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The imperative of physics-based modeling and inverse theory in computational science

To best learn from data about large-scale complex systems, physics-based models representing the laws of nature must be integrated into the learning process. Inverse theory provides a crucial perspective for addressing the challenges of ill-posedness, uncertainty, nonlinearity and under-sampling.

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The notions of 'artificial intelligence (AI) for science' and 'scientific machine learning' (SciML) are gaining widespread attention in the scientific community. These initiatives target development and adoption of AI approaches in scientific and engineering fields with the goal of accelerating research and development breakthroughs in energy, basic science, engineering, medicine and national security. For the past six decades, these fields have been advanced through the synergistic and principled use of theory, experiments and physics-based simulations. Our increased ability to sense and acquire data is clearly a game-changer in these endeavors. Yet, in our excitement to define a new generation of data-centric approaches, we must be careful not to chart our course based entirely on the successes of data science and machine learning in the vastly different domains of social media, online entertainment, online retail, image recognition, machine translation and natural language processing — domains for which data are plentiful and physics-based models do not exist. In contrast, many of today's scientific grand challenges suffer from the lack of adequate sampling of the processes underlying the complex, large-scale systems. Yet, for many of these systems, a great deal is known regarding the underlying physical principles or governing equations; we must continue to appeal to computational science to unleash this information. As Coveney et al. argue elegantly[1], big data need big theory — and big physics-based simulation models — too.

The unreasonable effectiveness of physics-based models

But what are physics-based models and why are they indispensable? A physics-based model is a representation of the governing laws of nature that innately embeds the concepts of time, space, causality and generalizability. These laws of nature define how physical, chemical, biological and geological processes evolve. Physics-based models typically encode knowledge in the form of conservation and constitutive laws, often based on decades if not centuries of theoretical development and experimental validation. These laws often manifest as systems of differential equations that are solved numerically with high-performance computing (HPC).

In his famous 1960 article, Eugene Wigner wrote about 'The unreasonable effectiveness of mathematics in the natural sciences'[2], pointing to "the 'laws of nature' being of almost fantastic accuracy but of strictly limited scope." As Wigner discusses, physics-based modeling is powerful and effective because it gives us a predictive window into the future based on understanding. It achieves this because any particular model limits its scope to a particular class of physical systems or processes, building a universal representation within that class. Armed with that universal representation, physics-based modeling is a way to simulate 'what if' scenarios and to issue predictions that have explanatory power or projections with quantified uncertainties that go beyond the current state and available data. For example, in our modern world, physics-based models are used to issue predictions about the future evolution of a cancer patient's tumor, or about the loads that a yet to be built aircraft may find itself experiencing under different operating conditions. They enable predictions of weather over the next five to ten days, or scenario-based projections about the future state of the Earth's climate in the decades to come.

The role of inverse theory in learning from data

As attention turns from simulation to learning from data (that is, from the forward problem to the inverse problem), we must bring these learned lessons — the big theory and the big physics-based simulation models — with us. Without physical constraints, purely data-driven approaches are unlikely to be predictive, no matter how expressive the underlying representation. Even when physical models are not well-established (such as for many biological processes, in constitutive laws for complex materials, or in subgrid scale models for unresolved physics), we know that certain universal properties and relationships must hold, such as conservation properties, material frame indifference, objectivity, symmetries, or other invariants. The learning-from-data problem is fundamentally an inverse problem that merges the partial knowledge reservoir of data with that of physics-based models in a systematic and rigorous way, and in a way that exploits the complementary and mutually reinforcing aspects of both data and models.

Data and models invariably come with uncertainties. Data are often noisy, sparsely and heterogeneously sampled, and representative of disparate observables. Experiments and data gathering are costly, time-consuming, and sometimes dangerous or impossible. Often data are hardest to acquire and are thus sparsest in the most decision-critical regions (for example, failure, instability, extreme environments). Even if it is possible to generate more data (for example, via simulation) a fundamental challenge remains: due to information loss in the forward problem and resulting ill-posedness of the inverse problem, data often contain only low-dimensional information about the physics, even when the data are large-scale[3].

In turn, physics-based models are typically characterized by uncertain parameters, which may include initial and boundary conditions, sources, material properties, geometry and model structure, all of which can be heterogeneous in space or time. In this setting, rather than ignore known physics, we must employ them to define the maps from parameters to observables, and invert them to project model and data uncertainties onto posterior parameter uncertainties. Embedding in a probabilistic framework leads to a problem of Bayesian inference[4]. Inverse theory also enables us to infer low-dimensional, data-informed subspaces, and to propagate posterior parameter uncertainties on key metrics related to prediction or reconstruction[5], thus providing an end-to-end uncertainty quantification framework[6]. It further provides a computational infrastructure for formal observing network design within which one may quantify uncertainty reduction from existing or hypothetical observational assets, optimal sensor deployment, and data complementarity versus redundancy[7].

Inverse problems abound in every area of science, engineering and medicine. As just a few examples of model-based inverse problems, we may infer: coalescing binary system properties from detected gravitational waves, earth structure from reflected seismic waves, reaction rates from measurements of chemically reacting flows, ice sheet basal friction from satellite observations of surface flow[5], three-dimensional bone structure from X-ray computed tomography measurements, subsurface contaminant plume spread from crosswell electromagnetic measurements, internal structural defects from measurements of structural vibrations, initial conditions for prediction from meteorological data[8], ocean state from satellite and in situ observations[9], biochemical reaction networks from observed species concentrations, and so forth.

In general, any endeavor to infer cause from effect — to extract knowledge from data — can be viewed as an inverse problem[3,4,9–11]. Indeed, inverse problems sit at the heart of the methods of machine learning, where models are inferred from training data by way of gradient-based optimization, with efficient gradient computation afforded by the adjoint method ('backpropagation') and reverse-mode automatic differentiation[12]. Yet, for a large class of scientific and engineering problems, it is intractable to approach the inverse problem with a black-box representation that ignores the properties of the underlying physics-based models. This intractability arises due to complex dynamics combined with high-dimensional parameter spaces, as well as the fundamental ill-posedness of the inverse problem. This is exacerbated by the fact that, despite the revolution in observational capabilities (remote sensing, autonomous sensing) and the apparent revolution in data streams, the underlying systems remain heavily under-sampled in practice. Instead, we must design methods that exploit the underlying structure of the inverse problem and the structure of the physics-based model that sits within it. Mathematically, this structure is reflected in the geometry, smoothness, invariance properties, sensitivity, local and global stability properties, intrinsic low dimensionality, and sparsity of the parameter-to-observable map. This is why it is crucial to interpret the data 'through the lens' of the physics-based model. An example of a seemingly 'big data' yet de facto sparsely sampled problem is encountered in numerical weather (and increasingly Earth system) prediction, which mandates advanced estimation or data assimilation (specific renderings of inverse methods) as core computational infrastructure[13]. It is also a good example of exploiting model structure to determine uncertainty growth due to non-normal transient amplification[14].

Intentionality meets serendipity

The core of the field of computational science has been the development of mathematical and numerical methods that exploit the structure of physics-based models — which manifests mathematically through properties such as geometry, regularity, asymptotic behavior, intrinsic low dimensionality, and sparsity — to achieve predictive and explanatory simulation and inversion of complex systems at scale[15]. For example, a partial differential equation (PDE) solver that is universally best does not exist; instead, PDE discretizations and algorithms are tailored to the nonlinearities, heterogeneities, anisotropies, diffusive-versus-convective nature, coupling, and so forth, of the underlying models. With the notion of governing equations comes a class of 'intentional models' — models constructed to universally represent a particular class of physical systems and with the ability to meaningfully interpolate sparse, disparate data, to issue predictions, and to generalize, within this class of systems.

In machine learning, it is this very lack of specified structure that has proven to be so powerful. AI driven by perception and learning has the power to discover and exploit structure that may not be known a priori — to create 'serendipitous models'. AI has the power to adapt to changing conditions, and importantly, to use data to drive surrogate modeling when the governing equations are unknown or inadequate. Machine learning approaches have an added advantage in that their black-box nature makes them highly flexible and non-intrusive. Yet for grand challenge problems in science and engineering, most existing AI and machine learning approaches run the risk of lacking levels of robustness, reliability and interpretability to make them viable. In addition to the challenges of under-sampling, scientific and engineering decision-making often requires the characterization of rare events. For example, it is not unusual to require design of critical engineering systems to be certified against probabilities of failure in the range of 10^{-6} to 10^{-9}. Estimating a one-in-a-million event places extreme demands on prediction and generalization in a way that is very different from most applications of machine learning in computer science. These challenges are beginning to be widely appreciated, as indicated, for example, by the growing number of workshops and journal special issues on SciML, physics-informed machine learning, or theory-guided machine learning.

Indeed, much of the current effort in the research community is aimed at combining physics-based modeling with machine learning. What is required if we are to achieve rigorous, reliable, scalable, interpretable and generalizable methods for SciML? We believe that it is first important to disentangle three elements of the computational task of learning from data: (1) the representation of the parameter-to-observable map in the learning problem, (2) the optimization or search algorithm used to solve the learning problem, and (3) the nature of the underlying application and the characteristics of its data. Successes that hinge on the third element (that is, the data) should not be conflated with choices made for the first two elements, noting that machine learning has found substantial success in applications where data are voluminous using expressive but problem-agnostic representations (for example, a deep neural network) and simple search algorithms (for example, stochastic gradient descent). Let us also be cognizant of the fact that the more physics constraints are brought into the machine learning process, the closer the physics-guided machine learning formulation moves towards becoming a classical physics-constrained inverse problem. Indeed, there is a great opportunity to exploit the large body of theory and scalable algorithms for large-scale deterministic and Bayesian inverse problems governed by PDEs (or integral equations, or ordinary differential equations, or N-body problems, and so forth) to overcome the challenges of this merger of these two perspectives. Such inverse problem formulations have seen substantial successes in applications where the unknown parameters are high-dimensional but data are sparse. Machine learning representations (such as deep neural networks) offer the promise of efficiently and accurately representing high-dimensional parameter-to-observable maps. This is an advantage that could play an important role in crafting efficient surrogates for expensive computer models in order to tackle large-scale Bayesian inverse problems, provided these machine learning-based surrogates can be constructed with limited training data.

Future decision-making supported by computational science

The greatest challenges facing society — clean energy, climate change, sustainable urban infrastructure, access to clean water, poverty, personalized medicine, and more — by their very nature require predictions or scenario-based projections that go well beyond the available data. There is a critical need to quantify uncertainty and our associated confidence in predictions; there is a critical need to make informed decisions that account for risk. Advances in computational science, in partnership with data science, are required to support these needs. Forward simulations must be augmented with advanced inverse (or data assimilation) methods. Frequently, these inverse capabilities are not in place even in state-of-the-art simulation codes, in part due to the added computational complexity of inverse methods. Thus, approaches that address computational complexity are key, ranging from scalable search algorithms that use higher-order sensitivity information (for example, via adjoint PDEs), to surrogate modeling (including reduced models and deep networks) for simulation speed-ups, to innovations in computational algorithms (and the associated adaptation of legacy production codes) to next-generation heterogeneous HPC hardware. Furthermore, forward and inverse modeling frameworks must be endowed with rigorous (yet practical) uncertainty quantification frameworks. Again, this is a challenge that requires advances across methods, algorithms and computational implementations. Finally, we need ways to make our sparse-but-valuable data even more valuable, while recognizing the real-world constraints (expense, intrusivity, maintainability) of observational systems in the physical and natural world. Thus, research is needed to render practical optimal experimental design approaches for large-scale, real-world applications. Such approaches provide powerful conceptual frameworks for codesigning complex sensor networks, involving observationalists, modelers, data scientists and users. ❐

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