Abstract

The discovery of scientific formulae that parsimoniously explain natural phenomena and align with existing background theory is a key goal in science. Historically, scientists have derived natural laws by manipulating equations based on existing knowledge, forming new equations, and verifying them experimentally. In recent years, data-driven scientific discovery has emerged as a viable competitor in settings with large amounts of experimental data. Unfortunately, data-driven methods often fail to discover valid laws when data is noisy or scarce. Accordingly, recent works combine regression and reasoning to eliminate formulae inconsistent with background theory. However, the problem of searching over the space of formulae consistent with background theory to find one that fits the data best is not well-solved. We propose a solution to this problem when all axioms and scientific laws are expressible via polynomial equalities and inequalities and argue that our approach is widely applicable. We further model notions of minimal complexity using binary variables and logical constraints, solve polynomial optimization problems via mixed-integer linear or semidefinite optimization, and automatically prove the validity of our scientific discoveries via Positivestellensatz certificates. Remarkably, the optimization techniques leveraged in this paper allow our approach to run in polynomial time with fully correct background theory, or non-deterministic polynomial (NP) time with partially correct background theory. We experimentally demonstrate that some famous scientific laws, including Kepler’s Third Law of Planetary Motion, the Hagen-Poiseuille Equation, and the Radiated Gravitational Wave Power equation, can be automatically derived from sets of partially correct background axioms.
1 Introduction

A fundamental problem in science and engineering involves explaining natural phenomena in a manner consistent with noisy experimental data and a body of potentially inexact and incomplete background knowledge about the universe’s laws [31]. In the past few centuries, “The Scientific Method” [78] has led to significant progress in discovering new laws. Unfortunately, the rate of emergence of these laws and their contribution to economic growth is stagnating relative to the amount of capital invested in deducing them [21, 16]. Indeed, Dirac [33] noted that it is now more challenging for first-rate physicists to make second-rate discoveries than it was previously for second-rate physicists to make first-rate ones, while Arora et al. [7] found that the marginal value of scientific discoveries to large companies has declined since the fall of the Berlin Wall. This phenomenon can be partly explained by analogy to the work of Cowen [26], namely, that The Scientific Method has picked most of the “low-hanging fruit” in science and engineering, such as natural laws that relate physical quantities using a small number of low-degree polynomials. This calls for automated and more disciplined alternatives to The Scientific Method, which integrate background information and experimental data to generate and verify higher dimensional laws of nature, thereby promoting scientific discovery and hopefully leading to economic growth [c.f. 1, 52, 83].

On the other hand, the past thirty years have seen significant improvements in the scalability of global optimization methods — which, as we argue in this paper, can search over the space of scientific laws — owing to Moore’s law and significant theoretical and computational advances by the optimization community [see 17, 45, 12, for reviews]. Bertsimas and Dunn [13, Chap. 1] observed that the speedup in raw computing power between 1991 and 2015 is at least six orders of magnitude. Additionally, sum-of-squares and polynomial optimization methods have become much more scalable since the work of Parrilo [65], and primal-dual interior-point methods [62] have improved considerably, with excellent implementations now available in, for example, the Mosek solver [6].

In this paper, we propose a new and automated approach to scientific discovery that leverages these advances by the optimization community; see Figure 1 for a high-level overview of our approach. Given a set of background axioms, theorems, and laws expressible as a basic semialgebraic set (i.e., a system of polynomial equalities and inequalities) and observations from experimental data, we derive

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2 Code and data used for this work will be made available upon acceptance.

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Figure 1: Schematic illustration of discovering Kepler’s third law of planetary motion. Using partially correct background knowledge encoded as multivariate polynomials, experimental data, and a sparsity constraint on the background theory to control our model’s complexity, we formulate scientific discovery as a polynomial optimization problem, reformulate it as a semidefinite optimization problem, and solve to obtain both a symbolic model and its formal derivation.
new laws representable as polynomial expressions that are either exactly or approximately consistent with existing laws and experimental data by solving polynomial optimization problems via linear and semidefinite optimization. By leveraging fundamental results from real algebraic geometry, we obtain formal proofs of the correctness of our laws as a byproduct of the optimization problems. This is notable, because existing automated approaches to scientific discovery, as reviewed in Section 1.1, often rely upon deep learning techniques that do not provide formal proofs and are prone to “hallucinating” incorrect scientific laws that cannot be automatically proven or disproven, analogously to output from state-of-the-art Large Language Models such as GPT-4 [64]. As such, any new laws derived by these systems cannot easily be explained or justified. On the other hand, our approach is based on a new notion of distance that demonstrates the compatibility of a symbolic law with a set of background theories based on the distance between a law and its projection onto the set of symbolic laws derivable from our theory. Moreover, our approach is scalable; it runs in polynomial time (when the degree of the polynomial certificates we search over is bounded; see Section 2.2) with a complete and correct set of background theory.

We believe our approach could be a first step towards discovering new laws of the universe which involve higher degree polynomials and are impractical for scientists to discover without the aid of modern solvers and high-performance computing environments. Further, our approach is potentially useful for reconciling mutually inconsistent axioms. Indeed, if a system of scientific laws is mutually inconsistent (in the sense that no point satisfies all laws simultaneously), our polynomial optimization problem offers a formal proof of its inconsistency. Moreover, our approach allows scientists to make discoveries using at most $k$ laws out of a supplied list of $n$ laws (where $n > k$), meaning it is possible to select the $k$ laws that best explain the experimental data.

1.1 Literature Review

Our proposed approach to scientific discovery uses polynomial optimization to obtain provably correct scientific formulae from axioms and data and builds upon two areas typically considered in isolation: (a) semidefinite and sum-of-squares optimization techniques for solving polynomial optimization problems, and (b) data-driven techniques for symbolic discovery. We now review relevant literature.

Sum-of-Squares Optimization: Sum-of-squares optimization has been an important component of global optimization methods since the seminal work of Parrilo [65] (see also Lasserre [55]), which combines two key observations. First, sum-of-squares decompositions of multivariate polynomials can be computed via semidefinite optimization, so optimizing over sum-of-squares polynomials is no harder than performing semidefinite optimization. Second, owing to a fundamental result from real algebraic geometry, namely the Positivestellensatz [53, 79, 68], polynomials of bounded degree defined on basic semialgebraic sets can be certified as non-negative over these sets by representing them as systems of sum-of-squares polynomials (see Section 1.3). Consequently, optimizing over a real polynomial system is (under mild assumptions) equivalent to solving a (larger) sum-of-squares optimization problem, and thus a tractable convex problem. These observations have allowed an entire field of optimization to blossom; see Blekherman et al. [18], Hall [46] for reviews. However, to our knowledge, no works have proposed using sum-of-squares optimization to discover scientific formulae. The closest works are Clegg et al. [24], who propose using Gröbner bases to design proofs of unsatisfiability, Curmei and Hall [30], who propose a sum-of-squares approach to fitting a polynomial to data under very general constraints on the functional form of the polynomial, e.g., non-negativity of the derivative over a box, Ahmadi and El Khadir [3], who propose learning the behavior of noisy dynamical systems via semialgebraic techniques, and Fawzi et al. [36], who propose learning proofs of optimality of stable set problems by combining reinforcement learning with the Positivestellensatz. However, determining whether polynomial optimization is practically useful for scientific discovery remains open.

Data-Driven Approaches to Scientific Discovery: The availability of large amounts of scientific data generated and collected over the past few decades has spurred increasing interest in data-driven methods for scientific discovery that aim to identify symbolic equations that accurately explain high-dimensional datasets. Bongard and Lipson [19] and Schmidt and Lipson [75] proposed using heuristics and genetic programming to discover scientifically meaningful formulae, and implemented their approach in the Eureqa software system [34]. Other proposed approaches are based on mixed-integer global optimization [9, 28], sparse regression [20, 73, 14], Cylindrical Algebraic Decomposition [41],
neural networks [50, 54], and Bayesian Markov Chain Monte Carlo approaches [44]. See [51, 10] for reviews of data-driven scientific discovery in fundamental physics and chemistry.

Data-driven approaches have since been shown by several authors to perform well in highly overdetermined settings with limited amounts of noise. For instance, Udrescu et al. [81, 80] proposed a method called AI-Feynman, which combines neural networks with physics-based techniques to discover symbolic formulae. Moreover, they constructed a benchmark dataset of 100 scientific laws derived from Richard Feynman’s lecture notes [38], with 100,000 noiseless experimental observations of each scientific law, and demonstrated that while the Eurequa system could recover an already impressive 71/100 instances from the data, their approach could recover all one hundred; see the work of Cornelio et al. [25] for a review of scientific discovery systems.

Unfortunately, data-driven approaches to scientific discovery have at least three significant drawbacks. First, they are not data efficient [40] and only reliably recover scientific formulae in highly overdetermined settings with several orders of magnitude more data than a human would likely need to make the same discoveries. Indeed, Matsubara et al. [61] recently argued that the sampling regime used by AI-Feynman is unrealistic, because it samples values far from those observable in the real world. Moreover, Cornelio et al. [25] recently rebenchmarked AI-Feynman on 81 of the 100 aforementioned laws, but with 10 (rather than 100,000) observations per law, and where each experimental observation is contaminated with a small amount of noise. In this limited data setting, Cornelio et al. [25] found that AI-Feynman recovered 40 of the 81 laws considered, whereas they were able to recover 49/81 laws using their symbolic regression solver. This performance degradation is a significant issue in practice because scientific data is typically expensive to obtain and scarce and noisy. Second, purely data-driven methods are agnostic to important background information, such as existing literature, that valid scientific formulae should be consistent with unless there is extraordinary experimental evidence that the literature is incorrect. This implies that data-driven methods search over a larger space of laws than is necessary, require more data than a human would need to derive a valid law, and frequently propose laws that are not scientifically meaningful. Third, they typically do not provide interpretable explanations for why their discoveries are valid [c.f. 72], which makes diagnosing whether their discoveries are consistent with existing theory challenging.

To account for background theory in scientific discovery, Cornelio et al. [25] recently proposed an approach called AI-Descartes, which iteratively generates plausible scientific formulae using a mixed-integer nonlinear symbolic regression solver [see also 9], and tests whether these formulae are derivable from the background knowledge. In the case they are not, the method provides a set of reasoning-based measures to compute how distant the formulae induced from the data are from the background theory, but is unable to recover the correct formulae. This is because their approach derives potential scientific laws from data and subsequently tests the hypothesis against the background theory, rather than learning from axioms and data simultaneously.

1.2 Contributions and Structure

We propose a novel automated approach to scientific discovery, which we term AI-Hilbert, that utilizes techniques from the polynomial and sum-of-squares optimization literatures to derive polynomial scientific laws that best explain a set of experimental data while maintaining consistency with a body of background knowledge. Our approach is inspired by the generality of the sum-of-squares optimization framework and the work of David Hilbert, who was one of the first mathematicians to investigate the power and expressivity of sum-of-squares functions of polynomials.

Our approach automatically provides an axiomatic derivation of the correctness of the discovered scientific law derived, conditional on the correctness of our background theory. Moreover, in instances with inconsistent background theory, our approach is capable of successfully identifying the sources of inconsistency by performing best subset selection to determine the axioms which best explain the data. This is notably different from current data-driven approaches to scientific discovery, which often generate spurious laws in limited data settings and fail to differentiate between valid and invalid discoveries, or provide explanations of their derivations. We illustrate our approach by axiomatically deriving some of the most frequently cited natural laws in the scientific literature, including Kepler’s Third Law and Einstein’s Relativistic Time Dilation Law, among other scientific discoveries.

A second contribution of our approach is that it permits fine-grained control of the tractability of the scientific discovery process, by bounding the degree of the coefficients in the Positivstellensatz
certificates that are searched over (see Section 1.3, for a formal statement of the Positivestellensatz). This differs from prior work on automated scientific discovery, which offers more limited control over its time complexity. For instance, in the special case of scientific discovery with a complete body of background theory and no experimental data, to our knowledge, the only current alternative to our approach is symbolic regression [see, e.g., 28], which requires genetic programming or mixed-integer nonlinear programming techniques that are not guaranteed to run in polynomial time. On the other hand, our approach searches for polynomial certificates of a bounded degree by leveraging a fixed level of the sum-of-squares hierarchy [55, 65], which can be searched over in polynomial time [62, 69].

To contrast our approach with existing approaches to scientific discovery, Figure 2 depicts a stylized version of the scientific method. In this version, new laws of nature are proposed from background laws, and, therefore, likely requires less experimental data to make scientific discoveries than purely data-driven approaches.

1.3 Background and Notation

The notation is mostly standard to the polynomial optimization literature. We let non-boldface characters such as $b$ denote scalars, lowercase bold-faced characters such as $x$ denote vectors, uppercase bold-faced characters such as $A$ denote matrices, and calligraphic uppercase characters such as $Z$ denote sets. We let $[n]$ denote the set of indices $\{1, \ldots, n\}$. We let $e$ denote the vector of ones, $0$ denote the vector of all zeros, and $I$ denote the identity matrix. We let $\|x\|_p$ denote the $p$-norm of a vector $x$ for $p \geq 1$. We let $\mathbb{R}$ denote the real numbers, $S^n_+$ denote the cone of $n \times n$ symmetric matrices, and $S^n_{++}$ denote the cone of $n \times n$ positive semidefinite matrices.

We also use some notations specific to the sum-of-squares (SOS) optimization literature; see [18] for a general theory. Specifically, we let $\mathbb{R}[x]_{n,2d}$ denote the ring of real polynomials in the $n$-tuple of variables $x \in \mathbb{R}^n$ of degree $2d$, $P_{n,2d} := \{p \in \mathbb{R}[x]_{n,2d} : p(x) \geq 0 \ \forall x \in \mathbb{R}^n\}$ denote the convex cone of non-negative polynomials in $n$ variables of degree $2d$, and

$$
\Sigma[x]_{n,2d} := \left\{p(x) : \exists q_1, \ldots, q_m \in \mathbb{R}[x]_{n,d} \quad p(x) = \sum_{i=1}^m q_i^2(x)\right\}
$$

denote the cone of sum-of-squares polynomials in $n$ variables of degree $2d$, which can be optimized over via $\left(\binom{n+d}{d}\right)$ dimensional semidefinite matrices [c.f. 65] using interior point methods [62]. Note that $\Sigma[x]_{n,2d} \subseteq P_{n,2d}$, and the inclusion is strict unless $n \leq 2$, $2d \leq 2$ or $n = 3, 2d = 4$ [47]. Nonetheless, $\Sigma[x]_{n,2d}$ provides a high-quality approximation of $P_{n,2d}$, since each non-negative polynomial can be approximated (in the $\ell_1$ norm of its coefficient vector) to any desired accuracy $\epsilon > 0$ by a sequence of sum-of-squares [56]. If the maximum degree $d$ is unknown, we suppress the dependence on $d$ in our notation.

To define a notion of distance between polynomials, we also use several functional norms. Let $x^\alpha$ stand for the monomial $x_1^{\alpha_1} \cdots x_n^{\alpha_n}$. Then, for a polynomial $q \in \mathbb{R}[x]_{n,2d}$ with the decomposition $q(x) = \sum_{|\alpha| \leq 2d} a_\alpha x^\alpha$, we let the notation $|q|_p := \|a\|_p = \left(\sum_{|\alpha| \leq 2d} a_\alpha^p\right)^{1/p}$ denote the coefficient norm of the polynomial, where $\| \cdot \|_p$ denotes the $\ell_p$ norm of a vector.

Finally, to derive new laws of nature from existing ones, we repeatedly invoke a fundamental result from real algebraic geometry called the Positivestellensatz [see, e.g., 79]. Various versions of the Positivestellensatz exist, with stronger versions holding under stronger assumptions [see 57, for a review], and any reasonable version being a viable candidate for our approach. For simplicity, we invoke a compact version due to [68], which holds under some relatively mild assumptions but nonetheless lends itself to relatively tractable optimization problems:
Figure 2: The Scientific Method With Scientific Discoveries Made Via Classical Methods, Data-Driven Methods, or AI-Hilbert. AI-Hilbert proposes scientific laws consistent with a body of background theory formally articulated as polynomial equalities, inequalities, and relevant data sources. This likely allows scientific discoveries to be made using fewer data points than via state-of-the-art approaches, and for missing scientific axioms to be deduced via abductive reasoning as part of the scientific discovery process. On the other hand, existing approaches to scientific discovery propose laws that may be inconsistent with either background theory or existing data sources.
Theorem 1 (Putinar’s Positivestellensatz [68], see also Theorem 5.1 of [65]) Consider the basic (semi)algebraic sets
\[ G := \{ x \in \mathbb{R}^n : g_1(x) \geq 0, \ldots, g_m(x) \geq 0 \}, \]
\[ H := \{ x \in \mathbb{R}^n : h_1(x) = 0, \ldots, h_n(x) = 0 \}, \]
where \( g_i, h_j \in \mathbb{R}[x]_n \), and \( G \) satisfies the Archimedean property, i.e., there exists an \( R > 0 \) and \( \alpha_0, \ldots, \alpha_n \in \Sigma[x]_n \) such that \( R - \sum_{i=1}^n x_i^2 = \alpha_0(x) + \sum_{i=1}^m \alpha_i(x)g_i(x) \).

Then, for any \( f \in \mathbb{R}[x]_{n,2d} \), the implication
\[ x \in G \cap H \implies f(x) \geq 0 \]
holds if and only if there exist SOS polynomials \( \alpha_0, \ldots, \alpha_m \in \Sigma[x]_{n,2d} \) and real polynomials \( \beta_1, \ldots, \beta_n \in \mathbb{R}[x]_{n,2d} \) such that
\[ f(x) = \alpha_0(x) + \sum_{i=1}^m \alpha_i(x)g_i(x) + \sum_{j=1}^n \beta_j(x)h_j(x). \]

Remarkably, the Positivestellensatz implies that if we set the degree of \( \alpha_0 \) to be zero, then a wide subset of the set of polynomial laws consistent with a set of equality-constrained polynomials can be searched over via linear optimization. Indeed, this subset is sufficiently expressive that, as we demonstrate in our numerical results, it allows us to recover Kepler’s third law and Einstein’s dilation law axiomatically. Moreover, the set of polynomial natural laws consistent with polynomial inequalities can be searched via semidefinite or sum-of-squares optimization.

We close this section by remarking that one could develop an alternative version of the Positivestellensatz with only inequality constraints, by expressing each equality via two inequalities. However, this increases the number of decision variables in the optimization problems generated by the Positivestellensatz and solved in this paper, and thus decreases the tractability of these optimization problems; see also [18]. Accordingly, we treat equality and inequality constraints separately for convenience throughout the paper.

1.4 Structure

The rest of the paper is organized as follows: in Section 2, we describe \textsc{AI-Hilbert}, the scientific discovery system proposed in this paper, and present results from applying \textsc{AI-Hilbert} in different discovery contexts. We argue that it presents an exciting new approach to scientific discovery, by demonstrating that it can rediscover the Hagen-Poiseuille Equation, Einstein’s Relativistic Time Dilation Law, Kepler’s Third Law, the Radiated Gravitational Wave Power Equation, and the Bell Inequalities. In Section 3, we summarize our conclusions and discuss the limitations of and future research opportunities arising from this work.

2 Discovering Scientific Formulae Via Polynomial Optimization

In this section, we formally introduce \textsc{AI-Hilbert}, our scientific discovery system, and illustrate its capacity to rediscover five famous scientific laws. First, in Section 2.1, we define a new notion of the distance between a polynomial and a (possibly inconsistent or incomplete) set of background knowledge. Second, in Section 2.2, we formalize our approach as a polynomial optimization problem. Third, in Section 2.3, we specialize our approach to problem settings where a scientist has access to a complete set of background theory and no experimental data. Next, in Section 2.4, we derive the Hagen-Poiseuille Equation given a complete set of background theory and no experimental data, to demonstrate the ability of our approach to derive new polynomial expressions from background theory. Next, in Section 2.5, we derive Einstein’s Relativistic Time Dilation Law. Next, in Section 2.6, we derive Kepler’s Third Law of Planetary Motion, given a complete set of background knowledge.

\footnote{This assumption is stronger than the compactness assumption on \( G \) found for instance in the Positivestellensatz of [77], but is typically not restrictive in practice, as one could assume that \( g_i(x) = R - \sum_{i=1}^m x_i^2 \) for some constant \( R \). Moreover, it is arguably more tractable-it avoids the need to explicitly consider products of the form \( g_i g_j \) in the decomposition, although we may require SOS polynomials of a higher degree to generate a valid certificate.}
plus an incorrect candidate formula and a limited amount of scientific data from a binary star system. Further, in Section 2.7, we derive the Gravitation Power Wave Equation, and finally, in Section 2.8 the Bell Inequalities. In conclusion, we can derive five renowned polynomial laws, which state-of-the-art works on automated scientific discovery find very challenging to derive.

To illustrate the strength of our system, Table 1 compares AI-Hilbert with four state-of-the-art approaches in terms of their ability to recover two of the scientific laws studied in this section using experimental data, according to the literature. We denote a law successfully (unsuccessfully) recovered by a method with a "✓" ("✗"), and provide a reference to where this method was benchmarked on this problem. We do not report on the three laws studied in this section which we recover without using any experimental data, as all four state-of-the-art methods that AI-Hilbert is benchmarked against in Table 1 require experimental data to make any discoveries. We observe that our approach successfully recovers both scientific formulae given (potentially corrupted) background axioms and (a potentially limited) amount of experimental data, while this is not true for the other approaches.

Table 1: Comparison of AI-Hilbert with state-of-the-art discovery methods in terms of ability to recover scientific laws from background theory and experimental data. AI-Hilbert recovers both scientific laws by combining experimental data and background theory via polynomial optimization, while state-of-the-art approaches fail at discovering both. The symbol * denotes up to a constant approximation.

<table>
<thead>
<tr>
<th></th>
<th>Kepler's Third Law</th>
<th>Relativistic Time Dilation</th>
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<tbody>
<tr>
<td>AI-Feynman [81]</td>
<td>✗</td>
<td>✗ [25, S.Tab. 13]</td>
</tr>
<tr>
<td>AI-Descartes [25]</td>
<td>✓ [25, Tab. 1]</td>
<td>✗ [25, Tab. 1]</td>
</tr>
<tr>
<td>PySR [29]</td>
<td>✓ [25, S.Tab. 10]</td>
<td>✗ [25, S.Tab. 13]</td>
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<tr>
<td>BMS [44]</td>
<td>✗</td>
<td>✗ [25, S.Tab. 13]</td>
</tr>
<tr>
<td>AI-Hilbert</td>
<td>✓ (Sec. 2.6)</td>
<td>✓ (Sec. 2.5)</td>
</tr>
</tbody>
</table>

Note that, except where explicitly stated otherwise, all numerical experiments described in this section were conducted on a 2.9 GHz 6-core Intel® i9 processor using Julia version 1.7.2 and Gurobi version 9.5.1.

2.1 Distance to Background Theory and Model Complexity

In the investigation of scientific phenomena, researchers have access to a collection of experimental measurements and a set of polynomial equalities and inequalities (axioms), which they believe to be true with high confidence. From these axioms and measurements, they aim to deduce a new law of nature that explains their experiment, which includes one or more dependent variables (possibly raised to some power), some other independent variables, and excludes certain variables that either cannot be measured during the experiment or would make the formula trivial (e.g., excluding the frequency when developing a formula for the period). The simplest case of scientific discovery involves a consistent and correct set of axioms that fully characterize the problem. In this case, the previously described Positivestellensatz enables the discovery of new scientific laws via deductive reasoning, without even needing to examine any experimental data, as we argue in Section 2.3. Indeed, under an Archimedean assumption, the set of all valid scientific laws corresponds precisely to the preprime (see [27] for a definition) generated by our axioms [68], and searching for the simplest polynomial version of a law which features a given dependent variable corresponds to solving an easy linear or semidefinite feasibility problem.

Unfortunately, in scientific discovery contexts, the set of axioms is often inconsistent (meaning that there are no values of \( x \in \mathbb{R}^n \) that satisfy all laws simultaneously), or incomplete (meaning the axioms do not “span” the space of all derivable polynomials; we provide a formal definition later in this section). Therefore, we require a notion of a distance between a body of background theory (which, in our case, consists of a set of polynomial equalities and inequalities) and a polynomial. We now establish this definition, treating the inconsistent and incomplete cases separately. We remark that [18, 85] propose related notions of the distance between (a) a point and a variety defined by a set of equality constraints, and (b) the distance between two semialgebraic sets via their Hausdorff distance. However, to our knowledge, the distance metrics proposed in this paper have not previously been proposed in the literature.
Incomplete Case: Suppose we are given a set of axioms defined by the basic semi-algebraic sets:

\[ \mathcal{G} := \{ x \in \mathbb{R}^n : g_1(x) \geq 0, \ldots, g_m(x) \geq 0 \}, \]
\[ \mathcal{H} := \{ x \in \mathbb{R}^n : h_1(x) = 0, \ldots, h_n(x) = 0 \}, \]

where \( \mathcal{G} \) satisfies the previously defined Archimedean property (see Theorem 1) with constant \( R \), and the axioms are not inconsistent, meaning that \( \mathcal{G} \cap \mathcal{H} \neq \emptyset \). Then, a natural notion of distance is the \( \ell_2 \) coefficient distance \( d^e \) between \( f \) and \( \mathcal{G} \cap \mathcal{H} \), which is given by:

\[
d^e(f, \mathcal{G} \cap \mathcal{H}) := \min_{\alpha_0, \ldots, \alpha_m \in \Sigma_{n,2d}[x], \beta_1, \ldots, \beta_n \in \mathbb{R}_{\geq 0}} \| \text{Coefficients} \left( f - \alpha_0 - \sum_{i=1}^m \alpha_i g_i - \sum_{j=1}^n \beta_j h_j \right) \|_2,
\]

where Coefficients(·) is a linear operator which maps a polynomial’s coefficients to a vector. It follows directly from Putinar’s Positivestellensatz that \( d(f, \mathcal{G} \cap \mathcal{H}) = 0 \) if and only if \( f \) is derivable from \( \mathcal{G} \cap \mathcal{H} \). We remark that this distance has a geometric interpretation as the distance between a polynomial \( f \) and its projection onto the algebraic variety generated by \( \mathcal{G} \cap \mathcal{H} \). Moreover, by norm equivalence, this is equivalent to the Hausdorff distance [85] between \( f \) and \( \mathcal{G} \cap \mathcal{H} \).

With the above definition of \( d^e \), and the fact that \( \mathcal{G} \cap \mathcal{H} \neq \emptyset \), we say that \( \mathcal{G} \cap \mathcal{H} \) is an inconsistent set of axioms if there does not exist a polynomial \( p \) with a non-zero coefficient on a monomial which involves \( x_i \) raised to a non-zero power, such that \( d^e(f, \mathcal{G} \cap \mathcal{H}) = 0 \).

Inconsistent Case: Suppose now that we have an inconsistent set of axioms defined by the basic semi-algebraic sets

\[ \mathcal{G} := \{ x \in \mathbb{R}^n : g_1(x) \geq 0, \ldots, g_m(x) \geq 0 \}, \]
\[ \mathcal{H} := \{ x \in \mathbb{R}^n : h_1(x) = 0, \ldots, h_n(x) = 0 \}, \]

where \( \mathcal{G} \cap \mathcal{H} = \emptyset \), because the axioms are inconsistent.

Then, a very natural approach to scientific discovery is to assume that a subset of the equalities and inequalities constitute correct scientific axioms, while the remaining polynomials are scientifically invalid (or invalid in a specific context, e.g., micro vs. macro-scale). In line with the sparse regression literature [c.f. 15] and related work on discovering nonlinear dynamics [14], we assume that scientific discoveries can be made using at most \( k \) correct scientific laws and define the distance between the scientific law and the problem data as a best subset selection problem. Specifically, we introduce binary variables \( z_i \) to denote whether the \( i \)th law is consistent, and require that \( \alpha_i = 0 \) if \( z_i = 0 \) and \( \sum_i z_i \leq k \) for a sparsity budget \( k \). Furthermore, we allow a non-zero \( \ell_2 \) distance between the scientific law \( f \) and the reduced background theory, but penalize this distance in the objective. This gives the following notion of distance between a scientific law \( f \) and a body of background knowledge \( \mathcal{G} \cap \mathcal{H} \):

\[
d^e(f, \mathcal{G} \cap \mathcal{H}) := \min \left\| \text{Coefficients} \left( f - \alpha_0 - \sum_{i=1}^m \alpha_i g_i - \sum_{j=1}^n \beta_j h_j \right) \right\|_2, \quad \text{s.t.}
\]

\[
\alpha_i = 0 \text{ if } z_i = 0, \forall i \in \{0, \ldots, m\},
\beta_j = 0 \text{ if } y_j = 0, \forall j \in \{1, \ldots, n\},
\sum_{i=0}^m z_i + \sum_{j=1}^n y_m \leq k, \alpha_0, \ldots, \alpha_m \in \Sigma_{n,2d}[x],
\end{align*}

\[
\begin{array}{c}
z_0 \ldots z_m \in \{0, 1\}, \beta_1, \ldots, \beta_n \in \mathbb{R}_{\geq 0}, y_1, \ldots, y_n \in \{0, 1\}.
\end{array}
\]

It follows directly from the Positivestellensatz that \( d = 0 \) if and only if \( f \) can be derived from \( \mathcal{G} \cap \mathcal{H} \). If \( k = m + n \), then we certainly have \( d^e = 0 \), since the overall system of polynomials is inconsistent and the sum-of-squares proof system can deduce that \( "-1 \geq 0" \) from inconsistent proof systems, from which it can claim a distance of 0. However, by treating \( k \) as a hyper-parameter and including the quality of the law on experimental data as part of the optimization problem (see Section 2.2), scientific discoveries can be made from inconsistent axioms by incentivizing solvers to set \( z_i = 0 \) for inconsistent axioms \( i \). Provided there is a sufficiently high penalty cost on poorly explaining scientific data via the derived law, our optimization problem should prefer a subset of correct axioms with a non-zero distance \( d^e \) to the derived polynomial over a set of inconsistent axioms which gives a distance \( d^e = 0 \) to any polynomial.
2.2 Overall Problem Setting

We now describe the optimization problem solved by AI-Hilbert to discover scientific laws from background theory and experimental data. Formally, we are given a set of noisy measurements \( D = \{x_i\}_{i=1}^m \) from an experiment, where \( x_i \in \mathbb{R}^n \) is a vector which encodes both dependent and independent variables, and a (possibly inconsistent or incomplete) list of axioms defined by the basic closed (semi)algebraic sets \( G := \{ g_1(x) \geq 0, \ldots, g_m(x) \geq 0 \}, \mathcal{H} := \{ h_1(x) = 0, \ldots, h_n(x) = 0 \} \), where \( g_i(x) \in \Sigma(x)_{n,2d}, h_i(x) \in \mathbb{R}[x]_{n,2d} \) are polynomials representing existing laws of nature.

Given this information, our automated scientific discovery procedure (which we term AI-Hilbert) aims to discover an unknown polynomial model \( q \), which contains one or more dependent variables raised to some power within the expression (to avoid the trivial solution \( q = 0 \)), is approximately consistent with our axioms \( \mathcal{H} \) (resp. \( G \) and \( \mathcal{H} \)—meaning \( d^c \) is small), explains our experimental data well (meaning \( \| q(x_i) \| \) is small for each data point \( i \)), and is of low complexity.

Letting \( x_1 \) denote the dependent variable which we would like to ensure appears in our scientific law, and \( x_2, \ldots, x_l \) denote the independent variables which we would like to ensure appear in our scientific law, this can be formulated as solving the following polynomial optimization problem:

\[
\begin{align*}
\min_{q \in \mathbb{R}_{n,2d}} & \quad \sum_{x_i \in D} \| q(x_i) \| + \lambda \cdot d^c(q, G \cap \mathcal{H}) \\
\text{s.t.} & \quad \sum_{i:n_i \geq 1} a_i = 1 : q(x) = \sum_i a_i x_1^{\alpha_1} x_2^{\alpha_2} \ldots x_n^{\alpha_n}, \\
& \quad a_i = 0 \forall i : \sum_{t=i+1}^n \alpha_t \geq 1, \ q(x) = \sum_i a_i x_1^{\alpha_1} x_2^{\alpha_2} \ldots x_n^{\alpha_n},
\end{align*}
\]

where \( d^c \) is the optimal value of an inner minimization problem defined in the previous section, \( \lambda > 0 \) is a hyperparameter that balances the relative importance of model fidelity to the data against model fidelity to a set of axioms, the first constraint ensures that \( x_1 \), our dependent variable of interest, appears in \( q \), and the second constraint ensures that we do not include any symbolic variables which are part of our background theory but would render \( q \) uninteresting if they appeared in \( q \) (e.g., the frequency of revolution when aiming to explain the orbital period). Note that the formulation of the first constraint implicitly controls the complexity of the scientific discovery problem via the degree of the Positivestellensatz certificate: a smaller bound on the maximum allowable degree in the certificate yields a more tractable optimization problem but a less expressive family of certificates to search over, which ultimately entails a trade-off that needs to be made by the user. Indeed, this trade-off has been formally characterized by Lasserre [56], who showed that every non-negative polynomial is approximable to any desired accuracy by a sequence of sum-of-squares polynomials, with a trade-off between the degree of the SOS polynomial and the quality of the approximation.

We might also choose to exclude certain variables from our formula \( q \) if they appear in our background information but not our experimental data, e.g., if observing this variable would be prohibitively expensive or even physically impossible due to a physical law such as Heisenberg’s uncertainty principle [c.f. 84]. Note that in certain problem settings, we constraint \( d^c = 0 \), rather than penalizing the size of \( d^c \) in the objective.

After solving Problem (3), one of two possibilities occurs. Either the distance between \( q \) and our background information is 0, or the Positivestellensatz provides a non-zero polynomial

\[
\begin{align*}
r(x) := & \quad f(x) - \sigma_0(x) - \sum_{i=1}^m \sigma_i(x) g_i(x) - \sum_{j=1}^n \beta_j(x) h_j(x)
\end{align*}
\]

which defines the discrepancy between our derived physical law and its projection onto our background information. In this sense, solving Problem (3) also provides information about the inverse problem of identifying a complete set of axioms that explain \( q \).

In either case, it follows from the Positivestellensatz (Theorem 1) that solving Problem (3) for different hyperparameter values and different bounds on the degree of \( q \) eventually yields polynomials that explain the experimental data well and are approximately derivable from background theory.

We close this section with two remarks on the generality and complexity of AI-Hilbert.
Implicit and Explicit Symbolic Discovery: AI-Hilbert takes a philosophically different approach to symbolic discovery than most prior works (e.g., [30, 25, 76]). Namely, prior works typically aim to identify an unknown symbolic model \( f \in \mathbb{R}^{n,2d} \) of the form \( f(x_i) = y_i \) for a set of independent variables of interest \( x_i \in \mathbb{R}^n \) and a dependent variable \( y_i \in \mathbb{R} \), while we take a more general approach of aiming to uncover an implicit polynomial function \( q \) which links the dependent and independent variables.

We search for implicit functions for two reasons. First, many scientific formulae of practical interest admit implicit representations as polynomials, but their explicit formulations (with a dependent variable as a function of the independent variables) are not polynomials [c.f. 2], e.g., due to square root terms. For instance, Kepler’s third law of planetary motion is of this form. Second, as originally proven by Artin [8] to partially resolve Hilbert’s 17th problem [c.f. 47], an arbitrary non-negative polynomial can be represented as a sum of squares of rational functions. Therefore, by multiplying by the denominator in Artin’s representation [8], the set of implicit representations of natural laws becomes a viable and computationally affordable space to search over.

Complexity of Scientific Discovery: Observe that, if the degree of our new scientific law \( q \) is fixed and the degree of the polynomial multipliers in the definition in \( d \) is also fixed, then Problem (3) can be solved in polynomial time\(^4\) with a consistent set of axioms (resp. nondeterministic polynomial time with an inconsistent set of axioms). This is because solving Problem (3) with a fixed degree and a consistent set of axioms corresponds to solving a semidefinite optimization problem of a polynomial size, which can be solved in polynomial time (assuming that a constraint qualification such as Slater’s condition holds) [62]. Moreover, although solving Problem (3) with a fixed degree and an inconsistent set of axioms corresponds to solving a mixed-integer semidefinite optimization problem, which is NP-hard, recent evidence [32] shows that integer optimization problems can be solved in polynomial time with high probability. This suggests that Problem (3) may also be solvable in polynomial time with high probability. However, if the degree of \( q \) is unbounded then, to the best of our knowledge, no existing algorithm solves Problem (3) in polynomial time, which suggests that searching for scientific laws of a fixed degree and iteratively increasing the degree of the polynomial laws searched over, in accordance with Occam’s Razor, is a key aspect of our approach.

2.3 Discovering Scientific Laws From Background Theory Alone

Suppose that \( G \cap H \) constitutes a complete set of axioms that fully describes our physical system. Then, any polynomial which contains our dependent variable \( x_i \) and is derivable from our system of axioms is a valid physical law. Therefore, we need not even collect any experimental data, and we can solve the following feasibility problem to discover a valid law:

\[
\exists \quad q(x) \in \Sigma[x]_{n,2d} \\
s.t. \quad q(x) = g_0(x) + \sum_{j=1}^{m} \alpha_i(x)g_i(x) + \sum_{j=1}^{n} \beta_j(x)h_j(x), \\
\sum_{i: \alpha_i \geq 1} a_i = 1 : q(x) = \sum_i a_i x_1^{\alpha_1} x_2^{\alpha_2} \ldots x_n^{\alpha_n}, \\
a_i = 0 \forall i : \sum_{i=1}^{n} \alpha_i \geq 1, \quad q(x) = \sum_i a_i x_1^{\alpha_1} x_2^{\alpha_2} \ldots x_n^{\alpha_n}, \\
q(x) \in \mathbb{R}[x]_{n,2d}, \alpha_i(x) \in \Sigma[x]_{n,2d}, \beta_j(x) \in \mathbb{R}[x]_{n,2d},
\]

where the second and third constraints ensure that we include the dependent variable \( x_1 \) in our formula \( q \) and rule out the trivial solution \( q = 0 \), and exclude any solutions \( q \) which contain uninteresting symbolic variables respectively.

\(^4\)Under the real number complexity model, and under the bit number complexity model under some mild regularity conditions on the semidefinite optimization problems that arise from our sum-of-squares optimization problems. Note that, under the bit complexity model, semidefinite optimization problems cannot always be solved in polynomial time due to the existence of ill-behaved semidefinite problems where all feasible solutions are of doubly exponential size. We refer to Ramana [69] or Laurent and Rendl [58] for a complete characterization of the complexity of semidefinite optimization.
Note that if we do not have any inequality constraints in either problem, then we may replace $q \in \Sigma_{n,2d}$ with $q \in \mathbb{R}_{n,2d}$ and obtain a linear optimization problem.

### 2.4 Deriving the Hagen-Poiseuille Equation

We consider the problem of deriving the velocity of laminar fluid flow through a circular pipe, from a simplified version of the Navier-Stokes equations, an assumption that the velocity can be modeled by a degree-two polynomial in the radius of the pipe, and a no-slip boundary condition. Letting $u$ model the velocity in the pipe, $r$ denote the distance from the center of the pipe, $R$ denote the width of the pipe, $\Delta p$ denote the pressure differential throughout the pipe, $L$ denote the length of the pipe, and $\mu$ denote the viscosity of the fluid, we have the following velocity profile for $r \in [0, R]$:

$$u(r) = \frac{\Delta p}{4L\mu}(r^2 - R^2).$$

We now derive this law axiomatically, by assuming that the velocity profile can be modeled by a symmetric polynomial, and iteratively increasing the degree of the polynomial until we obtain a polynomial solution, consistent with Occam’s Razor. Accordingly, we set the degree of $u$ to be two and add together the following terms with appropriate polynomial multipliers:

1. $u = c_0 + c_2r^2$,
2. $\mu \frac{\partial}{\partial r} (r \frac{\partial}{\partial r} u) - r \frac{dp}{dx} = 0$,
3. $c_0 + c_2R^2 = 0$,
4. $L \frac{dp}{dx} = -\Delta p$,

where Equation (6) posits a quadratic velocity profile in $r$, Equation (7) imposes a simplified version of the Navier-Stokes equations in spherical coordinates, Equation (8) imposes a no-slip boundary condition on the velocity profile of the form $u(R) = 0$, and Equation (9) posits that the pressure gradient throughout the pipe is constant. Further, we treat $c_0, c_2, \frac{dp}{dx}$ as symbolic variables which should not appear in our final expression, and use the 

differentiate

function in Julia to symbolically differentiate $u = c_0 + c_2r^2$ with respect to $r$ in Equation (7) before solving the problem, giving the equivalent expression $4c_2r\mu = r \frac{dp}{dx}$. Solving Problem (4) with $u$ as the dependent variable, and searching for a formula involving $u, r, L, \mu, \Delta p$ with polynomial multipliers of degree at most 3 in each variable and an overall degree of at most 6 then yields the expression:

$$4rL\mu u = r\Delta p(R^2 - r^2),$$

which confirms the result. The associated polynomial multipliers for Equations (6)–(9) are:

- $4rL\mu$,
- $r^2L - LR^2$,
- $4rL\mu$,
- $r^3 - rR^2$.

### 2.5 Deriving Einstein’s Relativistic Time Dilation Law

Next, we consider the problem of deriving Einstein’s relativistic time dilation formula from a complete set of background knowledge plus an inconsistent “Newtonian” axiom, which posits that light behaves like a mechanical object. We distinguish between these axioms using data on the relationship between the velocity of a light clock and the relative passage of time, as measured experimentally by Chou et al. [23] and stated explicitly in the work of Cornelio et al. [25, Tab. 6].

Einstein’s law describes the relationship between how two observers in relative motion to each other observe time, and demonstrates that observers moving at different speeds experience time differently. Indeed, letting the constant $c$ denote the speed of light, the frequency $f$ of a clock moving at a speed $v$ is related to the frequency $f_0$ of a stationary clock via

$$\frac{f - f_0}{f_0} = \sqrt{1 - \frac{v^2}{c^2}} - 1.$$
We now derive this law axiomatically, by adding together the following five axioms with appropriate polynomial multipliers:

\[ c dt_0 - 2d = 0, \]  
\[ c dt - 2L = 0, \]  
\[ 4L^2 + 4d^2 - v^2 dt^2 = 0, \]  
\[ f dt_0 = 1, \]  
\[ f dt = 1, \]

plus the following (inconsistent) Newtonian axiom:

\[ dt^2 (v^2 + c^2) - 4L^2 = 0, \]

where \( dt_0 \) denotes the time required for a light to travel between two stationary mirrors separated by a distance \( d \), and \( dt \) denotes the time required for light to travel between two similar mirrors moving at velocity \( v \), giving a distance between the mirrors of \( L \).

These axioms have the following meaning: Equation (11) relates the time required for light to travel between two stationary mirrors to their distance, Equation (12) similarly relates the time required for light to travel between two mirrors in motion to the effective distance \( L \), Equation (13) relates the physical distance between the mirrors \( d \) to their effective distance \( L \) induced by the motion \( v \) via the Pythagorean theorem, and Equations (14)-(15) relate frequencies and periods. Finally, Equation (16) assumes (incorrectly) that light behaves like other mechanical objects, meaning if it is emitted orthogonally from an object traveling at velocity \( v \), then it has velocity \( \sqrt{v^2 + c^2} \).

By solving Problem (3) with a cardinality constraint that we include at most \( k = 5 \) axioms (corresponding to the exclusion of one axiom), a constraint that we must exclude either Equation (12) or Equation (16), \( f \) as the dependent variable, experimental data in \( f, f_0, v, c \) to separate the valid and invalid axioms (obtained from [25, Tab. 6] by setting \( f_0 = 1 \) to transform the data in \( (f - f_0)/f_0 \) into data in \( f, f_0 \), \( f_0, v, c \) as variables that we would like to appear in our polynomial formula \( q(x) = 0 \forall x \in G \cap H \), and searching the set of polynomial multipliers of degree at most 2 in each term, we obtain the law:

\[ -c^2 f_0^2 + c^2 f^2 + f_0^2 v^2 = 0, \]

in 6.04 seconds using Gurobi version 9.5.1. Moreover, we immediately recognize this as a restatement of Einstein's law. This shows that the correctness of Einstein's law can be verified by multiplying the (consistent relativistic set of) axioms by the following polynomials:

\[ 2df_0^2 f^2 + cf_0 f^2, \]  
\[ -cf_0^3 f - 2f_0^2 f^2 L, \]  
\[ -f_0^2 f^2, \]  
\[ -2cf_0 f^2 - c^2 f^2, \]  
\[ c^2 df_0 f - dt f_0^2 f v^2 + c^2 f_0^2 - f_0^2 v^2. \]

Moreover, it verifies that relativistic axioms, particularly the axiom \( c dt = 2L \), fit the light clock data of [23] better than Newtonian axioms, because, by the definition of Problem (3), AI-Hilbert selects the combination of \( k = 5 \) axioms with the lowest discrepancy between the discovered scientific formula and the experimental data.

2.6 Deriving Kepler’s Third Law of Planetary Motion

In this section, we consider the problem of deriving Kepler’s third law of planetary motion from a complete set of background knowledge plus an incorrect candidate formula, which is to be screened out using experimental data. To our knowledge, this paper is the first work that addresses this particularly challenging problem setting. Indeed, none of the approaches to scientific discovery reviewed in the introduction successfully distinguish between correct and incorrect axioms via experimental data by solving a single optimization problem. The primary motivation for this experiment is to demonstrate that AI-Hilbert provides a system for determining whether, given a set of background theory and experimental data, it is possible to improve upon a state-of-the-art scientific formula using background theory and experimental data.
Kepler’s law describes the relationship between the distance between two bodies, e.g., the sun and a planet, and their orbital periods and takes the form:

$$p = \sqrt[3]{\frac{4\pi^2(d_1 + d_2)^3}{G(m_1 + m_2)}}, \quad (23)$$

where $G = 6.6743 \times 10^{-11} \text{m}^3 \text{kg}^{-1} \text{s}^{-2}$ is the universal gravitational constant, $m_1$ and $m_2$ are the masses of the two bodies, $d_1$ and $d_2$ are the respective distances between $m_1$, $m_2$ and their common center of mass, and $p$ is the orbital period. We now derive this law axiomatically by adding together the following five axioms with appropriate polynomial multipliers:

$$d_1 m_1 - d_2 m_2 = 0, \quad (24)$$

$$(d_1 + d_2)^2 F_g - G m_1 m_2 = 0, \quad (25)$$

$$F_c - m_2 d_2 w^2 = 0, \quad (26)$$

$$F_c - F_g = 0, \quad (27)$$

$$w p = 1, \quad (28)$$

plus the following (incorrect) candidate formula proposed by Cornelio et al. [25] for the exoplanet dataset (where the mass of the planets can be discarded as negligible when added to the much bigger mass of the star):

$$p^2 m_1 - 0.1319(d_1 + d_2)^3 = 0. \quad (29)$$

Here $F_g$ and $F_c$ denote the gravitational and centrifugal forces in the system, and $w$ denotes the frequency of revolution. Note that we replaced $p$ with $2\pi p$ in our definition of revolution period in order that $\pi$ does not feature in our equations; we divide $p$ by $2\pi$ after deriving Kepler’s law.

The above axioms have the following meaning: Equation (24) defines the center of mass of the dynamical system, Equation (25) defines the gravitational force of the system, Equation (26) defines the centrifugal force of the system, Equation (27) matches the centrifugal and dynamical forces, and Equation (28) relates the frequency and the period of revolution.

Accordingly, we solve our polynomial optimization problem under a sparsity constraint that at most $k = 5$ axioms can be used to derive our model, a constraint that $d^e = 0$ (meaning we need not specify the hyperparameter $\lambda$ in (3)), by minimizing the objective

$$\sum_{i=1}^n |q(x_i)|,$$

where $q$ is our implicit polynomial and $\{x_i\}_{i=1}^n$ is a set of observations of the revolution period of binary stars stated in [25, Tab. 5]. Searching over the set of degree-five polynomials $q$ derivable using degree six certificates then yields a mixed-integer linear optimization problem in 18968 continuous and 6 discrete variables, with the solution:

$$m_1 m_2 G p^2 - m_1 d_1 d_2^2 - m_2 d_1^2 d_2 - 2 m_2 d_1 d_2^2 = 0, \quad (30)$$

which is precisely Kepler’s third law. The validity of this equation can be verified by adding together our axioms with the weights:

$$-d_2^2 p^2 w^2, \quad (31)$$

$$-p^2, \quad (32)$$

$$d_1^2 p^2 + 2 d_1 d_2 p^2 + d_2^2 p^2, \quad (33)$$

$$d_1^2 p^2 + 2 d_1 d_2 p^2 + d_2^2 p^2, \quad (34)$$

$$m_1 d_1 d_2^2 w + m_2 d_1^2 d_2 w + 2 m_2 d_1 d_2^2 w + m_1 d_1 d_2^2 + m_2 d_1^2 d_2 + 2 m_2 d_1 d_2^2, \quad (35)$$

as previously summarized in Figure 1. This is significant, because existing works on symbolic regression and scientific discovery [see, e.g., 81, 44] often struggle to derive Kepler’s law, even given observational data. Indeed, our approach is also more scalable than deriving Kepler’s law manually; Johannes Kepler spent four years laboriously analyzing stellar data to arrive at his law [74].
2.7 Radiation Gravitational Wave Power

We now consider the problem of deriving the power radiated from gravitational waves emitted by two point masses orbiting their common center of gravity in a Keplerian orbit, as originally derived by Peters and Mathews [67] and verified for binary star systems by Hulse and Taylor [49]. Specifically, Peters and Mathews [67] showed that the average power generated by such a system is:

\[ P = \frac{-32G^4}{5c^3\rho_0}(m_1m_2)^2(m_1 + m_2), \]

where \( P \) is the (average) power of the wave, \( G = 6.6743 \times 10^{-11} \text{ m}^3 \text{ kg}^{-1} \text{ s}^{-2} \) is the universal gravitational constant, \( c \) is the speed of light, \( m_1, m_2 \) are the masses of the objects, and we assume that the two objects orbit a constant distance of \( r \) away from each other. Note that this equation is one of the twenty so-called bonus laws considered in the work introducing AI-Feynman [81], and notably, is one of only two such laws that neither AI-Feynman nor Eureqa [34] were able to derive. We now derive this law axiomatically, by combining the following axioms with appropriate multipliers:

\[ \omega^2 r^3 - G(m_1 + m_2) = 0, \quad (36) \]

\[ 5(m_1 + m_2)^2 c^5 P + G tr \left( \frac{d^3}{dt^3} \left( m_1 m_2 r^2 \left( \begin{array}{ccc} x^2 - \frac{1}{3} & xy & 0 \\ xy & y^2 - \frac{1}{3} & 0 \\ 0 & 0 & -\frac{1}{3} \end{array} \right) \right) \right) = 0, \quad (37) \]

where we make the variable substitution \( x = \cos \phi, y = \sin \phi \), and manually define the derivative of a bivariate degree-two trigonometric polynomial in \( \phi = \phi_0 + \omega t \) in \((x, y)\) in terms of \((x, y, \omega)\) as the following linear operator:

\[
\frac{d}{dt} \left( \begin{array}{c} \sin \phi \\ \cos \phi \end{array} \right) ^{\top} \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \left( \begin{array}{c} \sin \phi \\ \cos \phi \end{array} \right) = \omega \left( \begin{array}{c} \sin \phi \\ \cos \phi \end{array} \right) ^{\top} \begin{pmatrix} a_{12} + a_{21} & a_{11} - a_{22} \\ a_{11} - a_{22} & -a_{12} - a_{21} \end{pmatrix} \left( \begin{array}{c} \sin \phi \\ \cos \phi \end{array} \right)
\]

Note that Equation (36) is a restatement of Kepler’s previously derived third law of planetary motion, Equation (37) provides the gravitational power of a wave when the wavelength is large compared to the source dimensions, by linearizing the equations of general relativity, the third equation defines the quadruple moment tensor, and Equation (38) (which we state as \( x^2 + y^2 = 1 \) within our axioms) is a standard trigonometric identity. Solving Problem (4) with \( P \) as the dependent variable, and searching for a formula involving \( P, G, r, c, m_1, m_2 \) with polynomial multipliers of degree at most 20, and allowing each variable to be raised to a power for the variables \((P, x, y, \omega, G, r, c, m_1, m_2)\) of at most \((1, 4, 4, 4, 3, 6, 1, 5, 5)\) respectively, then yields the following equation:

\[ \frac{1}{4} P r^5 e^5 (m_1 + m_2)^2 = \frac{-8}{5} G^4 m_1^2 m_2^2 (m_1 + m_2)^3, \quad (39) \]

which verifies the result. Note that this equation is somewhat expensive to derive, owing to fact that searching over the set of degree 20 polynomial multipliers necessitates generating a large number of linear equalities, and writing these equalities to memory is both time and memory intensive. Accordingly, we solved Problem (4) using the MIT SuperCloud environment [70] with 640 GB RAM. The resulting system of linear inequalities involves 416392 candidate monomials, and takes 14368s to write the problem to memory and 6.58s to be solved by Mosek. This shows that the correctness of the universal gravitational wave equation can be confirmed via the following multipliers:

\[ -\frac{8}{5} G m_1^2 m_2^2 (\omega^4 r^6 (x^2 + y^2)^2 + \omega^2 r^3 G(m_1 + m_2) + G^2 (m_1 + m_2)^2), \quad (40) \]

\[ 1 \quad (41) \]

\[ -\frac{8}{5} \omega^4 r^6 G^2 m_1^2 m_2^2 (m_1 + m_2) (x^2 + y^2 + 1). \quad (42) \]

Finally, Figure 3 illustrates how the Positivestellensatz derives this equation, by demonstrating that (setting \( m_1 = m_2 = c = G = 1 \)), the gravitational wave equation is precisely the set of points \((\omega, r, P)\) where our axioms hold with equality.
\( \omega^2 r^3 = 2 \)
\( 20 P + 32 r^4 \omega^6 = 0 \)
\( 5 P r^5 + 64 \omega^0 = 0 \)

Figure 3: Illustration of the Positivestellensatz and its ability to recover the Radiation Gravitational Wave Power Equation in the special case where \( m_1 = m_2 = c = G = 1 \). Keeping other variables constant, the points that obey the power equation are the intersection of the points that obey Kepler’s Third Law and the points of a linearized equation from general relativity, and the wave equation is recoverable by adding these other equations with appropriate polynomial multipliers.

2.8 Bell Inequalities

We now consider the problem of deriving Bell Inequalities in quantum mechanics. Bell Inequalities [11] are well-known in physics, because they provide bounds on the correlation of measurements in any multi-particle system which obeys local realism (i.e., for which a joint probability distribution exists), that are violated experimentally, thus demonstrating that the natural world does not obey local realism. For ease of exposition, we prove a version called the GHZ inequality [42]. Namely, given random variables \( A, B, C \) which take values on \( \{ \pm 1 \} \), for any joint probability distribution describing \( A, B, C \), it follows that

\[
\mathbb{P}(A = B) + \mathbb{P}(A = C) + \mathbb{P}(B = C) \geq 1,
\]

but this bound is violated experimentally [35].

We derive this result axiomatically, using Kolmogorov’s probability axioms and the specialization of our sum-of-squares framework to linear optimization proposed in Section 2.3, which is a valid specialization because the entire problem is linear. In particular, letting \( p_{-1,1,-1} = \mathbb{P}(A = -1, B = 1, C = -1) \), deriving the largest lower bound for which this inequality holds is equivalent to solving the following linear optimization problem:

\[
\begin{align*}
\min \ p_{AB} + p_{BC} + p_{AC} \quad \text{s.t.} \quad p \in S,
\end{align*}
\]

where \( S := \{ p \geq 0, e^\top p = 1 \} \), \( p_{AB} := p_{-1,-1,-1} + p_{-1,-1,1} + p_{1,1,-1} + p_{1,1,1} \) and \( p_{AC}, p_{BC} \) are defined similarly.

We solve this problem using Gurobi and Julia, which verifies that \( \gamma = 1 \) is the largest value for which this inequality holds, and obtains the desired inequality. Moreover, the solution to its dual problem yields the certificate \( 2p_{-1,-1,-1} + 2p_{1,1,1} \geq 0 \) which verifies that 1 is indeed a valid lower bound for \( p_{AB} + p_{BC} + p_{AC} \), by adding \( e^\top p \) to the left-hand side of this certificate and 1 to the right-hand side.

To further demonstrate the generality and utility of our approach, we now derive a more challenging Bell inequality, namely the so-called I3322 inequality (c.f. [39]). Given particles \( A_1, A_2, A_3, B_1, B_2, B_3 \) which take values on \( \{ \pm 1 \} \), the inequality reveals that for any joint probabil-
ity distribution, we have:

\[
\mathbb{E}[A_1] - \mathbb{E}[A_2] + \mathbb{E}[B_1] - \mathbb{E}[B_2] - \mathbb{E}[(A_1 - A_2)(B_1 - B_2)] + \mathbb{E}[(A_1 + A_2)B_3] + \mathbb{E}[A_3(B_1 + B_2)] \leq 4.
\]

Using the same approach as previously, and defining \( p \) to be an arbitrary discrete probability measure on \( \{\pm 1\}^6 \), we verify that the smallest such upper bound which holds for each joint probability measure is 4, with the following polynomial certificate modulo \( e^T p = 1 \):

\[
4p_{1,1,1,1,1,1} + 4p_{1,2,1,1,1,1} + 8p_{2,1,1,1,1,1} + 4p_{1,2,1,2,1,1} + 8p_{1,2,2,1,1,1} + 4p_{2,2,1,1,1,1} + 8p_{2,1,2,1,1,1} + 4p_{2,2,2,1,1,1} + 4p_{1,1,1,1,2,1} + 4p_{1,2,1,1,2,1} + 4p_{2,1,1,1,2,1} + 4p_{2,2,1,1,2,1} + 8p_{1,2,1,1,2,1} + 12p_{2,1,1,1,2,1} + 8p_{1,2,1,2,1,1} + 12p_{2,1,2,1,1,1} + 8p_{2,2,1,1,1,1} + 8p_{1,1,2,2,1,1} + 12p_{1,2,1,2,2,1} + 12p_{2,1,1,2,2,1} + 4p_{1,2,2,2,2,1} + 4p_{2,2,2,2,2,1}
\]

\[
+ 4p_{1,1,2,1,1,2} + 4p_{1,2,2,1,1,2} + 4p_{2,1,2,1,1,2} + 4p_{2,2,2,1,1,2} + 4p_{1,1,1,1,2,2} + 4p_{1,2,1,1,1,2} + 8p_{1,2,1,2,1,2} + 8p_{1,2,2,1,1,2} + 8p_{2,1,1,1,2,2} + 8p_{2,1,2,2,1,2} + 4p_{2,1,1,2,2,2} + 8p_{1,2,2,1,2,2} + 4p_{2,1,1,2,2,2} + 4p_{2,1,2,2,2,2} + 4p_{2,2,1,1,2,2} + 4p_{2,2,1,2,2,2} + 4p_{2,2,2,1,2,2} + 4p_{2,2,2,2,1,2} \geq 0
\]

where an index of 1 denotes that a random variable took the value \(-1\) and an index of 2 denotes that a random variable took the value \(1\), and the random variables are indexed in the order \(A_1, A_2, A_3, B_1, B_2, B_3\).

3 Discussion and Future Developments

In this work, we proposed a new approach to scientific discovery that leverages ideas from real algebraic geometry and mixed-integer optimization to discover new scientific laws from a possibly inconsistent or incomplete set of scientific axioms and experimental data. Our approach offers a promising direction for advancing the field of automated scientific discovery and could be applied to discover new scientific laws in the future. We hope our approach serves as an exciting tool that assists the scientific community in efficiently and accurately explaining the natural world.

Inspired by the success of AI-Hilbert in rediscovering existing scientific laws, we conclude by discussing some exciting research directions that are natural extensions of this work.

Improving the Generality of AI-Hilbert: This work proposes a symbolic discovery framework that combines background theory expressible as a system of polynomial equalities and inequalities, or that can be reformulated as such a system (e.g., in a Polar coordinate system, by substituting \( x = r \cos \theta, y = r \sin \theta \) and requiring that \( x^2 + y^2 = r^2 \)). However, many scientific discovery contexts involve background theory that cannot easily be expressed via polynomial equalities and inequalities, including differential operators, integrals, and limits, among other operators. Therefore, extending AI-Hilbert to encompass these non-polynomial settings would be of interest.

We point out that several authors have already proposed extensions of the sum-of-squares paradigm beyond polynomial basis functions, and these works offer a promising starting point for performing such an extension. Namely, Löfberg and Parrilo [60] propose an extension to trigonometric basis functions, and Fawzi et al. [37] propose approximating univariate non-polynomial functions via their Gaussian quadrature and Padé approximants. Moreover, Huchette and Vielma [48] advocate modeling non-convex functions via piecewise linear approximations with strong dual bounds. Using such polynomial approximations of non-polynomial operators offers one promising path for extending AI-Hilbert to the non-polynomial setting.

Automating AI-Hilbert: The version of AI-Hilbert proposed in this paper requires hyperparameter optimization by the user, to trade-off the importance of fidelity to a model, fidelity to experimental data, and complexity of the symbolic model discovered. Therefore, one extension of this work could be to automate this hyperparameter optimization process, by automatically solving mixed-integer and semidefinite optimization problems with different bounds on the degree of the proof certificates and different weights on the relative importance of fidelity to a model and fidelity to data, and using machine learning techniques to select solutions most likely to satisfy a scientist using AI-Hilbert.
Improving the Scalability of AI-Hilbert: One limitation of our implementation of AI-Hilbert is that it relies on reformulating sum-of-squares optimization problems as semidefinite problems and solving them via primal-dual interior point methods (IPMs) [62, 63]. This arguably presents a limitation, because the Newton step in IPMs [see, e.g., 5] requires performing a memory-intensive matrix inversion operation. Indeed, this matrix inversion operation is sufficiently expensive that, in our experience, AI-Hilbert was unable to perform scientific discovery tasks with more than \( n = 15 \) variables and a constraint on the degree of the certificates searched over of \( d = 20 \) or greater (in general, runtime and memory usage is a function of both the number of symbolic variables and the degree of the proof certificates searched over).

To address this limitation and enhance the scalability of AI-Hilbert, there are at least three future directions to explore. First, one could exploit ideas related to the Newton polytope (or convex hull of the exponent vectors of a polynomial) [71] to reduce the number of monomials in the sum-of-squares decompositions developed in this paper, as discussed in detail in [18, Chap 3.3.4]. Second, one could use presolving techniques such as chordal sparsity [43, 82] or partial facial reduction [66, 86] to reduce the number of variables in the semidefinite optimization problems that arise from sum-of-squares optimization problems. Third, one could attempt to solve sum-of-squares problems without using computationally expensive interior point methods for semidefinite programs, e.g., by using a Burer-Monteiro factorization approach [22, 59] or by optimizing over a second-order cone inner approximation of the positive semidefinite cone [4].

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References


