Complexity

Special Issue on

Complex Algorithms for Data-Driven Model Learning in Science and Engineering

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In their first centuries, scientific and engineering developments were dominated by empirical understanding which encapsulated the first paradigm of scientific discovery. After the Renaissance, the scientific revolution and the development of calculus led to a new scientific viewpoint whereby physical principles, laws of nature, and engineering models were established by proposing new theoretical constructs that could be verified through specific experiments. This was the second paradigm of scientific discovery. More recently, the computational era, or the third paradigm of discovery, has allowed us to solve complex and nonlinear scientific and engineering problems that were beyond our analytically tractable methodologies. Today, there is a new fourth paradigm of discovery, which is a data-driven science and engineering framework whereby complex models and physical laws are directly inferred from data.

Therefore, there is increasing change in the objective of computational algorithms used in simulations. Until now, the purpose was to accurately discretize systems of linear and nonlinear continuum equations derived from physical laws, models, and principles frequently established prior to the computational era; these equations were inferred from observation on limited experimental data and significantly simplified to make them analytically tractable. Today, the available experimental data and the complexity of the equations are no longer a major limitation to the point that we may compute physical processes without resorting to analytical laws, principles, or models; we just need to predict the correct output from the system for a given input even when there is not a well-defined model. However, for this endeavor, we need new computational algorithms capable of learning the complex behavior of the system and of establishing those governing equations of the system directly from experimental data, with the flexibility of not having to rely on analytical equations. An example is the determination of the nonlinear behavior of solids and fluids under general conditions directly from measured data, without specifying the form of the constitutive relations. Many fields already have started to capitalize on such methods, developing algorithms for fuzzy relations, leading to data-driven decision making in many fields by constructing purely computational predictive analytics in such complex fields as economics, consumer behavior and dynamics, security, and even web utilities. The engineering sciences are now poised to also take advantage of data-driven methods in obtaining physical principles and models which yield reliable laws and accurate predictions, using fewer hypotheses and fewer analytical relations and balancing the parametrization of physical models with the amount of available measurements.

The purpose of this special issue is to explore the different computational complex algorithms and methodological themes as chaos, genetic algorithms, cellular automata, neural networks, and evolutionary game theory in establishing data-driven models and relations between physical variables to produce accurate numerical predictions with less hypotheses.

Potential topics include but are not limited to the following:

- Data-driven determination of complex constitutive relations in solids and fluids
- Neural network approach for data-driven design of materials
- Data-driven chemistry, biology, and drug-discovery
- Data-driven solution of complex engineering and science systems
- Data-driven reduction of complex scientific and engineering problems and their solutions
- Complex mathematical algorithms and methods supporting the previous topics

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