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Editorial

Information processing as a paradigm to model and simulate complex systems

Computational science transforms observed complex phenomena into conceptual models which are formulated into algorithms that can be executed to yield predictions and estimate hidden parameters. These predictions can be compared to the observations, revealing to what extent the model is an accurate description. This generates an additional understanding of the phenomenon and leads to more specific models of the phenomenon. It is an iterative and creative process [1–3] largely based on intuition and experience of the scientist. Fundamental questions arise: What is the right level of abstraction? Should the model be continuous or discrete [4]? What type of predictions could be verified against observations and assist in a better understanding of the phenomenon?

It is the purpose of this editorial letter to introduce a more or less novel way to look at the computational science cycle through the use of information theory. This may be a surprising statement at first, but hints toward this link already exist. For instance, a natural phenomenon can be viewed as a (hidden) storage of information that is transmitted through space and time [5–7], and our attempt to model it corresponds to decrypting its hidden structure from observations [8,9]. Crutchfield and Feldman use statistical complexity to show that modeling is a necessary ingredient to make sense of observations, but at the same time it makes the phenomenon seem more random than it actually is [10]. Gu et al. use similar techniques to find the minimum memory requirements that a model can have while still retaining its predictive power [11].

More research into this link between information theory and computational science is needed, especially in the modeling phase and in the phase of understanding a phenomenon based on the predictions of such a model [e.g. 12]. This becomes ever more important as the field moves away from continuous mathematics and makes use of discrete models with increased complex. Next we take a closer look at this problem and discuss possible ways to address it.

In the past two centuries, continuous mathematics has been the most successful paradigm for describing and understanding physical systems. We understand these systems because we can describe their behavior with continuous models, such as partial differential equations, by exploiting their regularity and the mathematics of large numbers. These equations predict how the system behaves; bypassing the need to repeatedly prepare the systems and watch them evolve. In the words of Baierlein [13]: 'it all works because Avogadro's number is closer to infinity than to 10'.

This does not work, however, for systems with a 'less-than-infinite' number of elements or irregular interactions [14], for instance if each 'particle' has unique characteristics and there is a need to take into account individual behavior rather than bulk behavior. Contemporary science increasingly tries to study such systems, including the human brain [15], biological signaling systems [16,17], financial markets [18–20], social interaction [21–24], social computational systems [25], spreading of epidemics [26–29], city logistics [30], and the flow of fluids [14,31–35]. The irregularity of the interactions is a common denominator for many of these systems and is a research in its own right [23,36–39]. Classical mathematics is not well suited to predict the behavior of such systems.

The current trend therefore is to build models which are more complex, that is, which allow for unique interacting components that show behavior more like our idea of how the real system works. Well-established models are networks of cellular automata [40,41] and agent-based modeling [42]. Such models can be constructed even if we do not understand the macroscopic behavior: we need only to know how an individual 'particle' behaves and how it interacts with each other particle. Then we can set the model to an initial configuration and watch it evolve over time *in silico*. Given the microscopic state of the real system, we can even guess its future state before the real system reaches it.

But insofar the model becomes as complex as the real system, we still do not understand why the complex model behaves the way it does. Consider the example of opinion forming in a social network of friendships. A simple model that yields complex behavior is a heterogeneous network of Ising spins [43], where each person has two possible opinions and can 'persuade' their friends through a magnetic coupling. If we observe the model evolve over time then we see that many persons constantly change their opinion. We can zoom in on a particular spin flip of a particular person and ask questions like: 'why did this person change his opinion?' At first the answer may be that it is because his neighbor previously changed his opinion. But the question transfers: why did his neighbor change opinion? After a few such recurring questions we start to wonder: how far does this social influence reach? How long does it echo back and forth? Does it depend on the connectivity? What fraction of the observed dynamics is actually noise?

In the ideal case we could measure such characteristics of complex models in a unified manner. Not only would it help us in understanding the behavior of the real system, it would also allow us to compare such disparate systems as brain networks and financial markets. Perhaps we find that brain networks depend more on their underlying topology than financial markets, and perhaps the dynamics of a brain is on a more local scale whilst the financial markets operate on a global scale. At the same time, events in the financial markets might be quickly forgotten whereas the brain can remember a signal for a long time. Ultimately one could

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imagine a ‘taxonomy of complex systems’, an arrangement of natural phenomena along the dimensions of their behavior.

A general theory to answer such questions is still lacking. The current practice is to formulate specific measures for specific systems, and a natural choice is a ‘what-if’ scenario. For an N-body gravity simulation of planets, the ‘influence’ of a planet could be to what extent the trajectories of other planets deviate from the situation that a specific planet is not there [44,45]. In social networks, a person’s social influence could be taken as the number of people that will not change their opinion if this person were isolated [46,47]. In protein–protein interactions, the influence of one type of proteins could be the difference in concentrations of all other proteins in its absence (‘knock-out’ experiments) [48,49]. In addition to being application-specific, however, such ‘what-if’ scenarios are typically not observed in the natural setting which we try to understand. Planets do not suddenly disappear.

Perhaps the answer comes from describing the physics of complex systems using one of the earliest principles of informatics: information theory. In 1948, Shannon described how much information the receiving end of a noisy communication channel obtains from the sender of a message [50]. The unit of information is general-purpose: the number of yes/no questions that can be answered based on the message. Its converse, ‘uncertainty’, is measured as the number of unanswered yes/no questions. Nowadays, information theory is typically used for statistical inference, where an external observer attempts to describe the state of a system and its behavior [10,51,52]. The system state is the sender, and the measuring device of the external observer is the noisy communication channel.

Now suppose that we consider each ‘particle’ in a system as an observer in its own right. After all, each particle ‘measures’ the state of each neighbor particle through their interaction. Initially the state of each particle stores only the information that answers the question of what state the particle itself is in. But as time passes, particles receive information about the state of other particles and store it in their own state, which is in turn measured by other particles. As a result, the state of one particle can now partly answer the question of what state another particles is in. This is a measure of how much the state of the particle was influenced by the state of another particle: the more influence, the better the ‘measuring device’, and hence the more information is transmitted.

For example, let us apply this notion to social opinion forming, modeled by a network of Ising spins. We are interested to know how much the opinion (state) of a single person influences the dynamics of the entire system – a ubiquitous question in science. The goal is to be able to understand the observed dynamics of the system, i.e., the constant changing of opinions during a period of time. In particular, we would like to know which persons dictate these system dynamics.

To know the opinion of a person means to answer a single yes/no question. A person’s opinion s_0 at time zero influences the system state S_t at time t to the extent that the system state is capable of answering this question. We can say that the system ‘remembers’ the instantaneous state of each person. The longer a person’s state is remembered, the more the system dynamics are a reflection of the person’s state, and hence the more dynamics are explained by the state. Let us calculate how long a social network remembers the state of a person.

At time t the state of the social network stores $I(s_0 \mid S_t)$ bits of information about a person’s opinion s_0 at time 0, where

$$I(s_0|S_t) = H(s_0) - H(s_0|S_t)$$

is the mutual information and H is Shannon’s entropy [52]. To see how this quantity behaves, we first observe that at time 0 the network stores the maximum $I(s_0 \mid S_0) = 1$, for the trivial reason that

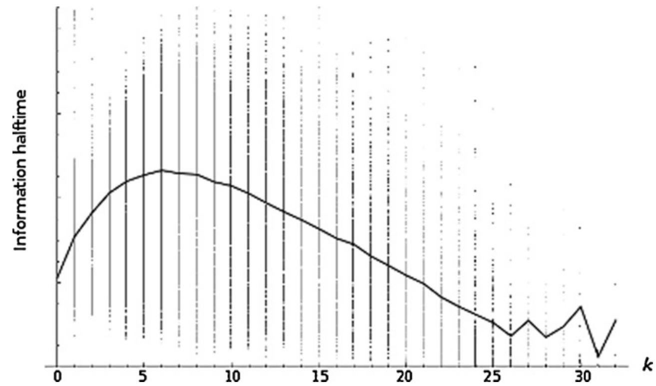

Fig. 1. The time that a social network remembers the state of a person with k connections. Here we simulated the Ising-spin dynamics in a network of 6000 nodes with a degree distribution $P(k) \propto k^{-1.6}$ using the Metropolis algorithm. The plot shows the average over six simulations.

the state s_0 is part of S_0 and is uniquely identified. Ultimately, as $t \to \infty$, S_t becomes independent of s_0 and $I(s_0 \mid S_0) \to 0$. In between these two extremes is a rate of losing information about s_0. We can then numerically calculate the halftime of the information that the network stores about a person. This is shown in Fig. 1 as function of the person’s connectivity.

This information theoretical point of view reveals an interesting feature of opinion forming in heterogeneous social networks: intermediately connected persons are best remembered by the network. This means that such a person contributes more to the observed system dynamics than hubs and peripheral persons. A possible explanation could be that Ising spins with only few connections behave too random, so the information that they transmit is mostly noise. The opinions of the hubs are ‘pinned’ by the many persons that influence them, so the information they transmit is redundant and already present in the network. Apparently there is a trade-off between these two extremes that optimizes the transmission of information through the network.

This is an example of how a computational model can lead to additional understanding about a phenomenon in a formal manner, using information theory. We used the concept that any physical system stores and processes bits of information [5–7], a concept explored in the context of quantum computing but not so much yet in classical systems. We hypothesize that the characteristics of this information processing might tell us how a system behaves. Combined with the other examples mentioned in our introduction, we conjecture that the field of information theory offers a promising opportunity to formalize the cycle of computational science. We hope that this viewpoint inspires our readers and we encourage the submission of novel research papers to the *Journal of Computational Science* that explores this exciting connection.

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Peter M.A. Sloot [a,b,c,*]
[a] *Computational Science, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, The Netherlands*
[b] *National Research University ITMO, Kronverkskiy 49, 197101, Saint Petersburg, Russian Federation*
[c] *Nanyang Technological University, 50 Nanyang Avenue, 639798, Singapore*

Rick Quax
Computational Science, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, The Netherlands

[*] Corresponding author at: Computational Science, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, The Netherlands.
E-mail address: p.m.a.sloot@uva.nl (P.M.A. Sloot)

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