Disentangling high-order mechanisms and high-order behaviours in complex systems

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Battiston *et al.* [1] provide a comprehensive overview of how investigations of complex systems should take into account interactions between more than two elements, which can be modelled by hypergraphs and studied via topological data analysis. Following a separate line of enquiry, a broad literature has developed information-theoretic tools to characterise high-order interdependencies from observed data. While these could seem to be competing approaches aiming to address the same question, in this correspondence we clarify that this is *not* the case, and that a complete account of higher-order phenomena needs to embrace both.

The approaches reviewed by Battiston and colleagues put a special focus on what could be described as *high-order mechanisms*, which are usually modelled via Hamiltonians or dynamical laws involving beyond-pairwise interactions. A distinct, but complementary perspective is to focus on the resulting *high-order behaviour*, i.e. patterns of activity that can be explained in terms of the whole but not the parts. Put simply, high-order mechanisms refer to the modelling of the data-generating process, while high-order behaviours refer to emergent properties within the resulting multivariate statistics. For example, in a spin glass system, high-order mechanisms would correspond to high-order terms in the system's Hamiltonian, while high-order behaviours would refer to the emergent patterns resulting from the corresponding Boltzmann distribution (Figure 1A).

The investigation of high-order behaviour in data has a long history, stemming from foundational work in information theory [2] and its early applications in biophysics [3, 4]. These early efforts led to the formalisation of high-order behaviour into the framework of partial information decomposition (PID) and its subsequent developments [5–7]. This literature has established formal bases for the analysis of high-order interdependencies exhibited by groups of three or more variables, and a description of their (synergistic or redundant) nature. While our primary focus here is on information-theoretic techniques, a number of other frameworks exist for probing the dynamics of complex systems beyond pairwise interactions — for a comprehensive review, see Ref. [8].

Mechanisms and behaviours address fundamentally different questions: the former address how the system is structured, while the latter focus on emergent properties related to what the system "does." Crucially, these questions are not interchangeable — intuition might suggest that high-order behaviour necessarily rests upon high-order mechanisms, but this is not the case (Figure 1B). Therefore, neglecting high-order behaviour risks missing important aspects of complex phenomena. Furthermore, when the goal is to identify high-order behaviour, high-order methods relying only on pairwise statistics (e.g. simplicial complexes built from a correlation matrix) may be in principle insufficient as significant information can be present only in the joint probability distribution and not the pairwise marginals (Figure 1B). There is a great need for inferential tools that can connect these two worlds — e.g. model selection methods to identify higher-order mechanisms that best match observed high-order behaviour, extending prior work on pairwise networks [9].

In summary, differentiating between high-order mechanisms and behaviours allows greater precision in articulating hypotheses, and in choosing the right tools to probe them. This distinction will facilitate the collaboration between different communities devoted to the study of complex systems, as the complementarity of these perspectives will provide a more powerful and encompassing avenue for deepening our understanding of high-order phenomena.

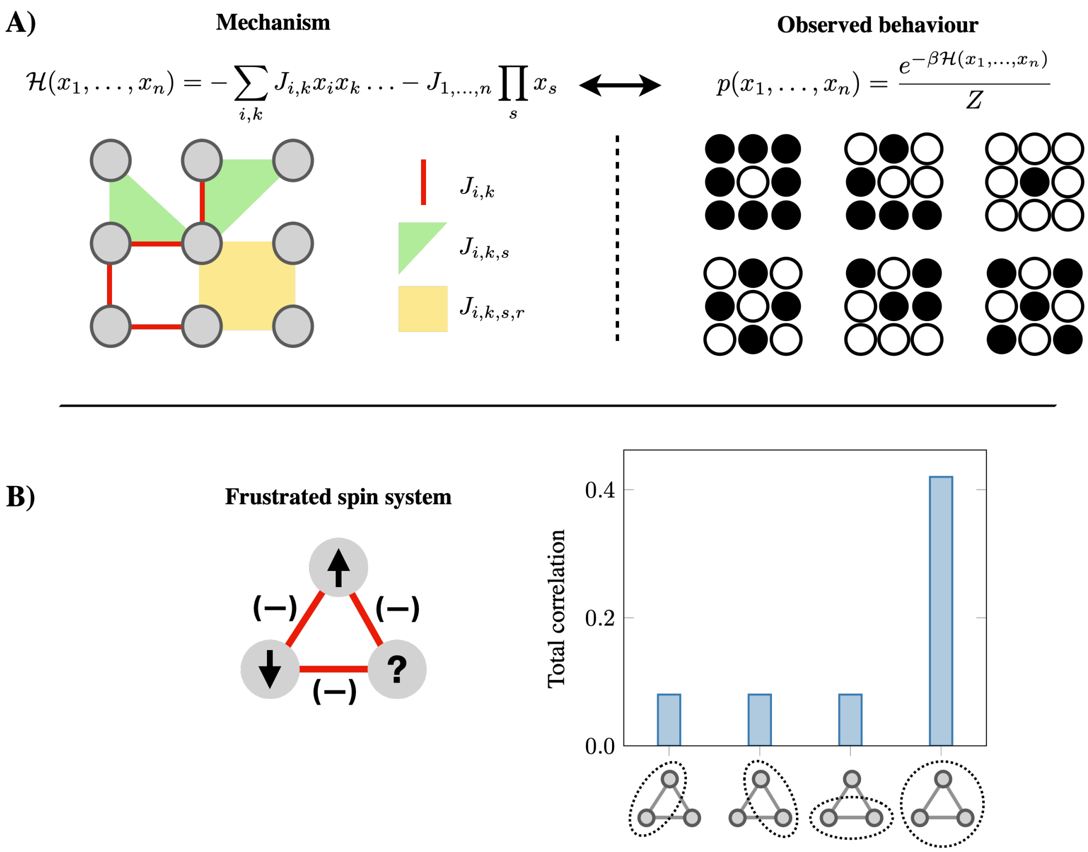

FIG. 1. **A)** The mechanism of a spin glass model is determined by a Hamiltonian $\mathcal{H}$ that accounts for pairwise and higher-order interactions, forming a hypergraph. The behaviour of the system is instead given by the frequencies of observed patterns, which can manifest as high-order interdependencies such as synergy or redundancy [5–7]. **B)** A small frustrated spin model, wherein spins cannot satisfy their tendency to differ from their neighbours [10]. The total interdependency (measured by Total Correlation [2]) significantly exceeds the sum of the three pairwise interdependencies, illustrating how low-order mechanisms can give rise to higher-order behaviour that cannot be explained from pairwise statistics.

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