

**Artificial intelligence for science: parsimony, Bayesianity, causality**

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Over the last decade, machine learning (ML) and artificial intelligence (AI) methods boosted by the unprecedented growth of computational power have entered, and have often become foundational, in the fields such as medicine, sociology, finance and climate modeling. The vast majority of ML applications are built on correlative models, enabled by the availability of large volumes of data inherent to these areas. However, this correlative data driven nature of the ML tools limits their incorporation in traditional scientific domains, dominated by hypothesis-driven research processes and relying heavily on past knowledge and history. We believe that the coming decade opens tremendous opportunities in ML areas that surpass this correlative paradigm, including parsimony, Bayesianity, and causality, and their introduction in theory and experimental domains. Beyond acceleration of traditional scientific workflows, this holds the potential for creation of fundamentally new ones, for example a near term realization could be via autonomous experimentation whereby causal-based directions in materials/chemical space are determined based on in-line measurements.

**1. Parsimony and physics extraction:** The classical correlative machine learning models often rely on the existence of large volumes of training data to establish relationships, and perform interpolation in high dimensional spaces. However, the intrinsic nature of material world is that it is often built on underlying simplicity – whether in the nature of elementary building blocks, or in the laws defining their interactions. Methods such as Independent Component Analysis (ICA) or Autoencoders implement the concept of simplicity via constraints on the latent variables or their distributions. However, much like infinitely complex geometries of the Mandelbrot set can be described by several lines of code, we ultimately seek to extract and analyze the physical equivalents of Kolmogorov complexity– whether it is the exchange Hamiltonians in lattice models or force fields between atoms and molecules. The forward prediction is possible only when the laws defining physical and chemical functionalities for defined atomic arrangements and configurations are known. We can postulate that they are “simple” in some sense, even though we do not necessarily know what they are. Ideally, we aim to discover these laws from the experiment while satisfying the known physics of the problem, including rigid (e.g., mass conservation), and soft (e.g., local electroneutrality), constraints.

**2. Bayesianity:** Scientific research relies on the preponderance of prior knowledge, either in the form of theoretical models and associated parameters, past observations and data, and “domain intuition” integrating the past observations and experience. This very rich structure of scientific domains naturally lends itself towards adoption of Bayesian methods that incorporate prior knowledge in the form of priors for model selection, parameters, etc., and enable establishing predictability of studied behaviors, etc. The required corollary for this is the incorporation of data integration methods that allow to systematically construct and verify such models. Moreover, the framework readily allows for uncertainty quantification, which is critical in for every scientific field, and which allows questions to be probed with answers produced to match required uncertainty targets.

**3. Causality.** Correlative ML methods are powerful tools for cases when causal links are known or when the confounding and bias factors are frozen or vary only weakly. However, in cases where causal links are unknown, ML methods can result in extreme problems, with the effects such as “Simpson paradox” hidden but not eliminated by complex algorithms. Correspondingly, determining the causal links from observed data, as is or in the Bayesian context of prior knowledge, is one of the key necessities for ML to develop. What’s notable is that determining the parsimonious functional forms of physical laws is insufficient to establish causal links, rendering parsimony, Bayesianity, and causality three major directions for AI in science during the next decade.

The incorporation of these trends into AI/ML driven experimental materials discovery, optimization, and design enabled transition to the AI-enabled research environment, both to enable fundamentally new science, significantly accelerate the scientific discovery workflows.