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Editorial by Peter Sloot

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 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? 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, and our attempt to model it corresponds to decrypting its hidden structure from observations. 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. Gu et al. use similar techniques to find the minimum memory requirements that a model can have while still retaining its predictive power.

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. 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: ‘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, 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, biological signaling systems, financial markets, social interaction, social computational systems, spreading of epidemics, city logistics, and the flow of fluids. The irregularity of the interactions is a common denominator for many of these systems and is a research in its own right. 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 and agent-based modeling. 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, 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.