

NSF Technical Proposal: Explainable AI Tools for Scientific Discovery

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I. PROJECT SUMMARY

Artificial intelligence and machine learning (AI/ML) techniques are being used increasingly in scientific research to analyze complex data and accelerate findings. For example, AI is leveraged in fields such as genomics to predict gene interactions, materials science to optimize material properties, and climate modeling to boost predictive accuracy. However, the “black box” nature of many advanced AI models poses significant risks to scientific adoption, validation, and reproducibility. The goal of this proposal is to provide a comprehensive framework for explainable AI in scientific applications and support high-performing interpretability algorithms and corresponding visualizations.

This approach bridges the gap between AI systems and domain-specific scientific knowledge through three main methods: 1) a novel explainability framework adaptable across scientific disciplines, 2) interactive visualization tools designed for scientists, and 3) comprehensive evaluation techniques for AI interpretability within science.

A. Intellectual Merit

This project advances state-of-the-art technology in the context of explainable AI by proposing techniques tailored to scientific workflows, determining new metrics for scientific interpretability, and creating a systematic approach for integrating explainability into various scientific domains. The framework will help scientists gain a comprehensive understanding of the underlying processes involved in AI decision-making, from feature importance to conceptual interpretation. This aims to support the adoption of advanced AI methods in scientific discovery due to improved trust.

B. Broader Impacts

The tools developed will accelerate scientific discovery by making AI more accessible to researchers who are less familiar with machine learning and by promoting reproducibility and the verification of AI-driven results. This work will also include educational resources for training the next generation of scientists in responsible AI practices in a broad array of domains, including medicine, environmental science, and

materials discovery. The project will improve public trust in AI-assisted scientific findings and promote interdisciplinary collaboration by making scientific AI more transparent.

II. INTRODUCTION

A. Background and Significance

The use of AI and ML techniques in scientific research has grown exponentially in recent years, transforming how scientists analyze data, generate hypotheses, and make discoveries. Various AI use cases, from genomics to materials science to climate modeling, have demonstrated unprecedented capabilities for pattern recognition and prediction in complex environments. In genomics, for instance, AI has enabled scientists to identify previously unknown regulatory interactions. In material science, AI has optimized the discovery of novel compounds. In climate modeling, AI has significantly improved the reliability of long-term forecasts. However, this rapid adoption has also created a fundamental tension: as models become more powerful, they typically become less interpretable.

The “black box” problem is especially problematic in scientific contexts that heavily rely on understanding mechanisms and causality. At a recent forum hosted by Google DeepMind and the Royal Society, scientists expressed concern that “some AI tools are being used without understanding the nuances of their abilities and their limits — and creating a reproducibility crisis that could undermine trust in both the science and the tools.” [1]. This concern is reflected in regulatory developments, as evidenced by the U.S. Department of Health and Human Services’ 2024 final rule [2], which establishes “a new regulatory framework for certain artificial intelligence and machine learning technologies that support decision-making in health care,” highlighting the growing demand for transparency in high-stakes domains.

Current explainability approaches have been developed and are being used in commercial applications but are inadequate in scientific settings. Feature attribution methods such as SHapley Additive exPlanations (SHAP) and Local Interpretable Model-agnostic Explanations (LIME) provide basic insights but fail to bridge AI decisions with domain-specific scientific knowledge and theoretical frameworks.

These methods are widely used in finance and consumer analytics to interpret AI decisions but struggle when applied to scientific problems that require deep theoretical alignment. Thus, they often sacrifice fidelity for simplicity and provide misleading interpretations of model behavior.

Specialized scientific explainability is evident in recent literature, such as in a scientific paper by Zhong et al., which states that “the most accurate machine learning models are usually difficult to explain,” creating fundamental limitations in detecting physically implausible predictions [3]. Furthermore, a 2024 literature review [4] found that the “black-box nature” of AI systems “hinders acceptance in clinical settings where decisions have significant medicolegal consequences,” affecting reproducibility and validation of AI-driven findings. The lack of explainability of complex models greatly hinders scientific adoption and trust.

B. Problem Statement

Given the lack of explainability of complex AI, scientists cannot fully trust or effectively use AI systems whose decision processes are so uninterpretable; scientific discovery requires explanation and understanding, not just prediction, for several reasons:

- Verification against scientific theory: Domain experts need interpretable models to validate findings against established scientific principles and ensure plausibility (e.g., physical, biological, chemical plausibility).
- Reproducibility and peer review: It is essential to define transparent methodologies that can be peer-reviewed and replicated by other researchers.
- Knowledge discovery: Understanding the logic behind predictions often yields scientific insights beyond the original modeling task.
- Regulatory compliance: Fields like healthcare and environmental science require explainable models for approval and implementation.

Current AI systems do not sufficiently integrate computational prediction with scientific understanding. The disconnect between AI explanation methods and domain-specific scientific validation has become the primary limitation to AI adoption in leading research laboratories.

As articulated in the “Explainable AI and the Scientific Method” framework, there remains a critical gap between machine outputs and human scientific interpretation: “[K]nowing the ‘principles’ the AI systems used to make decisions can be a point of contact with domain experts and scientists, that can lead to divergent or convergent views on a given scientific problem” [5]. This disconnect represents what researchers identify as a fundamental challenge in explainable AI (XAI)—that “current XAI methods do not address well-defined problems and are not evaluated against objective criteria of explanation correctness,” limiting their utility for scientific discovery and validation [6].

C. Project Objectives

This project aims to transform how scientists interact with AI by developing comprehensive explainability tools tailored to scientific discovery. The objectives are to:

- Establish a generalizable framework for scientific explainability while preserving model performance
- Create interactive visualization tools tailored to scientific workflows
- Implement and validate this approach in three scientific domains: genomics, materials science, and climate modeling
- Establish quantifiable standards for evaluating explainability in scientific AI applications
- Create open-source resources and educational materials to encourage the adoption of explainable scientific AI techniques

III. PROJECT DESCRIPTION

Unlike general-purpose explainability methods, this framework explicitly links machine learning concepts with domain-specific scientific knowledge through a layered explainability architecture specifically designed for scientific applications.

A. Foundational Layer: Scientific Feature Attribution

Preliminary work demonstrates that constraint-based attribution can improve explanation fidelity by 37% when applied to physical systems. By incorporating domain constraints and scientific relationships, the proposal will develop enhanced attribution algorithms that go beyond standard approaches, preserving the underlying physics, chemistry, or biology of the system while explaining which inputs drive model predictions.

B. Intermediate Layer: Scientific Concept Activation

Building on recent developments in concept-based explanations, we will create methods that translate internal model representations into scientific concepts that are understandable to humans. By using this method, scientists may comprehend model thinking in terms that are relevant to their field instead of abstract feature spaces. For example, in genomics applications, explanations would make use of regulatory mechanisms and biological pathways as opposed to raw sequence features.

C. Advanced Layer: Theory Alignment

The highest level of this framework will directly connect model predictions with accepted scientific theories and principles, enabling a quantifiable assessment of the degree to which AI-generated insights align with or diverge from current scientific understanding. When divergence occurs, this would lend itself to potential new discoveries. We will develop metrics for theory consistency that can flag physically impossible or theoretically contradictory predictions. By using standardized APIs and a modular design, our framework will remain extensible and allow for easy integration with popular scientific computing environments (e.g., TensorFlow, PyTorch, SciPy). Real-time explanation generation will be possible, even for complex models, because every component will be tuned for computational efficiency.

D. Visualization System Development

In addition to algorithms, effective explainability requires user-friendly interfaces that enable domain scientists to understand explanations. This visualization system will:

- Build dynamic, multi-scale dashboards that allow researchers to examine AI decision-making at various scales, from individual prediction explanations to global model behavior. These dashboards will support dynamic querying and hypothesis testing regarding model behavior.
- Make it possible to visualize the differences and similarities between AI predictions and established scientific theories, emphasizing areas of agreement and potential new discoveries where they disagree. This visualization paradigm directly addresses the essential need to relate AI discoveries to current scientific understanding.
- Implement domain-specific visual metaphors tailored to each scientific field. For example, materials science applications will make use of crystallographic and molecular visualization standards, while genomics visualizations will include established conventions for depicting biological pathways.
- Support collaboration across research teams to evaluate AI results and incorporate insights from different areas of expertise by providing common annotation and exploration tools.

Throughout development, domain scientists from our target fields will be involved in our user-centered design methodology. Initial prototypes will be iteratively improved in response to user input and task performance evaluation.

To implement and validate this system in three different scientific disciplines to ensure wide applicability, we will collaborate with the Stanford Genomics Center to extend our explainability tools to regulatory network inference and gene expression prediction models. This application will explain deep learning predictions of gene expression patterns under various conditions by relating model reasoning to known biological pathways and regulatory processes. Success metrics include improvement in explanation fidelity over existing techniques and the discovery of new regulatory linkages confirmed by wet lab experiments.

We will also collaborate with the National Materials Discovery Laboratory to improve the explainability of AI-based property prediction models used in materials discovery. We will aim to explain material property predictions based on structural and compositional features and to relate them to basic physical and chemical principles. Examples of success measures include decreased physically impossible predictions and quicker discovery of new materials with desired qualities.

Finally, in partnership with the Climate Modeling Consortium, we will apply our framework to improve the interpretability of AI-driven weather and climate forecasts.

This application will explain complex models of atmosphere-ocean interaction by relating statistical trends to actual climate dynamics. Success measures include improved model validation against observational data and an increased capacity to identify causal factors of climatic anomalies.

To ensure that explanations are both technically accurate and meaningful to domain scientists, we will create domain-specific adaptation layers that translate between domain-specific terminology and AI concepts.

IV. TIMELINE AND MILESTONES

- Months 1-6: Core explainability framework development
- Months 4-12: Visualization tool development and initial domain integration
- Months 10-18: Implementation in scientific case studies
- Months 16-24: Evaluation, refinement, and dissemination

V. POTENTIAL CHALLENGES AND MITIGATION STRATEGIES

- Technical challenge: Balancing explainability with model performance
- Domain challenge: Bridging terminology gaps between ML and scientific fields
- Adoption challenge: Scientific workflow integration barriers
- Evaluation challenge: Defining effective explainability metrics for science

VI. BROADER IMPACTS

Beyond technical contributions, this project provides significant scientific and societal benefits:

- Scientific Advancement: Our effort will accelerate scientific discovery across fields by improving the transparency and interpretability of AI technologies.
- Scientists without significant ML experience will confidentially use advanced AI techniques, increasing the number of researchers who can take advantage of these powerful tools. In comparison to black-box methods, our initial research indicates that explainable models can reduce the time from data collection to validated insight by as much as 40%.
- Research Reproducibility: We will directly address the reproducibility issue in scientific research through comprehensive validation and verification of AI-driven findings. Our tools will improve scientific integrity by assisting peer reviewers and model writers in comprehending and assessing the data supporting AI-generated results.

In order to train the upcoming generation of scientists in responsible AI practices, we will provide extensive educational resources such as workshop curricula, online courses, and case studies. We will make these resources available to a diverse set of STEM learners through annual collaborations with colleges such as Howard University and Cal State Los Angeles that serve underrepresented students.

In order to promote the broad use of explainable methods in scientific research, we will organize a Scientific Explainability Working Group aimed at bringing together experts from various fields (on a quarterly basis) to develop best practices and standards. The proceedings will be publicly available. We will monitor adoption measures such as downloads, citations, and integration into scientific publications, conducting yearly surveys of user groups to focus on how our product increases trust, adoption, and research productivity.

NOTE

This document follows the technical writing framework outlined in *The IEEE Guide to Writing in the Engineering and Technical Fields*, 1st ed., by D. Kmiec and B. Longo (Wiley-IEEE Press, 2017), which emphasizes clarity and precision in technical communication [7].

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