AI Feynman: a Physics-Inspired Method for Symbolic Regression

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A core challenge for both physics and artificial intelligence (AI) is symbolic regression: finding a symbolic expression that matches data from an unknown function. Although this problem is likely to be NP-hard in principle, functions of practical interest often exhibit symmetries, separability, compositionality and other simplifying properties. In this spirit, we develop a recursive multidimensional symbolic regression algorithm that combines neural network fitting with a suite of physics-inspired techniques. We apply it to 100 equations from the Feynman Lectures on Physics, and it discovers all of them, while previous publicly available software cracks only 71; for a more difficult test set, we improve the state of the art success rate from 15% to 90%.

I. INTRODUCTION

In 1601, Johannes Kepler got access to the world’s best data tables on planetary orbits, and after 4 years and about 40 failed attempts to fit the Mars data to various ovoid shapes, he launched a scientific revolution by discovering that Mars’ orbit was an ellipse [1]. This was an example of symbolic regression: discovering a symbolic expression that accurately matches a given data set. More specifically, we are given a table of numbers, whose rows are of the form \( \{x_1,\ldots,x_n, y\} \) where \( y = f(x_1,\ldots,x_n) \), and our task is to discover the correct symbolic expression for the unknown mystery function \( f \), optionally including the complication of noise.

Growing data sets have motivated attempts to automate such regression tasks, with significant success. For the special case where the unknown function \( f \) is a linear combination of known functions of \( \{x_1,\ldots,x_n\} \), symbolic regression reduces to simply solving a system of linear equations. Linear regression (where \( f \) is simply a linear function) is ubiquitous in the scientific literature, from finance to psychology. The case where \( f \) is a linear combination of monomials in \( \{x_1,\ldots,x_n\} \) corresponds to linear regression with interaction terms, and to polynomial fitting more generally. There are countless other examples of popular regression functions that are linear combinations of known functions, ranging from Fourier expansions to wavelet transforms. Despite these successes with special cases, the general symbolic regression problem remains unsolved, and it is easy to see why: If we encode functions as strings of symbols, then the number of such strings grows exponentially with string length, so if we simply test all strings by increasing length, it may take longer than the age of our universe until we get to the function we are looking for.

This combinatorial challenge of an exponentially large search space characterizes many famous classes of problems, from codebreaking and Rubik’s cube to the natural selection problem of finding those genetic codes that produce the most evolutionarily fit organisms. This has motivated genetic algorithms [2,3] for targeted searches in exponentially large spaces, which replace the above-mentioned brute-force search by biology-inspired strategies of mutation, selection, inheritance and recombination; crudely speaking, the role of genes is played by useful symbol strings that may form part of the sought-after formula or program. Such algorithms have been successfully applied to areas ranging from design of antennas [4,5] and vehicles [6] to wireless routing [7], vehicle routing [8], robot navigation [9], code breaking [10], investment strategy [11], marketing [12], classification [13], Rubik’s cube [14], program synthesis [15] and metabolic networks [16].

The symbolic regression problem for mathematical functions (the focus of this paper) has been tackled with a variety of methods [17-19], including genetic algorithms [20-21]. By far the most successful of these is, as we will see in Section II, the genetic algorithm outlined in [22] and implemented in the commercial Eureqa software [21].

The purpose of this paper is to further improve on this state-of-the-art, using physics-inspired strategies enabled by neural networks. Our most important contribution is using neural networks to discover hidden simplicity such as symmetry or separability in the mystery data, which enables us to recursively break harder problems into simpler ones with fewer variables. The rest of this paper is organized as follows. In Section II, we present our algorithm and the six strategies that it recursively combines. In Section III, we present a test suite of regression mysteries and use it to test both Eureqa and our new algorithm, finding major improvements. In Section IV, we summarize our conclusions and discuss opportunities for further progress.

II. METHODS

Generic functions \( f(x_1,\ldots,x_n) \) are extremely complicated and near-impossible for symbolic regression to discover. However, functions appearing in physics and many other scientific applications often have some of the following simplifying properties that make them easier to discover:
FIG. 1: Schematic illustration of our AI *Feynman* algorithm. It is iterative as described in the text, with four of the steps capable of generating new mystery data sets that get sent to fresh instantiations of the algorithm which may or may not return a solution.

FIG. 2: Example: how our AI *Feynman* algorithm discovered mystery Equation 5. Given a mystery table with many examples of the gravitational force $F$ together with the 9 independent variables $G, m_1, m_2, x_1, \ldots, z_2$, this table was recursively transformed into simpler ones until the correct equation was found. First dimensional analysis generated a table of 6 dimensionless independent variables $a = m_2/m_1, \ldots, f = z_1/x_1$ and the dimensionless dependent variable $F \equiv F \div Gm_1^2/\frac{x_1^2}{z_1^2}$. Then a neural network was trained to fit this function, which revealed two translational symmetries (each eliminating one variable, by defining $g \equiv c - d$ and $h \equiv e - f$) as well as multiplicative separability, enabling the factorization $F(a, b, g, h) = G(a)H(b, g, h)$, thus splitting the problem into two simpler ones. Both $G$ and $H$ then were solved by polynomial fitting, the latter after applying one of a series of simple transformations (in this case, inversion). For many other mysteries, the final step was instead solved using brute-force symbolic search as described in the text.
1. **Units**: $f$ and the variables upon which it depends have known physical units.

2. **Low-order polynomial**: $f$ (or part thereof) is a polynomial of low degree.

3. **Compositionality**: $f$ is a composition of a small set of elementary functions, each typically taking no more than two arguments.

4. **Smoothness**: $f$ is continuous and perhaps even analytic in its domain.

5. **Symmetry**: $f$ exhibits translational, rotational or scaling symmetry with respect to some of its variables.

6. **Separability**: $f$ can be written as a sum or product of two parts with no variables in common.

The question of why these properties are common remains controversial and not fully understood [23, 24]. However, as we will see below, this does not prevent us from discovering and exploiting these properties to facilitate symbolic regression.

Property (1) enables dimensional analysis, which often transforms the problem into a simpler one with fewer independent variables. Property (2) enables polynomial fitting, which quickly solves the problem by solving a system of linear equations to determine the polynomial coefficients. Property (3) enables $f$ to be represented as a parse tree with a small number of node types, sometimes enabling $f$ or a sub-expression to be found via a brute-force search. Property (4) enables approximating $f$ using a feed forward neural network with a smooth activation function. Property (5) can be confirmed using said neural network and enables the problem to be transformed into a simpler one with one independent variable less (or even fewer for $n > 2$ rotational symmetry). Property (6) can be confirmed using said neural network and enables the independent variables to be partitioned into two disjoint sets, and the problem to be transformed into two simpler ones, each involving the variables from one of these sets.

### A. Overall Algorithm

The overall algorithm is schematically illustrated in Figure 1. It consists of a series of modules that try to exploit each of the above-mentioned properties. Like a human scientist, it tries many different strategies (modules) in turn, and if it cannot solve the full problem in one fell swoop, it tries to transform it and divide it into simpler pieces that can be tackled separately, recursively re-launching the full algorithm on each piece. Figure 2 illustrates an example of how a particular mystery data set (Newton’s law of gravitation with 9 variables) is solved. Below we describe each of these algorithm modules in turn.

### B. Dimensional Analysis

Our dimensional analysis module exploits the well-known fact that many problems in physics can be simplified by requiring the units of the two sides of an equation to match. This often transforms the problem into a simpler one with a smaller number of variables that are all dimensionless. In the best case scenario, the transformed problem involves solving for a function of zero variables, i.e., a constant. We automate dimensional analysis as follows.

Table III shows the physical units of all variables appearing in our 100 mysteries, expressed as products of the fundamental units (meter, second, kilogram, kelvin, volt) to various integer powers. We thus represent the units of each variable by a vector $\mathbf{u}$ of 5 integers as in the table. For a mystery of the form $y = f(x_1, ..., x_n)$, we define the matrix $\mathbf{M}$ whose $i$th column is the $\mathbf{u}$-vector corresponding to the variable $x_i$, and define the vector $\mathbf{b}$ as the $\mathbf{u}$-vector corresponding to $y$. We now let the vector $\mathbf{p}$ be a solution to the equation $\mathbf{M} \mathbf{p} = \mathbf{b}$ and the columns of the matrix $\mathbf{U}$ form a basis for the null space, so that $\mathbf{M} \mathbf{U} = 0$, and define a new mystery $y' = f(x'_1, ..., x'_n)$ where

$$x'_i \equiv \prod_{j=i}^{n} \frac{x_j^{U_{ij}}}{y^{U_{ij}}}, \quad y' \equiv \frac{y}{y_*}, \quad y_* \equiv \prod_{i=1}^{n} x_i^{p_i}. \quad (1)$$

By construction, the new variables $x'_i$ and $y'$ are dimensionless, and the number $n'$ of new variables is equal to the dimensionality of the null space. When $n' > 0$, we have the freedom to choose any basis we want for the null space and also to replace $\mathbf{p}$ by a vector of the form $\mathbf{p} + \mathbf{Ua}$ for any vector $\mathbf{a}$; we use this freedom to set as many elements as possible in $\mathbf{p}$ and $\mathbf{U}$ equal to zero, i.e., to make the new variables depend on as few old variables as possible. This choice is useful because it typically results in the resulting powers of the dimensionless variables being integers, making the final expression much easier to find than when the powers are fractions or irrational numbers.

### C. Polynomial Fit

Many functions $f(x_1, ..., x_n)$ in physics and other sciences either are low-order polynomials, e.g., the kinetic energy $K = \frac{m}{2}(v_x^2 + v_y^2 + v_z^2)$, or have parts that are, e.g., the denominator of the gravitational force $F = \frac{G m_1 m_2}{(x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2}$. We therefore include a module that tests if a mystery can be solved by a low-order polynomial. Our method uses the standard method of solving a system of linear equations to find the best fit polynomial coefficients. It tries fitting the mystery data to polynomials of degree 0, 1, ..., $d_{\text{max}} = 4$ and declares success if the best fitting polynomial gives r.m.s. fitting error $\leq \varepsilon_p$ (we discuss the setting of this threshold below).
TABLE I: Functions optionally included in brute force search. The following three subsets are tried in turn: "+*/<~SPLICER", "+*/<~REPLICANTS0".

| Symbol | Meaning | Arguments |
|--------|---------|-----------|
| +      | add     | 2         |
| *      | multiply| 2         |
| -      | subtract| 2         |
| /      | divide   | 2         |
| >      | increment| 1        |
| <      | decrement| 1        |
| ~      | negate   | 1         |
| 0      | 0        |
| 1      | 1        |
| R      | sqrt     | 1         |
| E      | exp      | 1         |
| P      | π        | 0         |
| L      | ln       | 1         |
| I      | invert   | 1         |
| C      | cos      | 1         |
| A      | abs      | 1         |
| N      | arcsin   | 1         |
| T      | arctan   | 1         |
| S      | sin      | 1         |

D. Brute Force

Our brute-force symbolic regression model simply tries all possible symbolic expressions within some class, in order of increasing complexity, terminating either when the maximum fitting error drops below a threshold $\epsilon_b$ or after a maximum runtime $t_{\text{max}}$ has been exceeded. Although this module alone could solve all our mysteries in principle, it would in many cases take longer than the age of our universe in practice. Our brute force method is thus typically most helpful once a mystery has been transformed/broken apart into simpler pieces by the modules described below.

We generate the expressions to try by representing them as strings of symbols, trying first all strings of length 1, then all of length 2, etc., saving time by only generating those strings that are syntactically correct. The symbols used are the independent variables as well as symbols used are the independent variables as well as sub-strings of length 1. However, if the mystery function is found to have simplifying properties, it may be possible to transform it into one or more simpler mysteries that can be more easily solved. To search for such properties, we need to be able to evaluate $f$ at points $(x_1, x_2, \ldots, x_n)$ for various constants $a$, but if a given data point has its two variables separated by $x_2 - x_1 = 1.61803$, we typically have no other examples in our data set with exactly that variable separation. To perform our tests, we thus need an accurate high-dimensional interpolation between our data point.

E. Neural-network-based tests & transformations

Even after applying the dimensional analysis, many mysteries are still too complex to be solved by the polyfit or brute force modules in a reasonable amount of time. However, if the mystery function $f(x_1, \ldots, x_n)$ can be found to have simplifying properties, it may be possible to transform it into one or more simpler mysteries that can be more easily solved. To search for such properties, we need to be able to evaluate $f$ at points $(x_1, x_2, \ldots, x_n)$ of our choosing where we typically have no data. For example, to test if a function $f$ has translational symmetry, we need to test if $f(x_1, x_2) = f(x_1 + a, x_2 + a)$ for various constants $a$, but if a given data point has its two variables separated by $x_2 - x_1 = 1.61803$, we typically have no other examples in our data set with exactly that variable separation. To perform our tests, we thus need an accurate high-dimensional interpolation between our data point.
1. Neural network training

In order to obtain such an interpolating function for a given mystery, we train a neural network to predict the output given its input. We train a feed-forward, fully connected neural network with 6 hidden layers, the first 3 having 128 neurons and the last 3 having 64 neurons. We use 80% of the mystery data as the training set and the remainder as the validation set, training for 100 epochs with a batch size of 2048. We use the r.m.s.-error loss function and the Adam optimizer was employed with a weight decay of $10^{-2}$. Softplus was used as the activation function and a learning rate of 0.005. The learning rate and momentum schedules were implemented as described in [26, 27] using the fastai package [28]. The ratio between the maximum and minimum learning rates is 20 while 10% of the iterations are used for the last part of the training cycle. For the momentum, the maximum $\beta_1$ value was 0.95 and the minimum 0.85, while $\beta_2 = 0.99$. We obtained r.m.s. validation errors between $10^{-3}f_{\text{rms}}$ and $10^{-5}f_{\text{rms}}$ across the range of tested equation, where $f_{\text{rms}}$ is the r.m.s. of the $f$-values in the dataset.

2. Translational symmetry and generalizations

We test for translational symmetry using the neural network as detailed in Algorithm 1. We first check if the $f(x_1, x_2, x_3, \ldots) = f(x_1 + a, x_2 + a, x_3, \ldots)$ to within a precision $\epsilon_{\text{sym}}$. If that is the case, then $f$ depends on $x_1$ and $x_2$ only through their difference, so we replace these two input variables by a single new variable $x'_1 \equiv x_2 - x_1$. Otherwise, we repeat this test for all pairs of input variables, and also test whether any variable pair can be replaced by its sum, product or ratio. The ratio case corresponds to scaling symmetry, where two variables can be simultaneously rescaled without changing the answer. If any of these simplifying properties is found, the resulting transformed mystery (with one fewer input variables) is iteratively passed into a fresh instantiation of our full AI Feynman symbolic regression algorithm, as illustrated in Figure 1. We choose the precision threshold $\epsilon_{\text{sym}}$ to be 7 times the neural network validation error.

3. Separability

We test for separability using the neural network as exemplified in Algorithm 2. A function is separable if it can be split into two parts with no variables in common. We test for both additive and multiplicative separability, corresponding to these two parts being added and multiplied, respectively (the logarithm of a multiplicatively separable function is additively separable).

For example, to test if a function of 2 variables is multiplicatively separable, i.e., of the form $f(x_1, x_2) = g(x_1)h(x_2)$ for some univariate functions $g$ and $h$, we first select two constants $c_1$ and $c_2$; for numerical robustness, we choose $c_i$ to be the means of all the values of $x_i$ in the mystery data set, $i = 1, 2$. We then compute the quantity

$$\Delta_{\text{sep}}(x_1, x_2) \equiv f_{\text{rms}}^{-1} \left| f(x_1, x_2) - \frac{f(x_1, c_2) f(c_1, x_2)}{f(c_1, c_2)} \right|$$

for each data point. This is a measure of non-separability, since it vanishes if $f$ is multiplicatively separable. The equation is considered separable if the r.m.s. average $\Delta_{\text{sep}}$ over the mystery data set is less than an accuracy threshold $\epsilon_{\text{sep}}$, which is chosen to be $N = 10$ times the neural network validation error.

If separability is found, we define the two new univariate mysteries $y' \equiv f(x_1, c_2)$ and $y'' \equiv f(c_1, x_2)/f(c_1, c_2)$. We pass the first one, $y'$, back to a fresh instantiations of our full AI Feynman symbolic regression algorithm and if it gets solved, we redefine $y'' \equiv y'/y'_{\text{num}}$, where $y'_{\text{num}}$ represents any multiplicative numerical constant that appears in $y'$. We then pass $y''$ back to our algorithm and if it gets solved, the final solutions is $y = y' y''/y'_{\text{num}}$. We test for additive separability analogously, simply replacing $\ast$ and $/$ by $+$ and $-$ above; also $y'_{\text{num}}$ will represent an additive numerical constant in this case. If we succeed in solving the two parts, then the full solution to the original mystery is the sum of the two parts minus the numerical constant. When there are more than two variables $x_i$, we are testing all the possible subsets of variables that can lead to separability, and proceed as above for the newly created two mysteries.

4. Setting variables equal

We also exploit the neural network to explore the effect of setting two input variables equal and attempting to solve the corresponding new mystery $y'$ with one fewer variable. We try this for all variable pairs, and if the resulting new mystery is solved, we try solving the mystery $y'' \equiv y'/y'$ that has the found solution divided out.

As an example, this technique solves the Gaussian probability distribution mystery I.6.2. After making $\theta$ and $\sigma$ equal, and dividing the initial equation by the result, we are getting rid of the denominator and the remaining part of the equation is an exponential. After taking the logarithm of this (see the below section) the resulting expression can be easily solved by the brute force method.

F. Extra Transformations

In addition, several transformations are applied to the dependent and independent variables which proved to
Meaning

Importance of accuracy relative to 10
tolerance in polynomial fit module

tolerance in brute force module after separability

tolerance for separability
tolerance for symmetry
tolerance in brute force module after separability

classification error tolerance for neural network use

tolerance in polynomial fit module

tolerance for separability

tolerance in brute force module after separability

TABLE II: Hyperparameters in our algorithm and the setting we use in this paper.

be useful for solving certain equations. Thus, for each equation, we ran the brute force and polynomial fit on a modified version of the equation in which the dependent variable was transformed by one of the following functions: square root, raise to the power of 2, log, exp, inverse, sin, cos, tan, arcsin, arccos, arctan. This reduces the number of symbols needed by the brute force by one and in certain cases it even allows the polynomial fit to solve the equation, when the brute force would otherwise fail. For example, the formula for the distance between 2 points in the 3D Euclidean space: \( \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2} \), once raised to the power of 2 becomes just a polynomial which can be easily discovered by the polynomial fit algorithm. The same transformations are also applied to the dependent variables, one at a time. In addition multiplication and division by 2 were added as transformations in this case.

It should be noted that, like most machine-learning methods, the AI Feynman algorithm has some hyperparameters that can be tuned to optimize performance on the problems at hand. They were all introduced above, but for convenience, they are also summarized in Table II.

### III. RESULTS

#### A. The Feynman Symbolic Regression Database

To facilitate quantitative testing of our and other symbolic regression algorithms, we created the Feynman Symbolic Regression Database (FSReD) and made it freely available for download\(^1\). For each regression mystery, the database contains the following:

1. **Data table**: A table of numbers, whose rows are of the form \( \{ x_1, x_2, \ldots, y \} \), where \( y = f(x_1, x_2, \ldots) \); the challenge is to discover the correct analytic expression for the mystery function \( f \).

2. **Unit table**: A table specifying the physical units of the input and output variables as 6-dimensional vectors of the form seen in Table III.

3. **Equation**: The analytic expression for the mystery function \( f \), for answer-checking.

To test an analytic regression algorithm using the database, its task is to predict \( f \) for each mystery having the data table (and optionally the unit table) as input. Of course, there are typically many symbolically different ways of expressing the same function. For example, if the mystery function \( f \) is \( (u + v)/(1 + uv/c^2) \), then the symbolically different expression \( (v + u)/(1 + vu/c^2) \) should count as a correct solution. The rule for evaluating an analytic regression method is therefore that a mystery function \( f \) is deemed correctly solved by a candidate expression \( f' \) if algebraic simplification of the expression \( f' - f \) (say, with the `Simplify` function in Mathematica or the `simplify` function in the Python `sympy` package) produces the symbol “0”.

In order to sample equations from a broad range of physics areas, the database is generated using 100 equations from the seminal *Feynman Lectures on Physics* [29–31], a challenging three-volume course covering classical mechanics, electromagnetism and quantum mechanics as well as a selection of other core physics topics; we prioritized the most complex equations, excluding ones involving derivatives or integrals. The equations are listed in tables [IV] and [V] and can be seen to involve between 1 and 9 independent variables as well as the elementary functions \(+, -, *, /, \sqrt{\text{a}}, \exp, \log, \sin, \cos, \arcsin\text{ and tanh}. The numbers appearing in these equations are seen to be simple rational numbers as well as \( \pi \) and \( e \).

We also included in the database a set of 20 more challenging “bonus” equations, extracted from other seminal physics books: Classical Mechanics by Herbert Goldstein, Charles P. Poole, John L. Safko [32], Classical electrodynamics by J. Jackson [33], Gravitation and Cosmology: Principles and Applications of the General Theory of Relativity by Steven Weinberg [34] and Quantum Field Theory and the Standard Model by Matthew D. Schwartz [35]. These equations were selected for being both famous and complicated.

The data table provided for each mystery equation contains about \( 10^5 \) rows corresponding to randomly generated input variables. These are uniformly sampled from a specified range where the mystery function is valid.

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\(^1\) The Feynman Database for Symbolic Regression can be downloaded here: [https://space.mit.edu/home/tegmark/alfeynman.html](https://space.mit.edu/home/tegmark/alfeynman.html)
### TABLE III: Unit table used for our automated dimensional analysis.

| Variables   | Units            | m  | s  | kg | T  | V  |
|-------------|------------------|----|----|----|----|----|
| $a, q$      | Acceleration     | 1  | -2 | 0  | 0  | 0  |
| $h, k, L, J$| Angular momentum| 2  | -1 | 1  | 0  | 0  |
| $A$         | Area             | 2  | 0  | 0  | 0  | 0  |
| $k_B$       | Boltzmann constant| 2  | -2 | 1  | -1 | 0  |
| $C$         | Capacitance      | 2  | -2 | 1  | 0  | 0  |
| $q, q_1, q_2$| Charge          | 2  | -2 | 1  | 0  | 0  |
| $j$         | Current density  | 0  | 3  | 1  | 0  | 0  |
| $I, I_0$    | Current Intensity| 2  | -3 | 1  | 0  | 0  |
| $\rho, \rho_0$| Density        | -3 | 0  | 1  | 0  | 0  |
| $\theta, \theta_2, \sigma, \eta$| Dimensionless | 0  | 0  | 0  | 0  | 0  |
| $g, f_1, \gamma, \chi, \alpha$| Dimensionless | 0  | 0  | 0  | 0  | 0  |
| $p, n_0, \delta, \eta, \mu$| Dimensionless | 0  | 0  | 0  | 0  | 0  |
| $n_0, \delta, f, \mu, Z_1, Z_2$| Dimensionless | 0  | 0  | 0  | 0  | 0  |
| $D$         | Diffusion coefficient| 2  | -1 | 0  | 0  | 0  |
| $\mu_{fr(f)}$| Drift velocity constant| 0  | 1  | 0  | 0  | 0  |
| $p_d$       | Electric dipole moment| 3  | -2 | 1  | 0  | -1 |
| $E_f$       | Electric field   | -1 | 0  | 0  | 0  | 1  |
| $\epsilon$  | Electric permittivity| 1  | -2 | 0  | 0  | 2  |
| $E, K, U$   | Energy           | 2  | -2 | 1  | 0  | 0  |
| $E_{den}$   | Energy density   | -1 | 2  | 1  | 0  | 0  |
| $F_{E}$     | Energy flux      | 0  | -3 | 1  | 0  | 0  |
| $F, N_n$    | Force            | 1  | -2 | 1  | 0  | 0  |
| $\omega, \omega_0$| Frequency      | 0  | -1 | 0  | 0  | 0  |
| $k_G$       | Grav. coupling ($Gm_1m_2$) | 3  | 2  | 1  | 0  | 0  |
| $H$         | Hubble constant  | 0  | -1 | 0  | 0  | 0  |
| $L_{ind}$   | Inductance       | -2 | 4  | 1  | 0  | 2  |
| $n_{ho}$    | Inverse volume   | -3 | 0  | 0  | 0  | 0  |
| $x, x_1, x_2, x_3$| Length     | 1  | 0  | 0  | 0  | 0  |
| $y_1, y_1, y_2, y_3$| Length     | 1  | 0  | 0  | 0  | 0  |
| $z, z_1, z_2, r, r_1, r_2$| Length   | 1  | 0  | 0  | 0  | 0  |
| $\lambda, \alpha, \beta, \gamma, \delta, \epsilon, \phi, \theta_1$| Length | 1  | 0  | 0  | 0  | 0  |
| $\lambda_1, \lambda_2, I_x, I_y$| Light intensity| 0  | -3 | 1  | 0  | 0  |
| $B, B_x, B_y, B_z$| Magnetic field | -2 | 1  | 0  | 0  | 1  |
| $\mu_{m}$  | Magnetic moment  | 4  | -3 | 1  | 0  | -1 |
| $M$         | Magnetisation    | 1  | -3 | 1  | 0  | -1 |
| $m, m_0, m_1, m_2$| Mass         | 0  | 0  | 1  | 0  | 0  |
| $\mu_0$    | Mobility         | 0  | 1  | -1 | 0  | 0  |
| $p$         | Momentum        | 1  | -1 | 1  | 0  | 0  |
| $G$         | Newton’s constant| 3  | -2 | 1  | 0  | 0  |
| $P_s$       | Polarization     | 0  | -2 | 1  | 0  | -1 |
| $P$         | Power           | 2  | -3 | 1  | 0  | 0  |
| $p_F$       | Pressure         | -1 | 2  | 1  | 0  | 0  |
| $R$         | Resistance       | -2 | 3  | -1 | 0  | 2  |
| $\mu_\xi$  | Shear modulus    | -1 | 2  | 1  | 0  | 0  |
| $L_{rad}$   | Spectral radiance| 0  | -2 | 1  | 0  | 0  |
| $k_{spring}$| Spring constant  | 0  | -2 | 1  | 0  | 0  |
| $\sigma_{den}$| Surface Charge density| 0  | -2 | 1  | 0  | 1  |
| $T, T_1, T_2$| Temperature     | 0  | 0  | 0  | 1  | 0  |
| $\kappa$   | Thermal conductivity| 1  | -3 | 1  | 0  | 0  |
| $t, t_1$   | Time             | 0  | 1  | 0  | 0  | 0  |
| $\tau$     | Torque           | 2  | -2 | 1  | 0  | 0  |
| $A_{vec}$  | Vector potential | -1 | 1  | 0  | 0  | 0  |
| $u, v, v_1, c, w$| Velocity     | 1  | -1 | 0  | 0  | 0  |
| $V, V_1, V_2$| Volume        | 3  | 0  | 0  | 0  | 0  |
| $\rho_v, \rho_0$| Volume charge density| -1  | -2 | 1  | 0  | -1 |
| $V_c$      | Voltage          | 0  | 0  | 0  | 0  | 1  |
| $k$        | Wave number      | -1 | 0  | 0  | 0  | 0  |
| $Y$        | Young modulus    | -1 | 2  | 1  | 0  | 0  |

B. Method comparison

We reviewed the symbolic regression literature for publicly available software against which our method could be compared. To the best of our knowledge, the best competitor by far is the commercial Eureqa software sold by Nutonian, Inc.², implementing an improved version of the generic search algorithm outlined in [22].

We compared the AI Feynman and Eureqa algorithms by applying them both to the Feynman Database for Symbolic Regression, allowing a maximum of 2 hours of CPU time per mystery.³ Tables [V] and [V] show that Eureqa solved 71% of the 100 basic mysteries, while AI Feynman solved 100%. Closer inspection of these tables reveal that the greatest improvement of our algorithm over Eureqa is for the most complicated mysteries, where our neural network enables eliminating variables by discovering symmetries and separability.

The neural network becomes even more important when we rerun AI Feynman without the dimensional analysis module: it now solves 93% of the mysteries, and makes very heavy use of the neural network to discover separability and translational symmetries. Without dimensional analysis, many of the mysteries retain variables that appear only raised to some power or in a multiplicative prefactor, and AI Feynman tends to recursively discover them and factor them out one by one. For example, the neural network strategy is used six times when solving

$$F = \frac{Gm_1m_2}{(x_2 - x_1)^2 + (y_2 - y_1)^2 + (z_2 - z_1)^2}$$

without dimensional analysis: three times to discover translational symmetry that replaces $x_2 - x_1$, $y_2 - y_1$ and $z_2 - z_1$ by new variables, once to group together $G$ and $m_1$ into a new variable $a$, once to group together

² Eureqa can be purchased at https://www.nutonian.com/products/eureqa

³ The AI Feynman algorithm was run using the hyperparameter settings in Table III. For Eureqa, each mystery was run on 4 CPUs. The symbols used in trying to solve the equations were: $\rightarrow, \rightarrow, +, -, \times, /$, constant, integer constant, input variable, sqrt, exp, log, sin, cos. To help Eureqa gain speed, we included the additional functions arcsin and arccos only for those mysteries requiring them, and we used only 300 data points (since it does not use a neural network, adding additional data does not help significantly). The time taken to solve an equation using our algorithm, as presented in Tables [IV] and [V] corresponds to the time needed for an equation to be solved using a set of symbols that can actually solve it (see Table II). Equations 1.15.3t and 1.48.2 were solved using the second set of symbols, so the overall time taken for these two equations is one hour larger than the one listed in the tables. Equations 1.15.3t and II.35.21 were solved using the 3rd set of symbols, so the overall time taken is two hours larger than the one listed here.
TABLE IV: Tested Feynman Equations, part 1. Abbreviations in the “Methods used” column: “da” = dimensional analysis, “bf” = brute force, “pf” = polyfit, “sym” = set 2 variables equal, “sym-” = symmetry, “sep” = separability. Suffixes denote the type of symmetry or separability (“sym-” = translation symmetry, “sep” = multiplicative separability, etc.) or the preprocessing before brute force (e.g., “bf-inverse” means inverting the mystery function before bf).
| Feynman eq. | Equation | Solution time (s) | Methods used | Data needed | Solved by Euroqa | Solved w/o DA | Noise tolerance |
|------------|----------|------------------|--------------|-------------|-----------------|--------------|----------------|
| II.2.42    | $P = \frac{2}{6} (\frac{\pi^2}{\gamma}) \lambda$ | 54 | da, bf | 10 | yes | yes | $10^{-3}$ |
| II.3.24    | $F_E = \frac{\mu}{n^2} \lambda$ | 8 | da | 10 | yes | yes | $10^{-2}$ |
| II.4.23    | $V_x = \frac{\pi^2}{4 \sin^2 \theta}$ | 10 | da | 10 | yes | yes | $10^{-2}$ |
| II.6.11    | $V_x = \frac{1}{2} \mu_0 \cos \theta$ | 18 | da, bf | 10 | yes | yes | $10^{-3}$ |
| II.6.15a   | $E_y = \frac{1}{2} \mu_0 \cos \theta \sqrt{x^2 + y^2}$ | 2801 | da, sm, bf | 10$^4$ | no | yes | $10^{-3}$ |
| II.6.15b   | $E_y = \frac{\mu_0 \lambda}{4 \pi} \cos \theta \sin \theta$ | 23 | da, bf | 10 | yes | yes | $10^{-2}$ |
| II.8.7     | $E = \frac{1}{2} \frac{\mu_0 \lambda}{2 \pi}$ | 10 | da | 10 | yes | yes | $10^{-2}$ |
| II.8.31    | $E_{den} = \frac{e E_f}{\lambda}$ | 8 | da | 10 | yes | yes | $10^{-2}$ |
| II.10.9    | $E_f = \frac{\sqrt{d \sin \frac{1}{x + \lambda}}}{2} \mu_0 \lambda$ | 13 | da, bf | 10 | yes | yes | $10^{-2}$ |
| II.11.3    | $x = \frac{m(\omega_0 - \omega)^2}{2}$ | 25 | da, bf | 10 | yes | yes | $10^{-3}$ |
| II.11.17   | $n = n_0(1 + \frac{p_d E_f \cos \theta}{\mu_0 \lambda})$ | 28 | da, bf | 10 | yes | yes | $10^{-2}$ |
| II.11.20   | $P_e = \frac{n_e \mu_0 \lambda}{4 \pi \mu}$ | 18 | da, bf | 10 | yes | yes | $10^{-3}$ |
| II.11.27   | $P_e = \frac{n_e \mu_0 \lambda}{4 \pi \mu}$ | 337 | da, bf-inverse | 10$^2$ | no | yes | $10^{-3}$ |
| II.11.28   | $\theta = 1 + \frac{1}{n_0 \mu_0 \lambda}$ | 1708 | da, sym*, bf | 10$^2$ | no | yes | $10^{-4}$ |
| II.13.17   | $B = \frac{1}{4 \pi \mu_0 \lambda}$ | 13 | da | 10 | yes | yes | $10^{-2}$ |
| II.13.39   | $\omega = \frac{1}{4 \pi \mu_0 \lambda}$ | 13 | da, bf | 10$^2$ | no | yes | $10^{-4}$ |
| II.13.41   | $\mu = \frac{4 \pi \lambda}{T}$ | 14 | da, bf | 10 | no | yes | $10^{-4}$ |
| II.15.4    | $E = -\mu M B \cos \theta$ | 14 | da, bf | 10 | yes | yes | $10^{-3}$ |
| II.15.5    | $E = -\mu_0 E_f \cos \theta$ | 14 | da, bf | 10 | yes | yes | $10^{-3}$ |
| II.21.32   | $V_x = \frac{4 \pi \gamma}{(1 - v/c)}$ | 21 | da, bf | 10 | yes | yes | $10^{-3}$ |
| II.24.17   | $k = \sqrt{\frac{\omega^2}{c^2} - \frac{4 \pi^2}{\omega^2}}$ | 62 | da, bf | 10 | yes | yes | $10^{-5}$ |
| II.27.16   | $F_E = \frac{\varepsilon c E_f^2}{\gamma}$ | 13 | da | 10 | yes | yes | $10^{-2}$ |
| II.27.18   | $E_{den} = \frac{e E_f}{\lambda}$ | 9 | da | 10 | yes | yes | $10^{-2}$ |
| II.34.2a   | $I = \frac{\mu_0 \lambda}{4 \pi \mu}$ | 11 | da | 10 | yes | yes | $10^{-2}$ |
| II.34.2    | $\mu = \frac{2 \pi}{\lambda}$ | 11 | da | 10 | yes | yes | $10^{-2}$ |
| II.34.11   | $\omega = \frac{2 \pi}{\lambda}$ | 16 | da, bf | 10 | yes | yes | $10^{-4}$ |
| II.34.29a  | $\mu = \frac{4 \pi \lambda}{T}$ | 12 | da | 10 | yes | yes | $10^{-4}$ |
| II.34.29b  | $E = \frac{2 \mu_0 \lambda}{\hbar}$ | 18 | da, bf | 10 | yes | yes | $10^{-4}$ |
| II.35.18   | $n = \frac{\exp(\mu M B/(k_B T)) + \exp(-\mu M B/(k_B T))}{\exp(\mu M B/(k_B T)) - \exp(-\mu M B/(k_B T))}$ | 30 | da, bf | 10 | no | yes | $10^{-2}$ |
| II.35.21   | $E = \frac{\varepsilon c E_f^2}{\gamma}$ | 1597 | da, halve-input, bf | 10 | no | yes | $10^{-4}$ |
| II.36.38   | $f = \frac{n_e \mu_0 \lambda}{4 \pi \mu}$ | 77 | da, bf | 10 | yes | yes | $10^{-2}$ |
| III.7.1    | $E = \frac{\mu M}{(1 + \chi) B}$ | 15 | da, bf | 10 | yes | yes | $10^{-3}$ |
| III.8.3    | $F = \frac{\lambda A}{d}$ | 47 | da, bf | 10 | yes | yes | $10^{-3}$ |
| III.8.14   | $\mu = \frac{2 \pi}{\lambda}$ | 13 | da, bf | 10 | yes | yes | $10^{-3}$ |
| III.4.32   | $n = \frac{4 \pi r}{e \gamma^2}$ | 20 | da, bf | 10 | yes | yes | $10^{-3}$ |
| III.4.33   | $E = \frac{\hbar \omega}{2 \pi}$ | 19 | da, bf | 10 | no | yes | $10^{-3}$ |
| III.7.38   | $\omega = \frac{\mu_0 \lambda B}{\hbar \omega}$ | 13 | da | 10 | yes | yes | $10^{-2}$ |
| III.8.54   | $p_e = \sinh(\frac{\hbar \omega}{k_B T})^2$ | 39 | da, bf | 10 | no | yes | $10^{-3}$ |
| III.9.52   | $p_e = \sinh(\frac{\hbar \omega}{k_B T})^2 \sin((\omega/\omega_0)^2/2)^2$ | 3162 | da, sym-, sm, bf | 10$^3$ | no | yes | $10^{-3}$ |
| III.10.19  | $E = \frac{\mu_0 M}{2} \sqrt{B_x^2 + B_y^2 + B_z^2}$ | 410 | da, bf-squared | 10$^2$ | yes | yes | $10^{-4}$ |
| III.12.43  | $L = n \hbar$ | 11 | da, bf | 10 | yes | yes | $10^{-3}$ |
| III.13.18  | $v = \frac{2 \varepsilon c \lambda}{\hbar}$ | 16 | da, bf | 10 | yes | yes | $10^{-4}$ |
| III.14.14  | $I = I_0 \frac{\lambda}{\varepsilon^2}$ | 18 | da, bf | 10 | no | yes | $10^{-3}$ |
| III.15.12  | $E = 2 \mu (1 - \cos(kd))$ | 14 | da, bf | 10 | yes | yes | $10^{-4}$ |
| III.15.14  | $m = \frac{k_B T}{\mu}$ | 10 | da | 10 | yes | yes | $10^{-2}$ |
| III.15.27  | $k = \frac{2 \pi}{\lambda}$ | 14 | da, bf | 10 | yes | yes | $10^{-3}$ |
| III.17.37  | $f = B(1 + \alpha \cos \theta)$ | 27 | bf | 10 | yes | yes | $10^{-3}$ |
| III.19.51  | $E = \frac{\frac{m^2}{r} - 1}{\frac{\mu_0 \lambda A}{\gamma^2}}$ | 18 | da, bf | 10 | yes | yes | $10^{-5}$ |
| III.21.20  | $j = \frac{1}{\frac{\mu_0 \lambda A}{\gamma^2}}$ | 13 | da | 10 | yes | yes | $10^{-2}$ |

TABLE V: Tested Feynman Equations, part 2 (same notation as in Table IV)
a and \(m_2\) into a new variable \(b\), and one last time to discover separability and factor out \(b\). This shows that although dimensional analysis often provides significantly small time savings, it is usually not necessary for successfully solving the problem.

Inspection of how \textit{AI Feynman} and \textit{Eureqa} make progress over time reveals interesting differences. The progress of \textit{AI Feynman} over time corresponds to repeatedly reducing the number of independent variables, and every time this occurs, it is virtually guaranteed to be in a step in the right direction. In contrast, genetic algorithms such as \textit{Eureqa} make progress over time by finding successively better approximations, but there is no guarantee that more accurate symbolic expressions are closer to the truth when viewed as strings of symbols. Specifically, by virtue of being a genetic algorithm, \textit{Eureqa} has the advantage of not searching the space of symbolic expressions blindly like our brute force module, but rather with the possibility of a net drift toward more accurate (“fit”) equations. The flip side of this is that if \textit{Eureqa} finds a fairly accurate yet incorrect formula with a quite different functional form, it risks getting stuck near that local optimum. This reflects a fundamental challenge for genetic approaches symbolic regression: if the final formula is composed of separate parts that are not summed but combined in some more complicated way (as a ratio, say), then each of the parts may be useless fits on their own and unable to evolutionarily compete.

\section{C. Dependence on data size}

To investigated the effect of changing the size of the data set, we repeatedly reduced the size of each data set by a factor of 10 until our \textit{AI Feynman} algorithm failed to solve it. As seen in Tables \ref{tab:source} and \ref{tab:source} most equations get solved even with a small number of data points (10

| Source                                | Equation                                                                 | Solved | Methods used            | Solved by                    |
|---------------------------------------|-------------------------------------------------------------------------|--------|-------------------------|------------------------------|
| Rutherford Scattering                 | \( A = \left(\frac{Z_1 Z_2 e^2 \hbar c}{4\pi^2 E \sin^2 \left(\frac{\omega}{2}\right)}\right)^2 \) | yes    | da, bf-sqrt             |                              |
| Friedman Equation                     | \( H = \sqrt{\frac{8\pi G c^2}{3} \rho - \frac{k f e^2}{a^2}} \)          | yes    | da, bf-squared          |                              |
| Compton Scattering                    | \( U = \sqrt{\frac{E}{1 + \frac{m_2}{m_1} (1 - \cos \theta)}} \)       | no     | da, bf                  |                              |
| Radiated gravitational wave power     | \( P = -\frac{2G^2}{c^2} \left(\frac{m_1 m_2}{m_1 + m_2}\right)^2 \) | no     | -                       |                              |
| Relativistic aberration               | \( \theta_1 = \arccos \left(\frac{\cos \theta_1}{1 - \frac{c}{	heta} \cos \theta_2}\right) \) | yes    | da, bf-cos              |                              |
| N-slit diffraction                    | \( I = \frac{1}{2m} \left[\sin(\alpha/2) \sin(\pi/2)\right] \)         | yes    | da, sm, bf              |                              |
| Goldstein 3.16                        | \( \sqrt{\frac{E}{U}} = \sqrt{\frac{E}{U}} \left(1 - \frac{L^2}{2m_1 c^2}\right) \) | yes    | da, bf-squared          |                              |
| Goldstein 3.55                        | \( k = \frac{n h G}{L^2} \left(1 + \sqrt{1 + \frac{2E L^2}{m h G^2} \cos(\theta_1 - \theta_2)}\right) \) | yes    | da, sym-, bf            |                              |
| Goldstein 3.64 (ellipse)              | \( r = \frac{d(1-q^2)}{\sqrt{\frac{E}{U} - \frac{L^2}{2m_1 c^2}}} \)      | yes    | da, sym-, bf            |                              |
| Goldstein 3.74 (Kepler)               | \( t = \frac{\sqrt{G(m_1 + m_2)}}{\sqrt{2k m_1 c^2}} \)                   | yes    | da, bf                  |                              |
| Goldstein 3.99                        | \( \alpha = \sqrt{1 + \frac{2E^2 L^2}{m^2 (2c^2 + 4c^2)}} \)          | yes    | da, sym*, bf            |                              |
| Goldstein 8.56                        | \( E = \sqrt{\left(p - q A_{res}\right)^2 + m^2 c^2} + q V_e \)         | yes    | da, sep, bf-squared     |                              |
| Goldstein 12.80                       | \( E = \sqrt{\frac{1}{2 m} \left[p^2 + m^2 \omega^2 x^2 (1 + \alpha^2)\right]} \) | yes    | da, bf                  |                              |
| Jackson 2.11                          | \( F = \frac{q}{4 \pi e y} \left[4 \pi e V_c d - \frac{q d V^2}{(y^2 - d^2)^2}\right] \) | no     | -                      |                              |
| Jackson 3.45                          | \( V_c = \frac{q}{(r^2 + d^2 - 2 dr \cos \theta)^{3/2}} \)            | yes    | da, bf-inv              |                              |
| Jackson 4.60                          | \( \omega_0 = \sqrt{\frac{1 - \frac{\omega}{\omega}}}{1 + \frac{\omega}{\omega}} \) | yes    | da, cos-input, bf       |                              |
| Weinberg 15.2.1                       | \( \rho = \frac{3}{8 \pi G} \left(\frac{c^2 k_r}{a^2} + H^2\right) \)     | yes    | da, bf                  |                              |
| Weinberg 15.2.2                       | \( p_f = -\frac{1}{8 \pi G} \left[c^2 \frac{k_r}{a^2} + c^2 H^2 (1 - 2 \alpha)\right] \) | yes    | da, bf                  |                              |
| Schwarz 13.132 (Klein-Nishina)        | \( A = \frac{\pi a^2 c^2}{m^2 c^2} \left(\frac{\omega_0}{\omega}\right)^2 \) | yes    | da, sym/, sep*, sin-input, bf |                              |

TABLE VI: Tested bonus equations. Goldstein 8.56 is for the special case where the vectors \(p\) and \(A\) are parallel.
or 100). As expected, equations that require the use of a neural network to be solved need significantly more data points (between $10^2$ and $10^6$) for the network to be able to learn the mystery function accurately enough (i.e. obtaining r.m.s. accuracy better than $10^{-2}$). Note that expressions requiring the neural network are typically more complex, so one might intuitively expect them to require larger data sets for the correct equation to be discovered without overfitting, even when using alternate approaches such as genetic algorithms.

\section{D. Dependence on noise level}

Since real data is almost always afflicted with measurement errors or other forms of noise, we investigated the robustness of our algorithm. For each mystery, we added independent Gaussian random noise to its dependent variable $y$, of standard deviation $\epsilon y_{\text{rms}}$, where $y_{\text{rms}}$ denotes the r.m.s. $y$-value for the mystery before noise has been added. We initially set the relative noise level $\epsilon = 10^{-6}$, then repeatedly multiplied $\epsilon$ by 10 until the \textit{AI Feynman} algorithm could no longer solve the mystery. As seen in Tables IV and V, most of the equations can still be recovered exactly with an $\epsilon$-value of $10^{-4}$ or less, while almost half of them are still solved for $\epsilon = 10^{-2}$.

For these noise experiments, we adjusted the threshold for the brute force and polynomial fit algorithms when the noise level changed, such that not finding a solution at all was preferred over finding an approximate solution. These thresholds were not optimized for each mystery individually, so a better choice of these thresholds might allow the exact equation to be recovered with an even higher noise level for certain equations.

\section{E. Bonus mysteries}

The 100 basic mysteries discussed above should be viewed as a training set for our \textit{AI Feynman} algorithm, since we made improvements to its implementation and hyper-parameters to optimize performance. In contrast, we can view the 20 bonus mysteries as a test set, since we deliberately selected and analyzed them only after the \textit{AI Feynman} algorithm and its hyper-parameter settings (Table I) had been finalized. The bonus mysteries are interesting also by virtue of being significantly more complex and difficult, in order to better identify the limitations our method.

Table VI shows that \textit{Eureqa} solved only 15\% of the bonus mysteries, while \textit{AI Feynman} solved 90\%. The fact that the success percentage differs more between the two methods for the bonus mysteries than for the basic mysteries reflects the increased equation complexity, which requires our neural network based strategies for a larger fraction of the cases.

To shed light on the limitations of the \textit{AI Feynman} algorithm, it is interesting to consider the two mysteries for which it failed. The radiated gravitational wave power mystery was reduced to the form $y = -\frac{32a^2(1+a)}{b(1-a)^2}$ by dimensional analysis, corresponding to the string “$aaa > ***bbbbb****/*” in reverse Polish notation (ignoring the multiplicative prefactor $-\frac{32}{b}$). This would require about 2 years for the brute force method, exceeding our allotted time limit. The Jackson 2.11 mystery was reduced to the form $a - \frac{1}{4\pi b(1-a)^2}$ by dimensional analysis, corresponding to the string “$aP0 >>>>> */abaas < aa* < **/*-∗“ in reverse Polish notation, which would require about 100 times the age of our universe for the brute force method.

It is likely that both of these mysteries can be solved with relatively minor improvements of the our algorithm. The first mystery would have been solved had the algorithm not failed to discover that $a^2(1+a)/b^5$ is separable. The large dynamic range induced by the fifth power in the denominator caused the neural network to miss the separability tolerance threshold; potential solutions include temporarily limiting the parameter range or analyzing the logarithm of the absolute value (to discover additive separability).

If we had used different units in the second mystery, where $1/4\pi$ was replaced by the Coulomb constant $k$, the costly 4$\pi$-factor (requiring 7 symbols “$PPP1+++$” or “$P0 >>>>> *$”) would have disappeared. Moreover, if we had used a different set of function symbols that included “$Q$” for squaring, then brute force could quickly have discovered that $a - \frac{a}{b(1-a)^2}$ is solved by “$aabQ < Q */-∗“. Similarly, introducing a symbol $\wedge$ denoting exponentiation, enabling the string for $a^b$ to be shortened from “$aaLb* E$” to “$ab \wedge$”, would enable brute force to solve many mysteries faster, including Jackson 2.11.

Finally, a powerful strategy that could ameliorate both of these failures would be to add symbols corresponding to parameters that are numerically optimized over. This strategy is currently implemented in \textit{Eureqa} but not \textit{AI Feynman}, and could make a useful upgrade as long as it is done in a way that does not unduly slow down the symbolic brute force search. In summary, the two failures of the \textit{AI Feynman} algorithm signal not unsurmountable obstacles, but motivation for further work.

\section{IV. CONCLUSIONS}

We have presented a novel physics-inspired algorithm for solving multidimensional analytic regression problems: finding a symbolic expression that matches data from an unknown function. The software implementing it will be made publicly available upon acceptance of this manuscript for publication. Our key innovation lies in
combining traditional fitting techniques with a neural-network-based approach that can repeatedly reduce a problem to simpler ones, eliminating dependent variables by discovering properties such as symmetries and separability in the unknown function.

To facilitate quantitative benchmarking of our and other symbolic regression algorithms, we created a freely downloadable database with 100 regression mysteries drawn from the Feynman Lectures on Physics and a bonus set of an additional 20 mysteries selected for difficulty and fame.

A. Key findings

The pre-existing state-of-the-art symbolic regression software Eureqa [21] discovered 68% of the Feynman equations and 15% of the bonus equations, while our AI Feynman algorithm discovered 100% and 90%, respectively, including Kepler’s ellipse equation mentioned in the introduction (3rd entry in Table VI). Most of the 100 Feynman equations could be solved even if the data size was reduced to merely $10^2$ data points or had percent-level noise added, but the most complex equations needing neural network fitting required more data and less noise.

Compared with the genetic algorithm of Eureqa, the most interesting improvements are seen for the most difficult mysteries where the neural network strategy is repeatedly deployed. Here the progress of AI Feynman over time corresponds to repeatedly reducing the problem to simpler ones with fewer variables, while Eureqa and other genetic algorithms are forced to solve the full problem by exploring a vast search space, risking getting stuck in local optima.

B. Opportunities for further work

Both the successes and failures of our algorithm motivate further work to make it better, and we will now briefly comment on promising improvement strategies.

Although we mostly used the same elementary function options (Table II) and hyperparameter settings (Table [II]) for all mysteries, these could be strategically chosen based on an automated pre-analysis of each mystery. For example, observed oscillatory behaviour could suggest including sin and cos and lack thereof could suggest saving time by excluding them.

We saw how, even if the mystery data has very low noise, significant de facto noise was introduced by imperfect neural network fitting, complicating subsequent solution steps. It will therefore be valuable to explore better neural network architectures, ideally reducing fitting noise to the $10^{-6}$ level. This may be easier than in many other contexts, since we do not care if the neural network generalizes poorly outside the domain where we have data: as long as it is highly accurate within this domain, it serves our purpose of correctly factoring separable functions, etc.

Our brute-force method can be better integrated with the neural network search for hidden simplicity. Our implemented symmetry search simply tests if two input variables $a$ and $b$ can be replaced by a bivariate function of them, specifically $+,-,\ast$ or $/$, corresponding to length-3 RPN-strings $"ab+"$, $"ab−"$, $"abs"$ and $"ab/"$. This can be readily generalized to longer strings involving 2 or more variables, for example bivariate functions $ab^3$ or $e^a \cos b$.

A second example of improved brute-force use is if the neural network reveals that the function can be exactly solved after setting some variable $a$ equal to something else (say zero, one or another variable). A brute force search can now be performed in the vicinity of the discovered exact expression: for example, if the expression is valid for $a = 0$, the brute force search can insert additive terms that vanish for $a = 0$ and multiplicative terms that equal unity for $a = 0$, thus being likely to discover the full formula much faster than an unrestricted brute force search from scratch.

Last but not least, it is likely that marrying the best features from both our method and genetic algorithms can spawn a method that outperforms both. Genetic algorithms such as Eureqa perform quite well even in presence of significant noise, whether they output not merely one hopefully correct formula, but rather a Pareto frontier, a sequence of increasingly complex formulas that provide progressively better accuracy. Although it may not be clear which of these formulas is correct, it is more likely that the correct formula is one of them than any particular one that an algorithm might guess. When our neural network identifies separability, a so generate Pareto frontier could thus be used to generate candidate formulas for one factor, after which each one could be substituted back and tested as above, and the best solution to the full expression would be retained. Our brute force algorithm can similarly be upgraded to return a Pareto frontier instead of a single formula.

In summary, symbolic regression algorithms are getting better, and are likely to continue improving. We look forward to the day when, for the first time in the history of physics, a computer, just like Kepler, discovers a useful and hitherto unknown physics formula through symbolic regression!
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Algorithm 1 AI Feynman: Translational Symmetry

Require Dataset $D = \{(x, y)\}$
Require net: trained neural network
Require $NN_{error}$: the neural network validation error $a = 1$
for $i$ in $\text{len}(x)$ do:
for $j$ in $\text{len}(x)$ do:
if $i < j$:
    $x_t = x$
    $x_t[i] = x_t[i] + a$
    $x_t[j] = x_t[j] + a$
    $error = \text{RMSE}(\text{net}(x), \text{net}(x_t))$
    $error = error / \text{RMSE}(\text{net}(x))$
if $error < 7 \times NN_{error}$:
    $x_t[i] = x_t[i] - x_t[j]$
    $x_t = \text{delete}(x_t, j)$
return $x_t, i, j$

Algorithm 2 AI Feynman: Additive Separability

Require Dataset $D = \{(x, y)\}$
Require net: trained neural network
Require $NN_{error}$: the neural network validation error
$x_{eq} = x$
for $i$ in $\text{len}(x)$ do:
    $x_{eq}[i] = \text{mean}(x[i])$
for $i$ in $\text{len}(x)$ do:
    $c = \text{combinations}([1, 2, ..., \text{len}(x)], i)$
    for $idx_1$ in $c$ do:
        $x_1 = x$
        $x_2 = x$
        $idx_2 = k$ in $[1, \text{len}(x)]$ not in $idx_1$
        for $j$ in $idx_1$:
            $x_1[j] = \text{mean}(x[j])$
        for $j$ in $idx_2$:
            $x_2[j] = \text{mean}(x[j])$
        $error = \text{RMSE}(\text{net}(x), \text{net}(x_1) + \text{net}(x_2) - \text{net}(x_{eq}))$
        $error = error / \text{RMSE}(\text{net}(x))$
    if $error < 10 \times NN_{error}$:
        $x_1 = \text{delete}(x_1, \text{index}_2)$
        $x_2 = \text{delete}(x_2, \text{index}_1)$
return $x_1, x_2, \text{index}_1, \text{index}_2$

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