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Elucidating Material Dynamics with Deep Learning-based Inference

Abstract

Scientific inquiry seeks to understand how objects behave under varying conditions, yet objects are never accessed directly. They are encountered only through observations obtained under specific experimental settings, each capturing a partial and condition-dependent manifestation. As a result, object behavior cannot be identified from individual observations alone. Instead, behaviors and behavior patterns are articulated as characteristic responses of an object, inferred from structured variability across collections of observations as observing conditions change.

This dissertation formulates object inquiry as a process of organizing and interpreting observational variability. Observations, representations, relations, and behaviors are assigned distinct roles. Observations constitute empirical records and exhibit substantial variability due to experimental conditions. Learned representations are introduced as organizational structures that arrange observations so that specific kinds of relations become examinable, including similarity, continuity, progression, and contextual dependence. These relations organize how observations vary, but do not themselves define behavior. Behaviors are characterized at the observation level as coherent and condition-dependent patterns of variability revealed through how such relations evolve under applied conditions. In this sense, inference refers to the construction of behavior-level understanding from structured observational variation, rather than to prediction or parameter estimation from isolated data instances.

Material dynamics are examined as a primary instantiation of this inquiry formulation. In material systems, behaviors such as diffusion, deformation, and transformation are distributed across time, scale, and measurement modality, and are manifested through complex and coupled sources of variability. Direct comparison of observations is therefore unreliable, and inquiry requires organizing large collections of heterogeneous observations to expose condition-dependent patterns of change. This requirement motivates the integration of deep-learning models as inferential instruments, selected according to the representational properties they provide.

Two complementary deep-learning–integrated inquiry approaches are developed. A generative-inference approach employs deep generative models to organize admissible variability and continuity among observations, enabling systematic exploration of plausible transformation pathways and statistical characterization of behavior patterns beyond direct observation. An attentive-inference approach employs attention-based transformer models to organize contextual relations within observational data, emphasizing how localized features contribute to global responses across space, time, and modality. These approaches address the same notion of object behavior, while exposing complementary facets of how behaviors are manifested and constrained.

Across multiple case studies in material dynamics, the dissertation demonstrates how deep learning can support object inquiry not as a predictive endpoint, but as a means of organizing variability and relations in ways that make behaviors and behavior patterns interpretable. The central contribution is a clarified account of deep learning-based inference in object inquiry, specifying how representations support the organization of relations from which object behavior can be systematically articulated.

Keywords: *Scientific inquiry, Material dynamics, Time-resolved microscopy, Deep generative models, Attention mechanisms*