful and philosophically innocent framework to study

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causal emergence in multivariate data. Building on previous work [11], we take the perspective of an experimentalist who has no prior knowledge of the underlying phenomenon of interest, but has sufficient data of all relevant variables that allows an accurate statistical description of the phenomenon. In this context, we put forward a formal definition of causal emergence that doesn’t rely on coarse-graining functions as Ref. [6], but addresses the “paradoxical” properties of strong emergence based on the laws of information flow in multivariate systems.

The main contribution of this work is to enable a rigorous, quantitative definition of downward causation, and introduce a novel notion of causal decoupling as a complementary modality of causal emergence. Another contribution is to extend the domain of applicability of causal emergence analyses to include cases of observational data, in which case causality ought to be understood in the Granger sense, i.e. as predictive ability [12]. Furthermore, our framework yields practical criteria that can be effectively applied to large systems, bypassing prohibitive estimation issues that severely restrict previous approaches.

The rest of this paper is structured as follows. First, Section I introduces some fundamental intuitions by discussing minimal examples of emergence. Then, Section II presents the core of our theory, and Section III discusses practical methods to measure emergence from experimental data. Our framework is then illustrated on a number of case studies, presented in Section IV. Finally, Section V concludes the paper with a discussion of some of the implications of our findings.

I. FUNDAMENTAL INTUITIONS

To ground our intuitions, let us introduce minimal examples that embody a few key notions of causally emergent behaviour. Throughout this section, we consider systems composed of $n$ parts described by a binary vector $X_t = (X_t^1, \ldots, X_t^n) \in \{0, 1\}^n$, which undergo Markovian stochastic dynamics following a transition probability $p_{X_{t+1}|X_t}$. For simplicity, we assume that at time $t$ the system is found in an entirely random configuration (i.e. $p_{X_t}(x_t) = 2^{-n}$). From there, we consider three evolution rules.

Example 1: Consider a temporal evolution where the parity of $X_t$ is preserved with probability $\gamma \in (0, 1)$. Mathematically,

$$p_{X_{t+1}|X_t}(x_{t+1}|x_t) = \begin{cases} \frac{\gamma}{2^{n-1}}, & \text{if } \oplus_{j=1}^n x_{t+1}^j = \oplus_{j=1}^n x_t^j, \\ 1-\gamma, & \text{otherwise,} \end{cases}$$

for all $t \in \mathbb{N}$, where $\oplus_{j=1}^n a_j := 1$ if $\sum_{j=1}^n a_j$ is even and zero otherwise. Put simply: $x_{t+1}$ is a random sample from the set of all strings with the same parity as $x_t$ with probability $\gamma$; and is a sample from the strings with opposite parity with probability $1-\gamma$.

Causal decoupling

Downward causation

FIG. 1. Minimal examples of causally emergent dynamics. In Example 1 (left) the system’s parity tends to be preserved while no interactions occur between low-level elements, which is an example of causal decoupling. In Example 2 (right) the system’s parity determines one element only, corresponding to downward causation.

This evolution rule has a number of interesting properties. First, the system has a non-trivial causal structure, since some properties of the future state (its parity) can be predicted from the past state. However, this structure is noticeable only at the collective level, as no individual variable has any predictive power over the evolution of itself or any other variable (see Figure 1). Furthermore, even the complete past of the system $X_t$ has no predictive power over any individual future $X_{t+1}^i$. This case shows an extreme kind of causal emergence that we call “causal decoupling,” in which the parity predicts its own evolution but no element (or subset of elements) predicts the evolution of any other element.

Example 2: Consider now a system where the parity of $X_t$ determines $X_{t+1}^j$ (i.e. $X_{t+1}^1 = \oplus_{i=1}^n X_t^i$), and $X_{t+1}^j$ for $j \neq 1$ is a fair coin flip independent of $X_t$ (see Figure 1). In this scenario $X_t$ predicts $X_{t+1}^1$ with perfect accuracy, while it can be verified that $X_t^1 \perp X_{t+1}^j$ for all $i \in \{1, \ldots, n\}$. Therefore, under this evolution rule the whole system has a causal effect over a particular element, although this effect cannot be attributed to any individual part [13], being a minimal example of downward causation.

Example 3: Let us now study an evolution rule that includes the mechanisms of both Examples 1 and 2. Concretely, consider

$$p_{X_{t+1}|X_t}(x_{t+1}|x_t) = \begin{cases} 0 & \text{if } x_{t+1}^1 \neq \oplus_{j=1}^n x_{t+1}^j, \\ \frac{\gamma}{2^{n-1}} & \text{if } x_{t+1}^1 = \oplus_{j=1}^n x_{t+1}^j, \\ 1-\gamma & \text{and } \oplus_{j=1}^n x_{t+1}^j = \oplus_{j=1}^n x_t^j, \\ 2^{-n} & \text{otherwise.} \end{cases}$$

As in Example 1, the parity of $X_t$ is transferred to $X_{t+1}$ with probability $\gamma$; additionally, it is guaranteed that $X_{t+1}^1 = \oplus_{i=1}^n X_t^i$. Hence, in this case not only is there a macroscopic effect that cannot be explained from the parts, but at the same time there is another effect going from the whole to one of the parts. Importantly, both effects co-exist independently of each other.

The above are minimal examples of dynamical laws that cannot be traced from the interactions between their
elementary components: Example 1 shows how a collective property can propagate without interacting with its underlying substrate; Example 2 how a collective property can influence the evolution of specific parts; and Example 3 how these two kinds of phenomena take place in the same system. All these issues are formalised by the theory developed in the next section.

II. A FORMAL THEORY OF CAUSAL EMERGENCE

This section presents the main body of our theory of causal emergence. To fix ideas, we consider a scientist measuring a system composed of \( n \) parts. The scientist is assumed to measure the system regularly over time, and the results of those measurements are denoted by \( X_t = (X^1_t, \ldots, X^n_t) \), with \( X^i_t \in \mathcal{X}^i \) corresponding to the state of the \( i^{th} \) part at time \( t \in \mathbb{N} \) with phase space \( \mathcal{X}^i \). When referring to a collection of parts, we use the notation \( X^\alpha_t = (X^1_t, \ldots, X^n_t) \) for \( \alpha = \{i_1, \ldots, i_K\} \subset \{1, \ldots, n\} \). We also use the shorthand notation \( |n| := \{1, \ldots, n\} \).

Our analysis considers two time points of the evolution of the system, denoted as \( t \) and \( t' \), with \( t < t' \). The corresponding dynamics are encoded in the transition probability \( \mathbb{P}_{X_t}|_{X_{t'}|X_t} \). We consider features \( V_t \in \mathcal{V} \) generated via a conditional probability \( \mathbb{P}_V|X \), that are supervenient on the underlying system; i.e. that does not provide any predictive power for future states at times \( t' > t \) if the complete state of the system at time \( t \) is known with perfect precision. We formalise this condition by requiring \( V_t \) to be statistically independent of \( X_{t'} \) when \( X_t \) is given (equivalently, that \( V_t - X_{t'} \perp X_t \) form a Markov chain), for all \( t' > t \). This includes as particular cases deterministic functions \( F : \prod_{i=1}^n \mathcal{X}^i \to \mathcal{V} \) such that \( V_t = F(X_t) \), as well as aggregate properties affected by observational noise.

\[ I(X;Y) = \sum_{\alpha \in \mathcal{A}} I^\alpha_0(X;Y), \tag{1} \]

with \( \mathcal{A} = \{\alpha_1, \ldots, \alpha_L\} : \alpha_i \subseteq [n], \alpha_i \not\subseteq \alpha_j, \forall i, j \) being the set of antichain collections \([14]\). Intuitively, \( I^\alpha_0 \) for \( \alpha = \{\alpha_1, \ldots, \alpha_L\} \) represents the information that the collection of variables \( X^{\alpha_1}, \ldots, X^{\alpha_L} \) provide redundantly, but their sub-collections don’t. For example, for \( n = 2 \) source variables, \( \alpha = \{1\} \{2\} \) corresponds to the information about \( Y \) that is provided independently (and, hence, redundantly) by both of them, \( \alpha = \{1\} \) to the information provided uniquely by \( X_1 \), and, most interestingly, \( \alpha = \{\{1\} \{2\} \} \) corresponds to the information provided by both sources jointly but not separately — commonly referred to as informational synergy.

One of the drawbacks of PID is that the number of atoms (i.e. the cardinality of \( \mathcal{A} \)) grows super-exponentially with the number of sources, and hence it is useful to coarse-grain the decomposition according to specific criteria. Here we introduce the notion of \( k^{th}-order synergy \) between \( n \) variables, which is calculated as

\[ \text{Syn}^{(k)}(X;Y) := \sum_{\alpha \in \mathcal{S}^{(k)}} I^\alpha_0(X;Y), \]

with \( \mathcal{S}^{(k)} = \{\alpha_1, \ldots, \alpha_L\} \in \mathcal{A} : \min_j |\alpha_j| > k \). Intuitively, \( \text{Syn}^{(k)}(X;Y) \) corresponds to the information about the target that is provided by the whole \( X \) but is not contained in any set of \( k \) or less parts when considered separately from the rest. Accordingly, \( \mathcal{S}^{(k)} \) only contains collections with groups of more than \( k \) sources.

Similarly, we introduce the unique information of \( X^\beta \) with \( \beta \subset [n] \) with respect to sets of at most \( k \) other variables, which is calculated as

\[ \text{Un}^{(k)}(X^\beta;Y|X^{-\beta}) := \sum_{\alpha \in \mathcal{U}^{(k)}(\beta)} I^\alpha_0(X;Y). \]

Above, \( \mathcal{U}^{(k)}(\beta) = \{\alpha \in \mathcal{A} : \beta \in \alpha, \forall \alpha \not\subseteq \beta, \alpha \subseteq [n] \setminus \beta, |\alpha| > k\} \), and \( X^{-\beta} \) being all the variables in \( X \) whose indices are not in \( \beta \). Put simply, \( \text{Un}^{(k)}(X^\beta;Y|X^{-\beta}) \) represents the information carried by \( X^\beta \) about \( Y \) that no group of \( k \) or less variables within \( X^{-\beta} \) has on its own. Note that these coarse-grained terms can be used to build a general decomposition of \( I(X;Y) \) described in Appendix A, the properties of which are proven in Appendix B.

One peculiarity of PID is that it postulates the structure of information atoms and the relations between

A. Partial information decomposition

Our theory is based on the Partial Information Decomposition (PID) framework \([14]\), which provides powerful tools to reason about information in multivariate systems. In a nutshell, PID decomposes the information that \( n \) sources \( X = (X^1, \ldots, X^n) \) provide about a target variable \( Y \) in terms of information atoms as follows:

\[ I(X;Y) = \sum_{\alpha \in \mathcal{A}} I^\alpha_0(X;Y), \]
them, but it does not prescribe a particular functional form to compute $I^2_{\partial}$ [15]. Please note that there have been multiple proposals for specific functional forms of $I^2_{\partial}$ in the PID literature; see e.g. Refs. [16–19]. A particular method for fully computing the information atoms based on a recent PID [20] is discussed in Sec. III B.

Conveniently, our theory doesn’t rely on a specific functional form of PID, but only on a few basic properties that are precisely formulated in Appendix B. Therefore, the theory can be instantiated using any PID – as long as those properties are satisfied. Importantly, as shown in Section III A, the theory allows the derivation of practical metrics that are valid independently of the PID chosen.

\section{B. Defining causal emergence}

With the tools of PID at hand, now we introduce our formal definition of causal emergence.

**Definition 1.** For a system described by $X_t$, a supervenient feature $V_t$ is said to exhibit causal emergence of order $k$ if

$$\un^{(k)}(V_t; X'_t|X_t) > 0 \ .$$

Accordingly, causal emergence takes place when a supervenient feature $V_t$ has irreducible causal power, i.e. when it exerts causal influence that is not mediated by any of the parts of the system. In other words, $V_t$ represents some emergent collective property of the system if: 1) contains information that is dynamically relevant (in the sense that it predicts the future evolution of the system); and 2) this information is beyond what is given by the groups of $k$ parts in the system when considered separately.

To better understand the implications of this definition, let us study some of its basic properties.

**Lemma 1.** Consider a feature $V_t$ that exhibits causal emergence of order 1 over $X_t$. Then,

(i) The dimensionality of the system satisfies $n \geq 2$.

(ii) There exists no deterministic function $g(\cdot)$ such that $V_t = g(X^j_t)$ for any $j = 1, \ldots, n$.

**Proof.** See Appendix C. \hfill $\square$

These two properties establish causal emergence as a *fundamentally collective* phenomenon. In effect, property (i) states that causal emergence is a property of multivariate systems, and property (ii) that $V_t$ cannot have emergent behaviour if it can be perfectly predicted from a single variable.

In order to use Definition 1, one needs a candidate feature $V_t$ to be tested. However, in some cases there are no obvious candidates for an emergent feature, for which Definition 1 might seem problematic. Our next result provides a criterion for the existence of emergent features based solely on the system’s dynamics.

\section{C. A taxonomy of emergence}

Our theory, so far, is able to detect *whether* there is emergence taking place; the next step is to be able to characterise *which kind* of emergence it is. For this purpose, we combine our feature-agnostic criterion of emergence presented in Theorem 1 with Integrated Information Decomposition, ΦID, a recent extension of PID to multi-target settings [22].

Using ΦID, one can decompose a PID atom as

$$I^\alpha_\partial(X_t; X'_t) = \sum_{\beta \in \Lambda} I^{\alpha \rightarrow \beta}_\partial(X_t; X'_t) \ .$$

For example, if $n = 2$ then $I^{(1)}_{\partial} \rightarrow (1)_{\partial}^{(1)}$ represents the information shared by both time series at both timesteps (for example, when $X^1_t, X^2_t, X^1'_t, X^2'_t$ are all copies of each other); and $I^{(1)}_{\partial} \rightarrow (1)$ corresponds to the synergistic causes in $X_t$ that have a unique effect on $X^1_t$ (for example, when $X^1_t = X^1_t \oplus X^2_t$). More details and intuitions on ΦID can be found in Ref. [22].

With the fine-grained decomposition provided by ΦID one can discriminate between different kinds of synergies. In particular, we introduce the *downward causation* and

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causal decoupling indices of order \( k \), denoted by \( \mathcal{D}^{(k)} \) and \( \mathcal{G}^{(k)} \) respectively, as

\[
\mathcal{G}^{(k)}(X_t; X_{t'}) := \sum_{\alpha, \beta \in \mathcal{S}^{(k)}} I_{\alpha}^{\rightarrow \beta}(X_t; X_{t'}) , \tag{5}
\]
\[
\mathcal{D}^{(k)}(X_t; X_{t'}) := \sum_{\alpha \in \mathcal{S}^{(k)}} \sum_{\beta \in A \setminus \mathcal{S}^{(k)}} I_{\alpha}^{\rightarrow \beta}(X_t; X_{t'}) . \tag{6}
\]

From these definitions and Eq. (4), one can verify that

\[
\text{Syn}^{(k)}(X_t; X_{t'}) = \mathcal{G}^{(k)}(X_t; X_{t'}) + \mathcal{D}^{(k)}(X_t; X_{t'}) . \tag{7}
\]

Therefore, the emergence capacity of a system naturally decomposes in two different components: information about \( k \)-plets of future variables, and information about future collective properties beyond \( k \)-plets. The \( \Phi \)ID atoms that belong to these two terms are illustrated within the \( \Phi \)ID lattice for two time series in Figure 3. The rest of this section shows that \( \mathcal{D}^{(k)} \) and \( \mathcal{G}^{(k)} \) are natural metrics of downward causation and causal decoupling, respectively.

1. **Downward causation**

   Intuitively, downward causation occurs when collective properties have irreducible causal power over individual parts. More formally:

   **Definition 2.** A supervenient feature \( V_t \) exhibits downward causation of order \( k \) if, for some \( \alpha \) with \( |\alpha| = k \):

   \[
   \un^{(k)}(V_t; X^\alpha_t | X_t) > 0 . \tag{8}
   \]

   Note that, in contrast with Definition 1, downward causation requires the feature \( V_t \) to have unique predictive power over the evolution of specific subsets of the whole system. In particular, an emergent feature \( V_t \) that has predictive power over e.g. \( X^\alpha_t \) is said to exert downward causation, as it predicts something about \( X^\alpha_t \) that could not be predicted from any particular \( X^\alpha_i \) for \( i \in [n] \). Put differently, in a system with downward causation the whole has an effect on the parts that cannot be reduced to low-level interactions. A minimal case of this is provided by Example 2 in Section 1.

   Our next result formally relates downward causation with the index \( \mathcal{D}^{(k)} \) introduced in Eq. (6).

   **Theorem 2.** A system \( X_t \) admits features that exert downward causation of order \( k \) iff \( \mathcal{D}^{(k)}(X_t; X_{t'}) > 0 \).

   **Proof.** See Appendix C. \( \square \)

2. **Causal decoupling**

   In addition to downward causation, causal decoupling takes place when collective properties have irreducible causal power over other collective properties. In technical terms:

   **Definition 3.** A supervenient feature \( V_t \) is said to exhibit causal decoupling of order \( k \) if

   \[
   \un^{(k)}(V_t; V_{t'} | X_t, X_{t'}) > 0 . \tag{9}
   \]

   Furthermore, \( V_t \) is said to have pure causal decoupling if \( \un^{(k)}(V_t; X^\alpha_{t'} | X_t) > 0 \) and \( \un^{(k)}(V_t; X^\beta_{t'} | X_t) = 0 \) for all \( \alpha \subset [n] \) with \( |\alpha| = k \). Finally, a system is said to be perfectly decoupled if all the emergent features exhibit pure causal decoupling.

   Above, the term \( \un^{(k)}(V_t; V_{t'} | X_t, X_{t'}) \) refers to information that \( V_t \) and \( V_{t'} \) share that cannot be found in any microscopic element, either at time \( t \) or \( t' \). Note that features that exhibit causal decoupling could still exert influence over the evolution of individual elements, while features that exhibit pure decoupling cannot. In effect, the condition \( \un(V_t; X^\alpha_{t'} | X_t) = 0 \) implies that the high-order causal effect does not affect any particular part – only the system as a whole. Interestingly, a feature that exhibits pure causal decoupling can be thought of as having “a life of its own,” a sort of statistical ghost, that...
perpetuates itself over time without any individual part of the system influencing or being influenced by it. The system’s parity, in the first example of Sec. I, constitutes a simple example of perfect causal decoupling.

We close this section by formally establishing the connection between causal decoupling and the index $\mathcal{G}^{(k)}$ introduced in Eq. (5).

**Theorem 3.** A system possesses features that exhibit causal decoupling if and only if $\mathcal{G}^{(k)}(X_t; X_{t'}) > 0$. Additionally, the system is perfectly decoupled if $\mathcal{G}^{(k)}(X_t; X_{t'}) > 0$ and $\mathcal{D}^{(k)}(X_t; X_{t'}) = 0$.

**Proof.** See Appendix C.

## III. MEASURING EMERGENCE

This section explores methods to operationalise the framework presented in the previous section. We discuss two approaches: first, Section III A introduces sufficiency criteria that are practical for use in large systems; then, Section III B illustrates how further considerations can be made if one adopts a specific method of computing $\PhiID$ atoms. The latter approach provides accurate discrimination at the cost of being data-intensive and hence only applicable to small systems; the former can be computed in large systems and its results hold independently of the chosen PID, but is vulnerable to misdetections (i.e. false negatives).

### A. Practical criteria for large systems

While theoretically appealing, our proposed framework suffers from the challenge of estimating joint probability distributions over many random variables, and the computation of the $\PhiID$ atoms themselves. As an alternative, we consider approximation techniques that do not require the adoption of any particular PID or $\PhiID$ function and are data-efficient, since they are based on pairwise distributions only.

As practical criteria to measure causal emergence of order $k$, we introduce the quantities $\Psi_{t,t'}^{(k)}$, $\Delta_{t,t'}^{(k)}$, and $\Gamma_{t,t'}^{(k)}$. For simplicity, we write here the special case $k = 1$, and provide full formulae for arbitrary $k$ and accompanying proofs in Appendix D:

\[
\Psi_{t,t'}^{(1)}(V) \coloneqq I(V_t; V_{t'}) - \sum_j I(X^j_t; V_{t'}) , \tag{10a}
\]

\[
\Delta_{t,t'}^{(1)}(V) \coloneqq \max_j \left( I(V_t; X^j_t) - \sum_i I(X^i_t; X^j_{t'}) \right) , \tag{10b}
\]

\[
\Gamma_{t,t'}^{(1)}(V) \coloneqq \max_j I(V_t; X^j_{t'}) . \tag{10c}
\]

Our next result links these quantities with the formal definitions in Section II, showing their value as practical criteria to detect causal emergence.

### Proposition 1. $\Psi_{t,t'}^{(1)}(V) > 0$ is a sufficient condition for $V_t$ to be causally emergent. Similarly, $\Delta_{t,t'}^{(1)}(V) > 0$ is a sufficient condition for $V_t$ to exhibit downward causation. Finally, $\Psi_{t,t'}^{(k)}(V) > 0$ and $\Gamma_{t,t'}^{(k)}(V) = 0$ is sufficient for causal decoupling.

**Proof.** See Appendix D.

Although calculating whether a system has emergent features via Proposition 1 may be computationally challenging, if one has a candidate feature $V$ one believes may be emergent, one can compute the simple quantities in Eqs. (10) which depend only on standard mutual information and bivariate marginals, and scales linearly with system size (for $k = 1$). These quantities are easy to compute and test for significance using standard information-theoretic tools [23, 24]. Moreover, the outcome of these measures is valid for any choice of PID and $\PhiID$ that is compatible with the properties specified in Appendix B.

In a broader context, $\Psi_{t,t'}^{(1)}$ and $\Delta_{t,t'}^{(1)}$ belong to the same whole-minus-sum family of measures as the interaction information [14, 25], the redundancy-synergy index [26] and, more recently, the O-information $\Omega$ [27] – which cannot measure synergy by itself, but only the balance between synergy and redundancy. In practice, this means that if there is redundancy in the system it will be harder to detect emergence, since redundancy will drive $\Psi_{t,t'}^{(1)}$ and $\Delta_{t,t'}^{(1)}$ more negative. Furthermore, by summing all marginal mutual informations (e.g. $I(X^j_t; V_{t'})$ in the case of $\Psi_{t,t'}^{(1)}$), these measures effectively double-count redundancy up to $n$ times, further penalising the criteria. This problem of double-counting can be avoided if one is willing to commit to a particular PID or $\PhiID$ function, as we show next.

### B. Measuring emergence via synergistic channels

This section leverages recent work on information decomposition reported in Ref. [20], and presents a way of directly measuring the emergence capacity and the indices of downward causation and causal decoupling. The key takeaway of this section is that if one adopts a particular $\PhiID$, then it is possible to evaluate $\mathcal{D}^{(k)}$ and $\mathcal{G}^{(k)}$ directly, providing a direct route to detect emergence without double-counting redundancy, as the methods introduced in Section III A do. Moreover, additional properties may become available due to the characteristics of the particular $\PhiID$ chosen.

Let us first introduce the notion of $k$-synergistic channels: mappings $p_{V|X}$ that convey information about $X$ but not about any of the parts $X^\alpha$ for all $|\alpha| = k$. The set of all $k$-synergistic channels is denoted by

\[
\mathcal{C}_k(X) = \left\{ p_{V|X} \bigg| V \perp \perp X^\alpha, \forall \alpha \subseteq [n], |\alpha| = k \right\}. \tag{11}
\]
A variable $V$ generated via a $k$-synergistic channel is said to be a $k$-synergistic observable.

With this definition, we can consider the $k^{th}$-order synergy to be the maximum information extractable from a $k$-synergistic channel:

$$ \text{Syn}^{(k)}(X_t; X_{t'}) := \sup_{V \subset U} \sup_{V' \subset U} I(V; X_{t'}) .$$

This idea can be naturally extended to the case of causal decoupling by requiring synergistic channels at both sides, i.e.

$$ G^{(k)}(X_t; X_{t'}) := \sup_{V \subset U} \sup_{V' \subset U} I(V; U) .$$

Finally, the downward causation index can be computed from the difference

$$ D^{(k)}(X_t; X_{t'}) := \text{Syn}^{(k)}(X_t; X_{t'}) - G^{(k)}(X_t; X_{t'}) .$$

Note that $\text{Syn}^{(k)} \geq G^{(k)}$, which is a direct consequence of the data processing inequality applied on $V - X_t - X_{t'} - U$, and therefore $D^{(k)} \geq 0$.

By exploiting the properties of this specific way of measuring synergy, one can prove the following result. For this, let us say that a feature $V_i$ is auto-correlated if $I(V_i; V_i) > 0$.

**Proposition 2.** If $X_t$ is stationary, all auto-correlated $k$-synergistic observables are $k^{th}$-order emergent.

**Proof.** See Appendix D.

In summary, $D^{(k)}$ and $G^{(k)}$ provide data-driven tools to test — and possibly reject — hypotheses about emergence in scenarios of interest. Efficient algorithms to compute these quantities are discussed in Ref. [28]. Although current implementations allow only relatively small systems, this line of thinking shows that future advances in PID might make the computation of emergence indices more scalable, avoiding the limitations of Eqs. (10).

IV. CASE STUDIES

Let us summarise our results so far. We began by formulating a rigorous definition of emergent features based on PID (Section II B), and then used ΦID to break down the emergence capacity into the causal decoupling and downward causation indices (Section II C). Although these are not straightforward to compute, the ΦID framework allows us to formulate readily computable sufficiency conditions (Section III A). This section illustrates the usage of those conditions in various case studies.

### FIG. 4. Causal emergence in Conway’s Game of Life.

The system is initialised in a “particle collider” setting, and run until a stable configuration is reached after the collision. Using particle type as a supervenient feature $V$, we find the system meets our practical criterion for causal emergence.

#### A. Canonical examples of putative emergence

Here we present an evaluation of our practical criteria for emergence (Proposition 1) in two well-known systems: Conway’s Game of Life (GoL) [29], and Reynolds’ flocking boids model [30]. Both are widely regarded as paradigmatic examples of emergent behaviour, and have been thoughtfully studied in the complexity and artificial life literature [31]. Accordingly, we use these models as test cases for our methods. Technical details of the simulations are provided in Appendix E.

1. **Conway’s Game of Life**

A well-known feature of GoL is the presence of particles: coherent, self-sustaining structures known to be responsible for information transfer and modification [32]. These particles have been the object of extensive study, and detailed taxonomies and classifications exist [31, 33].

To test the emergent properties of particles, we simulate the evolution of 15x15 square cell arrays, which we regard as a binary vector $X_i \in \{0, 1\}^n$ with $n = 225$. As initial condition, we consider configurations that correspond to a “particle collider” setting, with two particles of known type facing each other (Figure 4). In each trial, the system is randomised by changing the position, type, and relative displacement of the particles. After an initial configuration has been selected, the well-known GoL evolution rule [29] is applied 1000 times, leading to a final state $X_{t'}$.

To use the criteria from Eqs. 10, we need to choose a candidate emergent feature $V_i$. In this case, we consider a symbolic, discrete-valued vector that encodes the type of
particle(s) present in the board. Specifically, we consider $V_t = (V_t^1, \ldots, V_t^L)$, where $V_t^j = 1$ iff there is a particle of type $j$ at time $t$—regardless of its position or orientation.

With these variables, we compute the quantities in Eqs. 10 using Bayesian estimators of mutual information [35]. The result is that, as expected, the criterion for causal emergence is met with $\Psi^{(1)}_{t,t'}(V) = 0.58 \pm 0.02$. Furthermore, we found that $\Gamma^{(1)}_{t,t'}(V) = 0.009 \pm 0.0002$, which is orders of magnitude smaller than $I(V_t; V_{t'}) = 0.99 \pm 0.02$. Using Proposition 1, these two results suggest that particle dynamics in GoL may not only be emergent, but causally decoupled with respect to their substrate.

2. Reynolds’ flocking model

As a second test case, we consider Reynolds’ model of flocking behaviour. This model is composed by boids (bird-oid objects), with each boid represented by three numbers: its position in 2D space and its heading angle. As candidate feature for emergence, we use the 2D coordinates of the center of mass of the flock, following Seth [5].

In this model boids interact with one another following three rules, each regulated by a scalar parameter [5]:

- aggregation ($a_1$), as they fly towards the center of the flock;
- avoidance ($a_2$), as they fly away from their closest neighbour; and
- alignment ($a_3$), as they align their flight direction to that of their neighbours.

Following Ref. [5], we study small flocks of $N = 10$ boids with different parameter settings to showcase some properties of our practical criterion of emergence. Note that this study is meant as an illustration of the proposed theory, and not as a thorough exploration of the flocking model, for which a vast literature exists (see e.g. the work of Vicsek [36] and references therein).

Figure 5 shows the results of a parameter sweep over the avoidance parameter, $a_2$, while keeping $a_1$ and $a_3$ fixed. When there is no avoidance, boids orbit around a slowly-moving center of mass, in what could be called an ordered regime. Conversely, for high values of $a_2$ neighbour repulsion is too strong for lasting flocks to form, and isolated boids spread across the space avoiding one another. For intermediate values, the center of mass traces a smooth trajectory, as flocks form and disintegrate. In line with the findings of Seth [5], our criterion indicates that the flock exhibits causally emergent behaviour in this intermediate range.

By studying separately the two terms that make up $\Psi$ we found that the criterion of emergence fails for both low and high $a_2$, but for different reasons (see Figure 5). In effect, for high $a_2$ the self-predictability of the center of mass (i.e. $I(V_t; V_{t'})$) is low; while for low $a_2$ it is high, yet lower than the mutual information from individual boids (i.e. $\sum_i^n I(X^i_t; V^i_{t'})$). These results suggest that the low-avoidance scenario is dominated not by a reduction in synergy, but by an increase in redundancy, which effectively increases the synergy threshold needed to detect emergence. However, note that, due to the limitations of the criterion, the fact that $\Psi^{(1)}_{t,t'} < 0$ is inconclusive and does not rule out the possibility of emergence. This is a common limitation of whole-minus-sum estimators like $\Psi$; further refinements may provide bounds that are less susceptible to these issues and perform accurately in these scenarios.

B. Mind from matter: Emergence, behaviour, and neural dynamics

A tantalising outcome of having a formal theory of emergence is the capability of bringing a quantitative angle to the archetype of emergence: the mind-matter relationship [38, 39]. As a first step in this direction, we conclude this section with an application of our emergence criteria to neurophysiological data.

We study simultaneous electrocorticogram (ECoG) and motion capture (MoCap) data of Japanese macaques performing a reaching task [37], obtained from the online Neurotycho database. Note that the MoCap data cannot be assumed to be a supervenient feature of the avail-

![FIG. 5. Causal emergence in the flocking boids model. As the avoidance parameter is increased, the flock transitions from an attractive regime (in which all boids orbit regularly around a stable center of mass), to a repulsive one (in which boids spread across space and no flocking is visible). a) Our criterion $\Psi$ detects causal emergence in an intermediate range of the avoidance parameter. b) Sample trajectories of boids (grey) and their center of mass (red).]
Causal emergence in motor behaviour of an awake macaque monkey. a) Position of electrocorticogram (ECoG) electrodes used in the recording (in blue) overlaid on an image of the macaque’s left hemisphere (front of the brain towards the top of the page). b) Sample time series from the 64-channel ECoG recordings used, which correspond to the system of interest $X_t \in \mathbb{R}^{64}$. c) 3D position of the macaque’s wrist, as measured by motion capture (blue) and as predicted by the regression model (orange), taken as a supervenient feature $X_t$, towards the top of the page). b) (ECoG) electrodes used in the recording (in blue) overlaid on an image of the macaque’s left hemisphere (front of the brain). c) 3D position of the macaque’s wrist, as measured by motion capture (blue) and as predicted by the regression model (orange), taken as a supervenient feature $V_t$, as measured by motion capture (blue) and as predicted by the regression model (orange), taken as a supervenient feature $V_t \in \mathbb{R}^3$. d) Our emergence criterion yields $\Psi_{t,t'}^{(1)}(V) > 0$, detecting causal emergence of the behaviour with respect to the ECoG sources. Original data and image from Ref. [37] and the Neurotycho database.

V. DISCUSSION

A large fraction of the modern scientific literature considers strong emergence to be impossible or ill-defined. This judgement is not fully unfounded: a property that is simultaneously supervenient (i.e. that can be computed from the state of the system) and that has irreducible causal power (i.e. that “tells us something” that the parts don’t) can indeed seem to be an oxymoron [4]. Nonetheless, by linking supervenience to static and causal power to dynamical properties, our framework shows that these two phenomena are perfectly compatible within the – admittedly counterintuitive – laws of multivariate information dynamics [22], providing a tentative solution to this paradox.

Our theory of causal emergence is about predictive power, not “explicability” [41], and therefore is not related to views on strong emergence such as Chalmers’ [41]. Nevertheless, our framework embraces aspects that are commonly associated with strong emergence – such as downward causation – and renders them quantifiable. Our framework also does not satisfy conventional definitions of weak emergence [42], but is compatible with more general notions of weak emergence, e.g. the one introduced by Seth (see Sec. V.C). Hence, our theory can be seen as an attempt at reconciling these approaches [39], showing how “strong” a “weak” framework can be.

An important consequence of our theory is the fundamental connection established between causal emergence and statistical synergy: the system’s capacity to host emergent features was found to be determined by how synergistic its elements are with respect to their future
evolution. Although previous ideas about synergy have been loosely linked to emergence in the past [43], this is (to the best of our knowledge) the first time such ideas have been formally laid out and quantified using recent advances in multivariate information theory.

Next, we examine a few caveats regarding the applicability of the proposed theory, its relation with prior work, and some open problems.

A. Scope of the theory

Our theory focuses on synchronic [44] aspects of emergence, analysing the interactions between the elements of dynamical systems and collective properties of them as they jointly evolve over time. As such, our theory directly applies to any system with well-defined dynamics, including systems described by deterministic dynamical systems with random initial conditions [11] and stochastic systems described by Fokker-Planck equations [45]. In contrast, the application of our theory to systems in thermodynamic equilibrium may not be straightforward, as their dynamics are often not uniquely specified by the corresponding Gibbs distributions [46]. Finding principled approaches to guide the application of our theory to those cases is an interesting challenge for future studies.

In addition, given the breadth of the concept of “emergence,” there are a number of other theories leaning more towards philosophy that are orthogonal to our framework. This includes, for example, theories of emergence as radical novelty (in the sense of features not previously observed in the system) [47], most prominently encapsulated in the aphorism “more is different” by Anderson [48], and also articulated in the work of Kauffman [49, 50]. Also, contextual emergence emphasises a role for macro-level constraints that cannot be described at the micro-level, but which impose constraints on the micro-level for the emergence of the macro [51, 52]. These are valuable philosophical positions, which have been studied from a statistical mechanics perspective in Ref. [51, 53]. Future work shall attempt to unify these other approaches with our proposed framework.

B. Causality

The de facto way to assess the causal structure of a system is to analyse its response to controlled interventions or to build intervention models (causal graphs) based on expert knowledge, which leads to the well-known do-calculus spearheaded by Judea Pearl [9]. This approach is, unfortunately, not applicable in many scenarios of interest, as interventions may incur prohibitive costs or even be impossible, and expert knowledge may not be available. These scenarios can still be assessed via the Wiener-Granger theory of statistical causation, which studies the blueprint of predictive power across the system of interest by accounting non-mediated correlations between past and future events [12]. Both frameworks provide similar results when all the relevant variables have been measured, but can nevertheless differ radically when there are unobserved interacting variables [9].

The debate between the Wiener-Granger and the Pearl schools has been discussed in other related contexts – see e.g. Refs. [54, 55] for a discussion regarding Integrated Information Theory (IIT), and Ref. [56] for a discussion about effective and functional connectivity in the context of neuroimaging time series analysis [57].

In our theory, the main object of analysis is Shannon’s mutual information, $I(X; V_r)$, which depends on the joint probability distribution $p_{X_t, X_{t'}}$. The origin of this distribution (whether it was obtained by passive observation or by active intervention) will change the interpretation of the quantities presented above, and will speak differently to the Pearl and the Wiener-Granger schools of thought; some of the implications of these differences are addressed when discussing Ref. [6] below. Nonetheless, since both methods of obtaining $p_{X_t, X_{t'}}$ allow synergy to take place, our results are in principle applicable in both frameworks – which allows us to formulate our theory of causal emergence without taking a rigid stance on a theory of causality itself.

C. Relationship with other quantitative theories of emergence

This work is part of a broader movement towards formalising theories of complexity through information theory. In particular, our framework is most directly inspired by the work of Seth [5] and Hoel et al. [6], and also related to recent work by Chang et al. [58]. This section gives a brief account of these theories, and discusses how they differ from our proposal.

Seth [5] proposes that a process $V_t$ is Granger-emergent (or G-emergent) with respect to $X_t$ if two conditions are met: (i) $V_t$ is autonomous with respect to $X_t$ (i.e. $I(V_t; V_r | X_t) > 0$), and (ii) $V_t$ is G-caused by $X_t$ (i.e. $I(X_t; V_r | V_t) > 0$). The latter condition is employed to guarantee a relationship between $X_t$ and $V_t$; in our framework an equivalent role is taken by the requirement of supervenience. The condition of autonomy is certainly related with our notion of causal decoupling. However, as shown in Ref. [14], the conditional mutual information conflates unique and synergistic information, which can give rise to undesirable situations: for example, it could be that $I(V_t; V_r | X_t) > 0$ while, at the same time, $I(V; V_r | X_t) = 0$, meaning that the dynamics of the feature $V_t$ are only visible when considering it together with the full system $X_t$, but not on its own. Our framework avoids this problem by refining this criterion via PID, and uses only the unique information for the definition of emergence.

Our work is also strongly influenced by the framework put forward by Hoel and colleagues in Ref. [6]. Their approach is based on a coarse-graining function $F(\cdot)$ re-
lating a feature of interest to the system, \( V_t = F(X_t) \), which is a particular case of our more general definition of supervenience. Emergence is declared when the dependency between \( V_t \) and \( V_{t'} \) is “stronger” than the one between \( X_t \) and \( X_{t'} \). Note that \( V_t - X_t - X_{t'} - V_{t'} \) is a Markov chain, and hence \( I(V_t; V_{t'}) \leq I(X_t; X_{t'}) \) due to the data processing inequality; therefore, a direct usage of Shannon’s mutual information would make the above criterion impossible to fulfill. Instead, this framework focuses on the transition probabilities \( p_{V_{t'}|V_t} \) and \( p_{X_{t'}|X_t} \), and hence the mutual information terms are computed using maximum entropy distributions instead of the stationary marginals. By doing this, Hoel et al. account not for what the system actually does, but for all the potential transitions the system could do. However, in our view this approach is not well-suited to assess dynamical systems, as it might account for transitions that are never actually explored [59]. Additionally, this framework relies on having exact knowledge about the microscopic transitions as encoded by \( p_{X_{t'}|X_t} \), which is not possible to obtain in most applications.

Finally, Chang et al. [58] consider supervenient variables that are “non-trivially informationally closed” (NTIC) to their corresponding microscopic substrate. NTIC is based on a division of \( X_t \) into a subsystem of interest, \( X^*_t \), and its “environment” given by \( X^{-\alpha}_t \). Interestingly, a system being NTIC requires \( V_t \) to be supervenient only with respect to \( X^*_t \) (i.e. \( V_t = F(X^*_t) \)), as well as information flow from the environment to the feature (i.e. \( I(X^{-\alpha}_t; V_{t'}) > 0 \)) mediated by the feature itself, so that \( X_t - V_t - V_{t'} \) is a Markov chain. Hence, NTIC requires features that are sufficient statistics for their own dynamics, which is akin to our concept of causal decoupling but focused on the interaction between a macroscopic feature, an agent, and its environment. Extending our framework to agent-environment systems involved in active inference is part of our future work.

D. Limitations and open problems

The framework presented in this paper focuses on features from fully observable systems with Markovian dynamics. These assumptions, however, often do not hold when dealing with experimental data – especially in biological and social systems. As an important extension, future work should investigate the effect of unobserved variables on our measures. This could be done, for example, leveraging Taken’s embedding theorem [60, 61] or other methods [62].

An interesting feature of our framework is that, although it depends on the choice of PID and \( \PhiID \), its practical application via the criteria discussed in Section IIIA is agnostic to those choices. However, they incur the cost of a limited sensitivity to detect emergence due to an overestimation of the microscopic redundancy; so they can detect emergence when it is substantial, but might miss it in more subtle cases. Additionally, these criteria are unable to rule out emergence, as they are sufficient but not necessary conditions. Therefore, another avenue of future work should search for improved practical criteria for detecting emergence from data. One interesting line of research is providing scalable approximations for \( \text{Syn}^{(k)} \) and \( \text{g}^{(k)} \) as introduced in Section III B, which could be computed in large systems.

Another open question is how the emergence capacity is affected by changes in the microscopic partition of the system (c.f. Section II B). Interesting applications of this includes scenarios where elements of interest have been subject to a mixing process, such as the case of electroencephalography where each electrode detects a mixture of brain sources. Other interesting questions include studying systems with non-zero emergence capacity for all reasonable microscopic partitions, which may correspond to a stronger type of emergence.

VI. CONCLUSION

This paper introduces a quantitative definition of causal emergence, which addresses the apparent paradox of supervenient macroscopic features with irreducible causal power using principles of multivariate statistics. We provide a formal, quantitative theory that embodies many of the principles attributed to strong emergence, while being measurable and compatible with the established scientific worldview. Perhaps the most important contribution of this work is to bring the discussion of emergence closer to the realm of quantitative, empirical scientific investigation, complementing the ongoing philosophical inquiries on the subject.

Mathematically, the theory is based on the Partial Information Decomposition (PID) framework [14], and on a recent extension, Integrated Information Decomposition (\( \PhiID \)) [22]. The theory allows the derivation of sufficiency criteria for the detection of emergence that are scalable, easy to compute from data, and based only on Shannon’s mutual information. We illustrated the use of these practical criteria in three case studies, and concluded that: i) particle collisions are an emergent feature in Conway’s Game of Life, ii) flock dynamics are an emergent feature of simulated birds; and iii) the representation of motor behaviour in the cortex is emergent from neural activity. Our theory, together with these practical criteria, enables novel data-driven tools for scientifically addressing conjectures about emergence in a wide range of systems of interest.

Our original aim in developing this theory, beyond the contribution to complexity theory, is to help bridge the gap between the mental and the physical, and ultimately understand how mind emerges from matter. This paper provides formal principles to explore the idea that psychological phenomena could emerge from collective neural patterns, and interact with each other dynamically in a causally decoupled fashion – perhaps akin to the “statistical ghosts” mentioned in Section II C 2. Put
simply: just as particles in the Game of Life have their own collision rules, we wonder if thought patterns could have their own emergent dynamical laws, operating at a larger scale with respect to their underlying neural substrate [63]. Importantly, the theory presented in this paper not only provides conceptual tools to frame this conjecture rigorously, but also provides practical tools to test it from data. The exploration of this conjecture is left as an exciting avenue for future research.

ACKNOWLEDGEMENTS

The authors thank Shamil Chandaria, Matthew Crosby, Martin Biehl and Acer Chang for insightful discussions, and the creators of the Neurotycho database for opening to the public such a valuable resource. P.M. and D.B. are funded by the Wellcome Trust (grant no. 210920/Z/18/Z). F.R. is supported by the Ad Astra Chandaria foundation. A.K.S. and A.B.B. are grateful to the Dr. Mortimer and Theresa Sacker Foundation, which supports the Sackler Centre for Consciousness Science.

Appendix A: Information decomposition in large multivariate systems

To formulate our theory of causal emergence for arbitrary order $k$, in Sec. II A we introduced definitions of $k$th-order synergy and unique information. In this appendix we complement these with a matching definition of $k$th-order redundancy, and show that these provide a full-fledged information decomposition for any $k = \{1, \ldots, n - 1\}$. For completeness, we present all definitions and examples here – including those that were necessary for the exposition of the main text and were previously presented in Sec. II A.

We begin by (re-)introducing the notion of $k$th-order synergy between $n$ variables, defined as

$$
\text{Syn}^{(k)}(X; Y) := \sum_{\alpha \in S^{(k)}} I^\beta_\beta(X; Y),
$$

with $S^{(k)} = \{\{\alpha_1, \ldots, \alpha_L\} \in A : |\alpha_j| > k, \forall j = 1, \ldots, L\}$. Intuitively, $\text{Syn}^{(k)}(X; Y)$ corresponds to the information about the target that is provided by the whole $X$ but is not contained in any set of $k$ or less parts when considered separately from the rest. Accordingly, $S^{(k)}$ only contains collections of more than $k$ sources. For example, for $n = 2$ we obtain the standard synergy $S^{(1)} = \{\{12\}\}$, and for $n = 3$ we have $S^{(1)} = \{\{12\}, \{13\}, \{23\}, \{12\}{13}, \{12\}{23}, \{13\}{23}, \{12\}{13\}{23}\}$. Similarly, the $k$th-order unique information of $X^\beta$ with $\beta \subseteq [n]$ is calculated as

$$
\text{Un}^{(k)}(X^\beta; Y|X^{-\beta}) := \sum_{\alpha \in U^{(k)}(\beta)} I^\beta_\beta(X; Y),
$$

with $U^{(k)}(\beta) = \{\alpha \in A : \beta \subseteq \alpha, \forall \beta, \alpha \subseteq [n] \backslash \beta, |\alpha| > k\}$, and $X^{-\beta}$ being all the variables in $X$ the indices of which are not in $\beta$. This corresponds to all the atoms where $\beta$ is the only source of size $k$ or less – which, importantly, is in general not just $I^\beta_\beta$. Intuitively, this is the information that $X^\beta$ has access to and no other subset of parts has access to on its own (although bigger groups of other parts may). And again, for $n = 2$ we recover $U^{(1)}(\{1\}) = \{\{1\}\}$, and for $n = 3$ we have e.g. $U^{(1)}(\{1\}) = \{\{1\}, \{1\}{12}\}$. Finally, the $k$th-order redundancy is given by

$$
\text{Red}^{(k)}(X; Y) := \sum_{\alpha \in R^{(k)}} I^\beta_\beta(X; Y),
$$

with $R^{(k)} = \{\alpha \in A : \exists j \neq \beta, |\alpha_j|, |\alpha_\beta| \leq k\}$. Intuitively, $\text{Red}^{(k)}(X; Y)$ is the information that is held by at least two different groups of size $k$ or less. Again, in the $n = 2$ case we recover the standard redundancy $R^{(1)} = \{\{1\}\{2\}\}$; and as an example for $n = 3$ we have $R^{(1)} = \{\{1\}\{2\}, \{1\}\{3\}, \{2\}\{3\}, \{1\}\{2\}\{3\}\}$. With the definitions above, we can build a coarse-grained PID which generalises the well-known construction for $n = 2$. This allows us to formulate decompositions with a small number of atoms that scale gracefully with system size, and, more interestingly, preserve the intuitive meaning that synergy, redundancy, and unique information have for $n = 2$.

**Lemma 2.** The $k$th-order synergy, redundancy, and unique information defined above provide an exact decomposition of mutual information:

$$
I(X; Y) = \text{Red}^{(k)}(X; Y) + \text{Syn}^{(k)}(X; Y) + \sum_{\beta \subseteq [n]; |\beta| \leq k} \text{Un}^{(k)}(X^\beta; Y|X^{-\beta}). \quad (A1)
$$

**Proof.** We will prove this by showing that the sets $R^{(k)}$, $S^{(k)}$ and $U^{(k)}(\beta)$ are a partition of $A$. We will do this in two steps: first, we show that their intersection is empty; and second, that their union is $A$.

Let us show that the intersections between every pair of sets is empty:

- $R^{(k)} \cap S^{(k)} = \emptyset$, since if $\alpha \in R^{(k)}$ it must contain at least one $\alpha \in A : |\alpha| \leq k$, and therefore $\alpha \notin S^{(k)}$.
- $U^{(k)}(\gamma) \cap U^{(k)}(\beta) = \emptyset$ if and only if $\gamma \neq \beta$, since every $\alpha \in U^{(k)}(\gamma)$ has either no other elements apart from $\gamma$ (in which case $\beta \notin \alpha$ and thus $\alpha \notin U^{(k)}(\beta)$), or other elements of cardinality greater than $k$ (in which case, again, $\beta \notin \alpha$ and thus $\alpha \notin U^{(k)}(\beta)$).
- $S^{(k)} \cup U^{(k)}(\beta) = \emptyset$ for all $|\beta| \leq k$, since every $\alpha \in U^{(k)}(\beta)$ contains at least one element with cardinality less than or equal to $k$ (specifically, $\beta$), and therefore $\alpha \notin S^{(k)}$.
We will show this by proving that every $\alpha$ need to prove that the union of those sets is indeed an exact decomposition of mutual information. This concludes the first part of the proof. Next, we will show that the union of those sets is indeed $A$.

We will show this by proving that every $\alpha \in A$ is in one of those sets:

- If $|\alpha| \leq k$, then $\alpha \in S^{(k)}$.
- If there is exactly one $\alpha \in A : |\alpha| \leq k$, then $\alpha \in U^{(k)}(\alpha)$.
- If there are more than one $\alpha \in A : |\alpha| \leq k$, then $\alpha \in R^{(k)}$.

The two possible decompositions for $n = 3$, together with the standard PID lattice, are shown in Figure 7.

Appendix B: Properties of high-order PI atoms

As discussed in Section II, our theory does not depend on a specific functional form of PID. Instead, it applies to any PID that satisfies the following properties:

- **Deterministic equality:** if there exists a function $f(\cdot)$ such that $X^i = f(X^j)$ with $i \neq j$, then the information decomposition of $X$ is isomorphic to that of $X^{-j}$ (see below).
- **Non-negativity:** $\text{Syn}^{(k)}(X; Y) \geq 0$, and $\min\{I(Z; Y), I(Z; Y|X)\} \geq \text{Un}^{(k)}(Z; Y|X)$ for all $W = Z - (X, Y)$ Markov chains.

To formulate the causal decoupling and downward causation indices in Section II C, we make use of $\PhiID$, a recent extension of PID to multi-target settings [22]. As with PID, our theory does not require a particular functional form of $\PhiID$, only the following property:

- $\sum_{|\alpha| = k} \text{Syn}^{(k)}(X_t; X_t^\beta) \geq D^{(k)}(X_t; X_t^\beta) \geq \text{Syn}^{(k)}(X_t; X_t^\alpha)$ for all $|\beta| = k$.

Finally, these properties are required to formulate the practical criteria for emergence in Section III A:

- **Whole-minus-sum:** $\text{Syn}^{(k)}(X; Y) \geq I(X; Y) - \sum_{|\alpha| = k} I(X^\alpha; Y)$. 

![Figure 7](image-url)
• Target data processing inequality: for all $X - Y - U$ Markov chains, $\text{Syn}^{(k)}(X; U) \leq \text{Syn}^{(k)}(X; Y)$.

For completeness, we present a precise definition of the deterministic equality property, as previously introduced in the PID literature [64].

Definition 4. A PID satisfies deterministic equality if
\[ I_{\beta}^{g} (X; Y) = I_{\beta}^{g} (X^{-j}; Y) \]
for all $\alpha \in A$ whenever there exists a function $f(\cdot)$ such that $f(X^i) = X^i$ with $i \neq j$, with $g_j(\alpha)$ removes $j$ from all the sets of indices in $\alpha$.

It is direct to check that a number of well-known information decompositions, including the Minimum Mutual Information PID [65], and the corresponding $\Phi$ID [22], satisfy these requirements.

With these properties at hand we can prove the following results, used in Sections II B and II C:

Lemma 3. If $X^{n+1} = X$, then the following holds:
\[ \text{Syn}^{(k)}(X; Y) = \text{Un}^{(k)}(X^{n+1}; Y|X) . \] (B1)

Above, the second term corresponds to a PID over a system of $n + 1$ elements.

Proof. Begin by considering the PID of $n$ sources $X^1, \ldots, X^n$ on the lattice $A^n$, and define its set $S^{(k)}$ as above. Now we add an additional $n + 1$st variable that is simply all of them concatenated, $X_{n+1} = X^n$, and build a PID on the lattice $A^{n+1}$. In the following, we consider the set $S^{(k)}$ to belong to the lattice $A^n$, and the set $U^{(k)}(\beta)$ to belong to the lattice $A^{n+1}$. To prove the lemma we need four ingredients, which we provide in the four paragraphs below.

1. First, note that the nodes in $A^{n+1}$ that precede \{n + 1\} are those in $A^n$, but with the singleton \{n + 1\} appended to them. More specifically, the mapping $f : A^n \to A^{n+1}$ of the form $f(\alpha) = \alpha \cup \{n + 1\}$ is such that for any $\alpha \in A^n$ then $f(\alpha) \times \{n + 1\}$. Additionally, due to the properties of the partial order, $\alpha \preceq \alpha'$ if and only if $f(\alpha) \preceq f(\alpha')$. This shows that $A^n$ is isomorphic to a sublattice of $A^{n+1}$.

2. Next, by the deterministic equality property it is direct to check that $I^{(f(\alpha))}_{\beta} = I^{(\alpha)}_{\beta}$. Since this equality holds for all $\alpha \in A^n$, then applying a Möbius inversion we directly obtain that $I^{(\alpha)}_{\beta} = I^{(\alpha)}_{\beta}$.

3. Additionally, by construction of $U^{(k)}$ and $S^{(k)}$, for all $\gamma \in S^{(k)}$ one has $f(\gamma) \in U^{(k)}(\{n + 1\})$. In other words, the set $U^{(k)}(\{n + 1\})$ includes all atoms in $S^{(k)}$, plus \{n + 1\}.

4. Finally, note that the node \{12...n\} + 1} is the only direct predecessor of \{n + 1\}, since there exists no node $\beta \in A^{n+1}$ such that $\beta \preceq \{n + 1\}$ and not $\beta \preceq \{12...n\} + 1$. By the deterministic equality property $I^{(\{12...n\})}(n + 1) = I^{(\{12...n\})} + 1$ and, therefore, $I^{(n+1)}_{\beta} = 0$.

With all of these, it is direct to see that
\[ \text{Un}^{(k)}(X^n; Y|X) = \sum_{\alpha \in U^{(k)}} I_{\beta}^{g} (X; Y) \]
\[ = \sum_{\alpha \in S^{(k)}} I_{\beta}^{g} (X; Y) = \text{Syn}^{(k)}(X; Y) . \]

□

Corollary 2. If $X^{n+1} = X$ and $Y^{n+1} = Y$, then the following holds:
\[ G^{(k)}(X; Y) = \text{Un}^{(k)}(X^{n+1}; Y^{n+1}|X, Y) \] (B2)

Above, the second term corresponds to a $\Phi$ID over a system of $n + 1$ elements.

Proof. Follows from a direct $\Phi$ID extension to the proof of Lemma 3, by formulating a decomposition
\[ I(X; Y) = \sum_{\alpha, \beta \in A^n} I_{\beta}^{g} (X; Y) , \]
and applying the proof above to both $\alpha$ and $\beta$. Strictly speaking, this also requires a natural multi-target extension of the Deterministic Equality property, namely that $I_{\beta}^{g} (X; Y) = I_{\beta}^{g} (X^{-j}; Y)$ if $X^i = f(X^j)$ with $j \neq i$, for any $\beta \in A^n$; as well as the symmetric $I_{\beta}^{g} (X; Y) = I_{\beta}^{g} (X; Y^{-j})$ if $Y^i = f(Y^j)$ with $j \neq i$, for any $\alpha \in A^n$.

□

Appendix C: Mathematical properties of causal emergence

Proof of Lemma 1. The first property can be easily proven by noting that there can be no synergy in a univariate system: i.e. if $n = 1$, then $S^{(k)} = \emptyset$ and therefore $\text{Syn}^{(k)}(X_t; X_{t'}) = 0$.

To prove the second property, let us assume that there exists a function $g(\cdot)$ such that $g(X^t_j) = V_t$ for some $j$. Then, one can show that
\[ \text{Un}^{(I)}(V_t; X_{t'}|X_t) \leq I(V_t; X_{t'}|X_t) \] (C1)
\[ \leq I(V_t; X_{t'}) \] (C2)
\[ \leq H(V_t|X^t_i) \] (C3)
\[ = 0 , \] (C4)

where (C1) is due to the non-negativity property of $\text{Un}^{(k)}$ introduced in Section II A. This shows that $V_t$ cannot exhibit emergent behaviour.

□

Proof of Theorem 1. If $\text{Syn}^{(k)}(X_t; X_{t'}) > 0$, then by Lemma 3 it is clear that the feature $V_t = X_t$ exhibits causal emergence.

To prove the converse, note that all supervenient features follow the Markov chain structure $X_t = X_t - X_{t'}$. 


Therefore, for any supervenient feature $V_t = f(X_t)$ the following holds:

\[
0 \leq \text{Un}^{(k)}(V_t; X_t | X_t) \leq \text{Un}^{(k)}(X_t; X_{t'} | X_t) = \text{Syn}(X_t; X_{t'}) \leq \text{D}(X_t; X_{t'}) \tag{C5}
\]

where (C5) is due to the data processing inequality of the unique information (c.f. Section II A), and (C6) is due to Lemma 3. Using this result, is clear that if $\text{Syn}^{(k)}(X_t; X_{t'}) = 0$ then $\text{Un}^{(k)}(V_t; X_t | X_t) = 0$ for any supervenient feature $V_t$.

The above proof implies that the system has emergent behaviour if and only if the system as a whole seen as a feature (i.e. $V_t = X_t$) is causally emergent. Note that the fact that this trivial feature is helpful for detecting the presence of emergence doesn’t imply that it is an appropriate way of representing it, as in most cases also carries non-interesting information, and in practice one may be interested in features that exhibit emergence but are shorter to describe than the microstate of the system, i.e. $H(V_t) < H(X_t)$.

**Proof of Theorem 2.** Let us first assume that there exists a supervenient feature $V_t$ such that $\text{Un}^{(k)}(V_t; X_{t'}^\alpha | X) > 0$ for some $\alpha : |\alpha| = k$. Then, one can find that

\[
0 < \text{Un}^{(k)}(V_t; X_{t'}^\alpha | X_t)
\leq \text{Un}^{(k)}(X_t; X_{t'}^\alpha | X_t) = \text{Syn}^{(k)}(X_t; X_{t'}^\alpha) \tag{C7}
\leq \text{D}^{(k)}(X_t; X_{t'}) \tag{C8}
\]

Above, (C7) is a consequence of the data processing inequality of the unique information, (C8) comes from Lemma 3, and (C9) is from the properties of $\text{D}^{(k)}$ stated in Section II C.

To prove the converse, let us assume that all supervenient features $V_t$ satisfy $\text{Un}^{(k)}(V_t; X_{t'}^\alpha | X_t) = 0$ for all $k$ and $|\alpha| = k$. In particular, this is true for the feature $V_t = X_t$. Then, another application of Lemma 3 shows that

\[
\text{D}^{(k)}(X_t; X_{t'}) \leq \sum_{|\alpha| = k} \text{Syn}^{(k)}(X_t; X_{t'}^\alpha) \tag{C10}
= \sum_{|\alpha| = k} \text{Un}^{(k)}(X_t; X_{t'}^\alpha | X_t)
= 0 .
\]

Above, (C10) is a consequence of the properties of $\text{D}^{(k)}$.

**Proof of Theorem 3.** We begin by proving that a system has a causally decoupled feature iff $G^{(k)}(X_t; X_{t'}) > 0$. This proof follows a similar structure to that of Theorem 2 for downward causation.

Let us first assume that there exists a supervenient feature $V_t$ with $\text{Un}^{(k)}(V_t; V_{t'}; X_t, X_{t'}) > 0$. Then,

\[
0 < \text{Un}^{(k)}(V_t; V_{t'} | X_t, X_{t'}) \leq \text{Un}^{(k)}(X_t; X_{t'} | X_t, X_{t'}) = G^{(k)}(X_t; X_{t'}) \tag{C11}
\leq \text{D}^{(k)}(X_t; X_{t'}) \tag{C12}
\]

Above, (C11) can be obtained through a combination of the data processing inequalities of the unique information and the synergy, as well as Lemma 3; and (C12) is an application of Corollary 2.

To prove the converse, assume that for all supervenient features $\text{Un}^{(k)}(V_t; V_{t'} | X_t, X_{t'}) = 0$. As before, this also includes $V_t = X_t$. Therefore, applying Corollary 2 we arrive at $G^{(k)}(X_t; X_{t'}) = \text{Un}^{(k)}(X_t; X_{t'} | X_t, X_{t'}) = 0$, which concludes the proof.

We now move on to prove the results on perfectly causally decoupled systems, where $G^{(k)}(X_t; X_{t'}) > 0$ and $\text{D}^{(k)}(X_t; X_{t'}) = 0$. As $\text{Syn}^{(k)}(X_t; X_{t'}) = G^{(k)}(X_t; X_{t'}) + \text{D}^{(k)}(X_t; X_{t'}) > 0$, thanks to Theorem 1 this is equivalent to the existence of at least one emergent feature $V_t$. Additionally, due to Theorem 2, $\text{D}^{(k)}(X_t; X_{t'}) = 0$ is equivalent to $\text{Un}^{(k)}(V_t; X_{t'}^\alpha | X_t) = 0$ for all emergent features and $\alpha : |\alpha| = k$.

**Appendix D: Mathematical properties of emergence criteria**

In this appendix we provide the necessary proofs linking the practical criteria for emergence in Eqs. (10) with the definitions in Section II. For completeness, we provide formulae of $\Psi, \Delta,$ and $\Gamma$ for arbitrary emergence order $k$:

\[
\Psi^{(k)}_{t,t'}(V) := I(V_t; V_{t'}) - \sum_{|\alpha| = k} I(X_t^\alpha; V_{t'}), \tag{D1a}
\]

\[
\Delta^{(k)}_{t,t'}(V) := \max_{|\alpha| = k} \left( I(V_t; X_{t'}^\beta) - \sum_{|\beta| = k} I(X_t^\beta; X_{t'}^\beta) \right), \tag{D1b}
\]

\[
\Gamma^{(k)}_{t,t'}(V) := \max_{|\alpha| = k} I(V_t; X_{t'}^\alpha). \tag{D1c}
\]

**Proof of Proposition 1.** To start, note that a direct calculation shows that

\[
\Psi^{(k)}_{t,t'}(V) \leq I(X_t; V_{t'}) - \sum_{|\alpha| = k} I(X_t^\alpha; V_{t'}) \tag{D2}
\leq \text{Syn}^{(k)}(X_t; V_{t'}) \tag{D3}
\leq \text{Syn}^{(k)}(X_t; X_{t'}). \tag{D4}
\]

Above, (D2) is due to the data processing inequality applied over the Markov chain $V_t - X_t - X_{t'} - V_{t'}$; (D3) is due to the whole-minus-sum property of the synergy; and (D4) is due to the data processing inequality of the
synergy. Therefore, it is clear that if $\Psi_{t,t'}^{(k)}(V) > 0$ for some feature $V_t$ then $\text{Syn}^{(k)}(X_t; X_{t'}) > 0$. This, combined with Theorem 1, guarantees that the system exhibits causal emergence.

To check the condition for downward causation, a direct calculation shows that, for some $|\alpha| = k$,

\[ \Delta^{(k)}_{t,t'}(V) \leq I(X_t; X^\alpha_{t'}) - \sum_{|\beta| = k} I(X^\beta_{t'; X_t}) \tag{D5} \]

\[ \leq \text{Syn}^{(k)}(X_t; X^\alpha_{t'}) \leq D^{(k)}(X_t; X_{t'}) . \tag{D7} \]

Above, (D5) is due to the data processing inequality applied over the Markov chain $V_t - X_t - X^\beta_{t'}$; (D6) to the whole-minus-sum property of the synergy; and (D7) to the properties of $D^{(k)}$. From here, is clear that if $\Delta^{(k)}_{t,t'}(V) > 0$ for some feature $V_t$ then $D^{(k)}(X_t; X_{t'}) > 0$. This, combined with Theorem 1, guarantees that the system exhibits downward causation.

Finally, for the condition for causal decoupling it is sufficient to note that

\[ \Gamma^{(k)}_{t,t'}(V) = \max_{|\alpha| = k} I(V_t; X^\alpha_{t'}) \geq 0 , \tag{D9} \]

where the inequality is due to the bounds of the unique information.

Proof of Proposition 2. Let us consider $V_t$ a $k$-synergistic observable. Due to stationarity, the fact that $V_t \in C_k(X_i)$ implies that $V_{t'} \in C_k(X_i)$. Using this fact, and noting that $V_t - X_t - X_{t'}$ is a Markov chain, it is direct to check that

\[ \Psi^{(k)}_{t,t'}(X_t; X_{t'}) \geq I(V_t; V_{t'}) > 0 , \tag{D10} \]

Additionally, since $D^{(k)}_{t,t'}(X_t; X_{t'}) \geq 0$, Eq. (D10) implies that $\text{Syn}^{(k)}_{t,t'}(X_t; X_{t'}) > 0$, proving the desired result.

Appendix E: Simulation details

Let us focus first on the Game of Life (GoL) simulations in Figure 4. For the initial state, two particles of three fixed types (nothing, a glider, or a lightweight spaceship) were selected at random, and placed at random positions in a 15x15 square cell array. The GoL evolution rule was run for 1000 steps, which, in most cases (judged by visual inspection) was enough for the system to settle on a stable configuration – which was typically either nothing, a small number of static structures, or a small number of particles in non-colliding tracks. To compute the emergent feature $V_{t'}$, particles were detected by simply pattern-matching the resulting system state against the known shapes of each particle. We considered five categories: still lifes, oscillators, gliders, lightweight spaceships, or nothing.

For static structures, we used a single symbol to represent all still lifes, and a single symbol for all oscillators. This particle detector was found to be very effective, with only 2% of runs resulting in unrecognised particles. A total of $5 \times 10^5$ independent runs were simulated and, due to the high number of possible states of $V_t$, to reduce bias we used the quasi-Bayesian estimator by Archer et al. [35].

For the boids simulation, $N = 10$ boids were simulated on a torus of side length $L = 200$. Boids are initialised with random positions, speeds, and head angles, and at each timestep each boid $i = 1, ..., N$ is updated according to the equations:

\[ x^{i}_{t'} = x^{i}_{t} + s^{i} \cos(\alpha^{i}_{t}) \]

\[ y^{i}_{t'} = y^{i}_{t} + s^{i} \sin(\alpha^{i}_{t}) \]

\[ \alpha^{i}_{t'} = \alpha^{i}_{t} + a_{1}\theta_{1} + a_{2}(\pi + \theta_{2}) + a_{3}\theta_{3} , \]

Where $\theta_{1}$ is the bearing to the flock’s center of mass, $\theta_{2}$ the bearing to the nearest boid, and $\theta_{3}$ the mean alignment of all boids within a 20 unit radius. The scalars $a_{1}, a_{2}, a_{3}$ are the aggregation, avoidance, and alignment parameters, respectively.

The results in Figure 5 were obtained averaging $\Psi$ across 25 independent runs of 5000 timesteps each, keeping $a_{1} = 0.15, a_{3} = 0.25$ fixed across all simulations. To compute $\Psi$, we pre-processed the trajectories using the same procedure as Seth [5] (i.e. each boid was described by its distance to the center of the environment and all time series were first-order differenced), and information-theoretic quantities were computed using the non-parametric estimator implemented in the JIDT toolbox [23, 24] using a dynamic correlation exclusion window of 10 samples [66].

Appendix F: ECoG preprocessing and decoding

ECoG signals were preprocessed following the steps presented in the original publication: specifically, the data was notch-filtered to remove line noise and band-pass filtered from 0.1 Hz to 600 Hz, and then downsampled to the same sampling frequency as the MoCap data (120 Hz) [37]. Then, data were divided into a 60/40 train/test split. To build the predictor, the training set was first standardised to zero mean and unit variance, and then it was dimensionality-reduced with a 20-component Partial Least Squares (PLS) regression using the three dimensions of the MoCap as dependent variables. We then trained a non-linear Support Vector Machine (SVM) [67] using a squared exponential kernel predicting the MoCap data from the 20-dimensional PLS scores. SVM and kernel hyperparameters were optimised through 5-fold cross-validation, and a model with the best hyperparameter configuration was trained on the full training set. This cross-validation and optimisation procedure was repeated for each dimension of the MoCap data, resulting in three separate SVMs [68].
The computation of Ψ was performed on the held-out test data set. ECoG signals were standardised and projected onto the PLS latent space (using the means, standard deviations, and projection matrix obtained from the training data), and mutual information terms involved in the computation of Ψ were calculated using the open-source JIDT toolbox [24].

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Note that the accuracy of this model is lower than the model presented in Ref. [37], for a precise reason: to predict position at time $t$, Chao et al. use a wavelet transform to obtain features that have represent ECoG from $t-1.1s$ to $t$. Unlike Chao et al., we work under the constraint of using supervenient features: for the axioms of the theory (in its current form) to hold, $V_t$ needs to be a function of $X_t$ only. This limits the possibilities for feature extraction, and naturally may result in lower-accuracy decoders.