

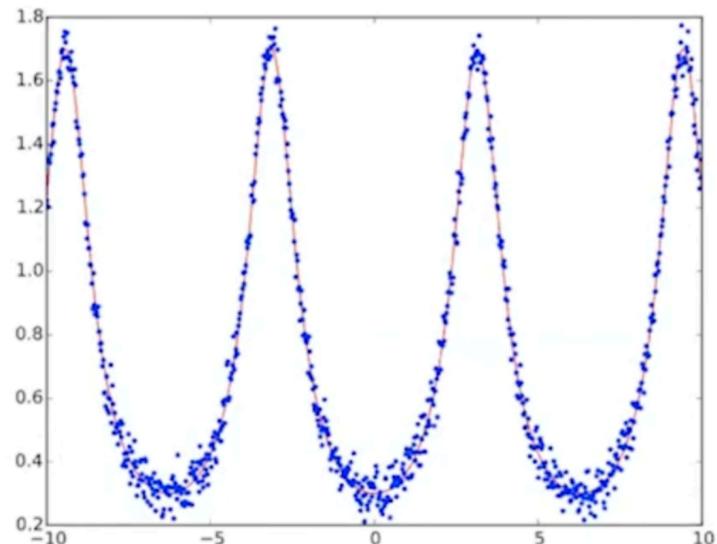
Symbolic Regression and Polynomial Optimization in Scientific Discovery

Karan Srivastava

Aim

- To discover meaningful laws of nature from experimental data

i.e. Given some data $\{(x_1, \dots, x_n, y)_i\}_{i \in \mathcal{D}}$ we want to find a function f so that $y = f(x_1, \dots, x_n)$ for each data point.



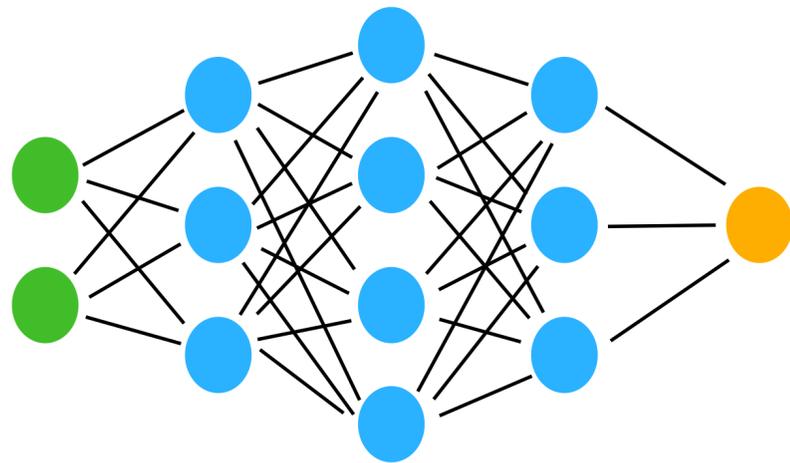
$$r = \frac{a(1 - e^2)}{1 + e \cos(\theta_1 - \theta_2)}$$

Aim

- Given some data $\{(x_1, \dots, x_n, y)_i\}_{i \in \mathcal{D}}$ we want to find a function f so that $y = f(x_1, \dots, x_n)$ for each data point.

Some ideas

Deep Learning



Pros: Good for discovering patterns in data

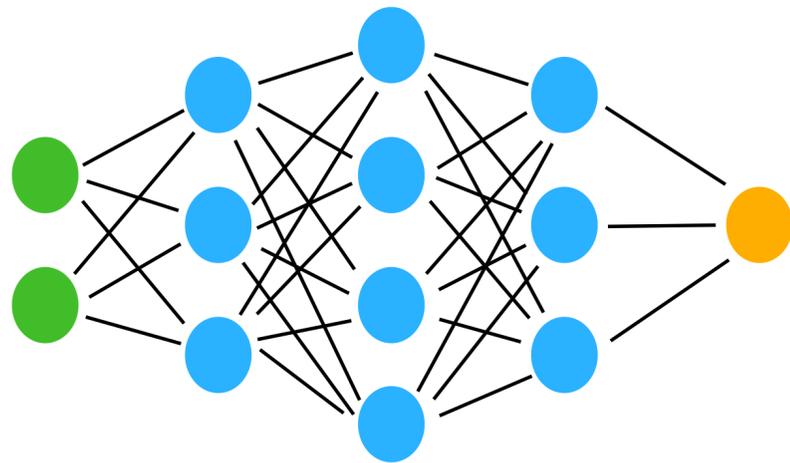
Drawback: Model itself is uninterpretable

Aim

- Given some data $\{(x_1, \dots, x_n, y)_i\}_{i \in \mathcal{D}}$ we want to find a function f so that $y = f(x_1, \dots, x_n)$ for each data point.

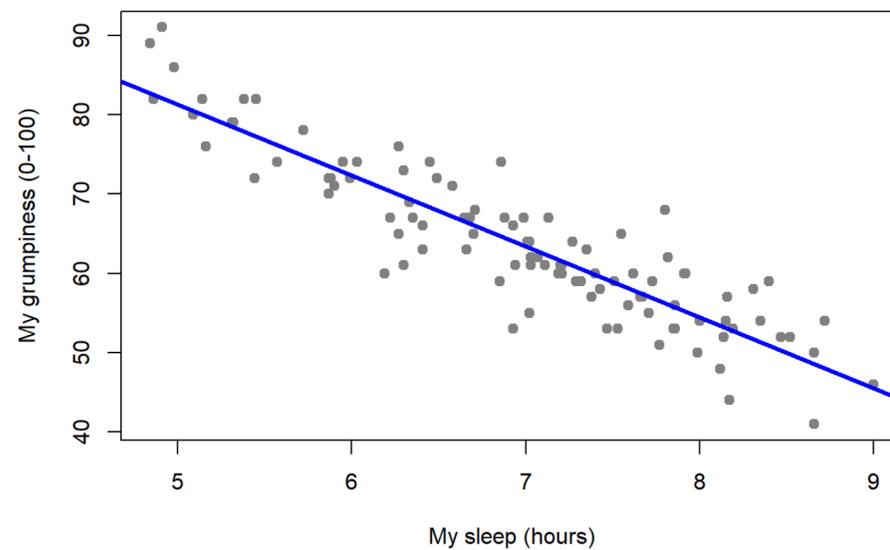
Some ideas

Deep Learning

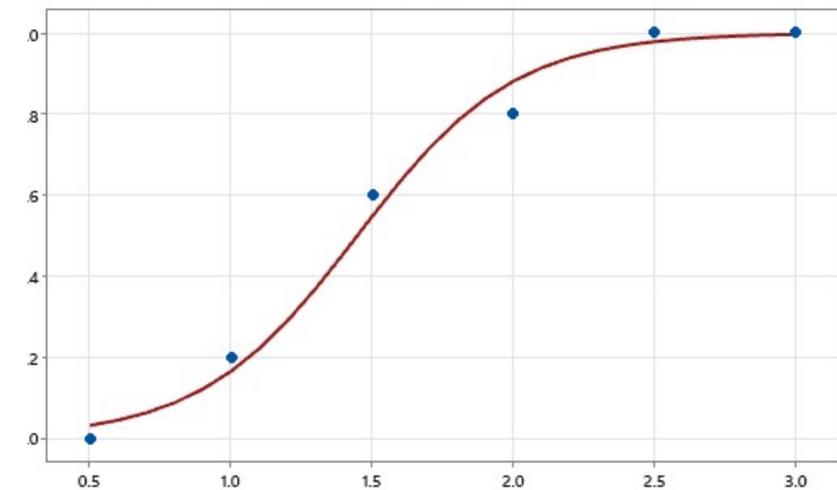


Pros: Good for discovering patterns in data
Drawback: Model itself is uninterpretable

Standard Regression



Pros: Models are very interpretable
Drawback: Functional form is fixed



Approach 1: Symbolic Regression

Approach 1: Symbolic Regression

In particular, we will look at the approach in this paper:

AI Feynman: a Physics-Inspired Method for Symbolic Regression

Silviu-Marian Udrescu, Max Tegmark*
Dept. of Physics & Center for Brains, Minds & Machines,
Massachusetts Institute of Technology, Cambridge, MA 02139; sudrescu@mit.edu and
Theiss Research, La Jolla, CA 92037, USA

(Dated: Published in *Science Advances*, 6:eaay2631, April 15, 2020)

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 physics-based test set, we improve the state of the art success rate from 15% to 90%.

I. INTRODUCTION

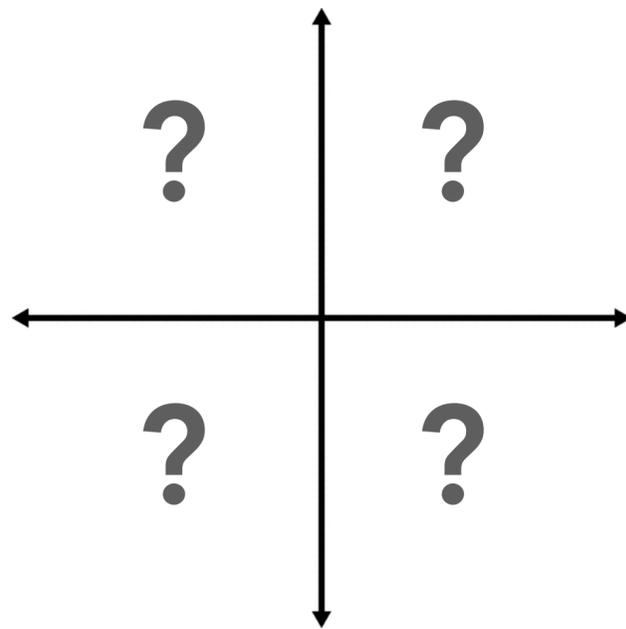
In 1601, Johannes Kepler got access to the world's best data tables on planetary orbits, and after 4 years and about 40 failed attempts to fit the Mars data to various ovoid shapes, he launched a scientific revolution by discovering that Mars' orbit was an ellipse [1]. This was an example of *symbolic 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 $\{x_1, \dots, x_n, y\}$ where $y = f(x_1, \dots, x_n)$, 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

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], discovering partial differential equations [11], investment strategy [12], marketing [13], classification [14], Rubik's cube [15], program synthesis [16] and metabolic networks [17].

Symbolic Regression

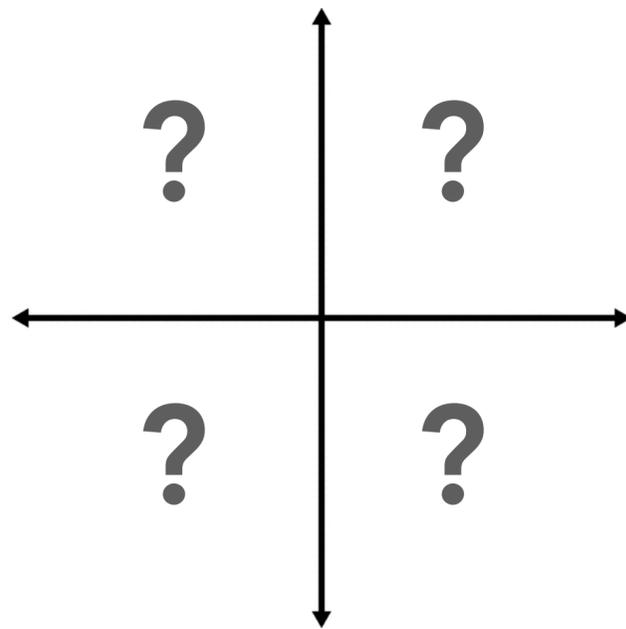
- Given some data $\{(x_1, \dots, x_n, y)_i\}_{i \in \mathcal{D}}$ we want to find a function f so that $y = f(x_1, \dots, x_n)$ for each data point **when the functional form of f is unknown.**



- In particular, given a set S of symbols (e.g. $+$, $-$, \div , $\sqrt{\quad}$, etc), find a function (string) f built from these symbols so that $y = f(x_1, \dots, x_n)$ fits the data.

Symbolic Regression

- Given some data $\{(x_1, \dots, x_n, y)_i\}_{i \in \mathcal{D}}$ we want to find a function f so that $y = f(x_1, \dots, x_n)$ for each data point **when the functional form of f is unknown.**



- In particular, given a set S of symbols (e.g. $+$, $-$, \div , $\sqrt{\quad}$, etc), find a function (string) f built from these symbols so that $y = f(x_1, \dots, x_n)$ fits the data.

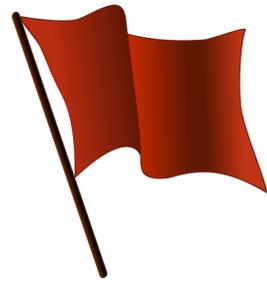


For generic functions $f(x_1, \dots, x_n)$, this is NP hard



Symbolic Regression

- In particular, given a set S of symbols (e.g. $+$, $-$, \div , $\sqrt{\quad}$, etc), find a function (string) f built from these symbols so that $y = f(x_1, \dots, x_n)$ fits the data.



For generic functions $f(x_1, \dots, x_n)$, this is NP hard



- Search grows exponentially with the number of symbols.
- Brute force search becomes infeasible very quickly

$$f = \frac{e^{-\frac{x^2}{2}}}{\sqrt{2\pi}} \sim 30 \text{ years}, \quad \omega = \frac{1 + \frac{v}{c}}{\sqrt{1 - \frac{v^2}{c^2}}} \sim 10^6 \text{ years, and so on.}$$

Symbolic Regression

Feynman eq.	Equation
I.6.20a	$f = e^{-\theta^2/2} / \sqrt{2\pi}$
I.6.20	$f = e^{-\frac{\theta^2}{2\sigma^2}} / \sqrt{2\pi\sigma^2}$
I.6.20b	$f = e^{-\frac{(\theta-\theta_1)^2}{2\sigma^2}} / \sqrt{2\pi\sigma^2}$
I.8.14	$d = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}$
I.9.18	$F = \frac{Gm_1m_2}{(x_2-x_1)^2+(y_2-y_1)^2+(z_2-z_1)^2}$
I.10.7	$m = \frac{m_0}{\sqrt{1-\frac{v^2}{c^2}}}$
I.11.19	$A = x_1y_1 + x_2y_2 + x_3y_3$
I.12.1	$F = \mu N_n$
I.12.2	$F = \frac{q_1q_2}{4\pi\epsilon r^2}$
I.12.4	$E_f = \frac{q_1}{4\pi\epsilon r^2}$
I.12.5	$F = q_2 E_f$
I.12.11	$F = q(E_f + Bv \sin \theta)$
I.13.4	$K = \frac{1}{2}m(v^2 + u^2 + w^2)$
I.13.12	$U = Gm_1m_2\left(\frac{1}{r_2} - \frac{1}{r_1}\right)$
I.14.3	$U = mgz$
I.14.4	$U = \frac{k_{spring}x^2}{2}$
I.15.3x	$x_1 = \frac{x-ut}{\sqrt{1-u^2/c^2}}$

BUT
SCIENCE IS
NOT
GENERIC

Symbolic Regression

In physics and in lots of science applications, functions we care about tend to be nice in the following ways:

1. Units: f and its variables have to be dimensionally consistent
2. Low degree polynomials: Parts of f tend to have low degree polynomials
3. Compositionality: f is a composition of elementary functions
4. Smoothness: f is continuous and often analytic on its domain
5. Symmetry: f comes with translational, rotational, and scaling symmetry with respect to some variables
6. Separability: f can be written as the sum or product of two parts with no common variables

Symbolic Regression

In physics and in lots of science applications, functions we care about tend to be nice in the following ways:

1. Units: Can use this to transform the problem to fewer independent variables
2. Low degree polynomials: Parts of f tend to have low degree polynomials
3. Compositionality: f is a composition of elementary functions
4. Smoothness: f is continuous and often analytic on its domain
5. Symmetry: f comes with translational, rotational, and scaling symmetry with respect to some variables
6. Separability: f can be written as the sum or product of two parts with no common variables

Symbolic Regression

In physics and in lots of science applications, functions we care about tend to be nice in the following ways:

1. Units: Can use this to transform the problem to fewer independent variables
2. Low degree polynomials: Parts of f tend to have low degree polynomials
3. Compositionality: f is a composition of elementary functions
4. Smoothness: f is continuous and often analytic on its domain
5. Symmetry: f comes with translational, rotational, and scaling symmetry with respect to some variables
6. Separability: f can be written as the sum or product of two parts with no common variables

Symbolic Regression

In physics and in lots of science applications, functions we care about tend to be nice in the following ways:

1. Units: Can use this to transform the problem to fewer independent variables
2. Low degree polynomials: Can use this to do polynomial fits for parts of f
3. Compositionality: f is a composition of elementary functions
4. Smoothness: f is continuous and often analytic on its domain
5. Symmetry: f comes with translational, rotational, and scaling symmetry with respect to some variables
6. Separability: f can be written as the sum or product of two parts with no common variables

Symbolic Regression

In physics and in lots of science applications, functions we care about tend to be nice in the following ways:

1. Units: Can use this to transform the problem to fewer independent variables
2. Low degree polynomials: Can use this to do polynomial fits for parts of f
3. Compositionality: f is a composition of elementary functions
4. Smoothness: f is continuous and often analytic on its domain
5. Symmetry: f comes with translational, rotational, and scaling symmetry with respect to some variables
6. Separability: f can be written as the sum or product of two parts with no common variables

Symbolic Regression

In physics and in lots of science applications, functions we care about tend to be nice in the following ways:

1. Units: Can use this to transform the problem to fewer independent variables
2. Low degree polynomials: Can use this to do polynomial fits for parts of f
3. Compositionality: Can use brute force for parts of the function
4. Smoothness: f is continuous and often analytic on its domain
5. Symmetry: f comes with translational, rotational, and scaling symmetry with respect to some variables
6. Separability: f can be written as the sum or product of two parts with no common variables

Symbolic Regression

In physics and in lots of science applications, functions we care about tend to be nice in the following ways:

1. Units: Can use this to transform the problem to fewer independent variables
2. Low degree polynomials: Can use this to do polynomial fits for parts of f
3. Compositionality: Can use brute force for parts of the function
4. Smoothness: f is continuous and often analytic on its domain
5. Symmetry: f comes with translational, rotational, and scaling symmetry with respect to some variables
6. Separability: f can be written as the sum or product of two parts with no common variables

Symbolic Regression

In physics and in lots of science applications, functions we care about tend to be nice in the following ways:

1. Units: Can use this to transform the problem to fewer independent variables
2. Low degree polynomials: Can use this to do polynomial fits for parts of f
3. Compositionality: Can use brute force for parts of the function
4. Smoothness: f can be learned by a NN
5. Symmetry: f comes with translational, rotational, and scaling symmetry with respect to some variables
6. Separability: f can be written as the sum or product of two parts with no common variables

Symbolic Regression

In physics and in lots of science applications, functions we care about tend to be nice in the following ways:

1. Units: Can use this to transform the problem to fewer independent variables
2. Low degree polynomials: Can use this to do polynomial fits for parts of f
3. Compositionality: Can use brute force for parts of the function
4. Smoothness: f can be learned by a NN
5. Symmetry: f comes with translational, rotational, and scaling symmetry with respect to some variables
6. Separability: f can be written as the sum or product of two parts with no common variables

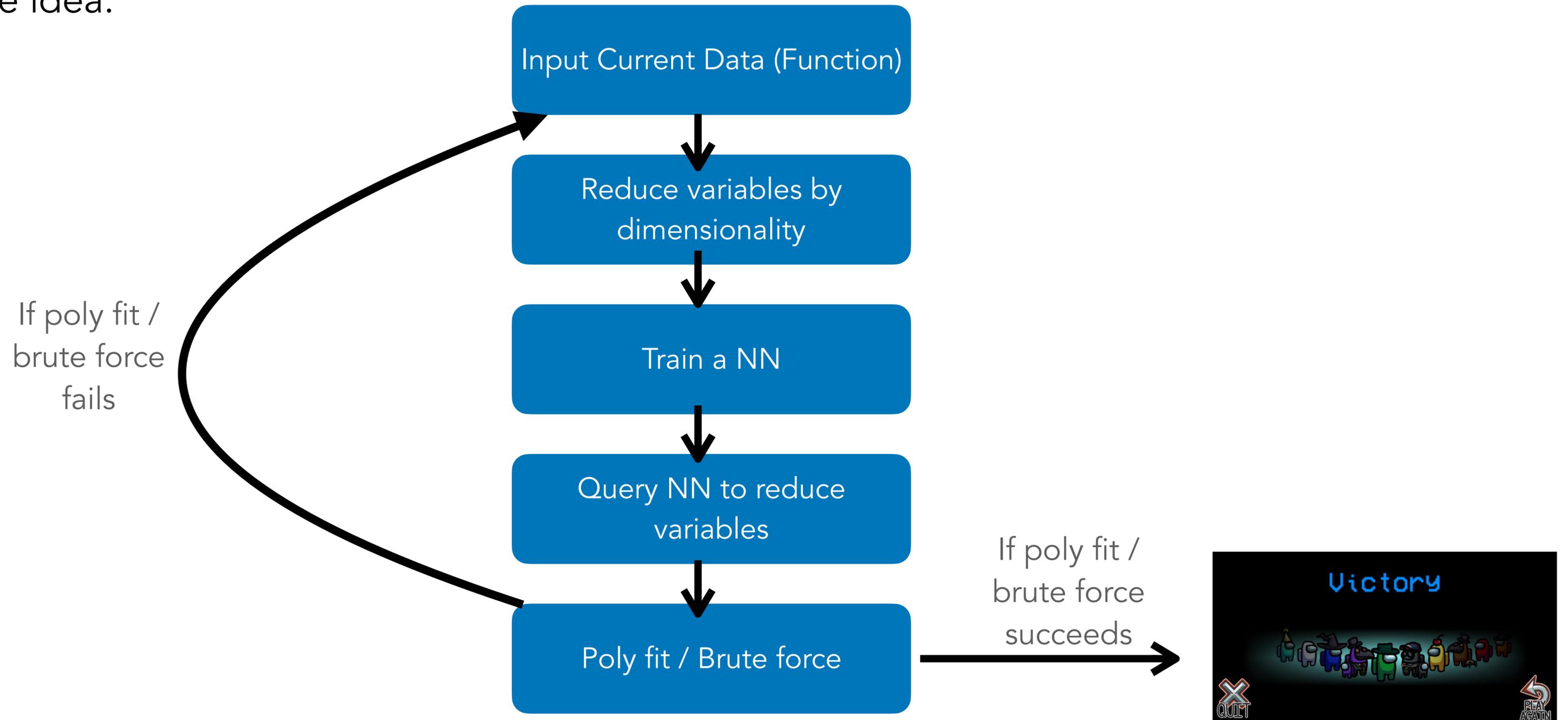
Symbolic Regression

In physics and in lots of science applications, functions we care about tend to be nice in the following ways:

1. Units: Can use this to transform the problem to fewer independent variables
2. Low degree polynomials: Can use this to do polynomial fits for parts of f
3. Compositionality: Can use brute force for parts of the function
4. Smoothness: f can be learned by a NN
5. Symmetry: Can be tested by a neural network trained on the data
6. Separability: Can be tested by a neural network trained on the data

Symbolic Regression

The idea:

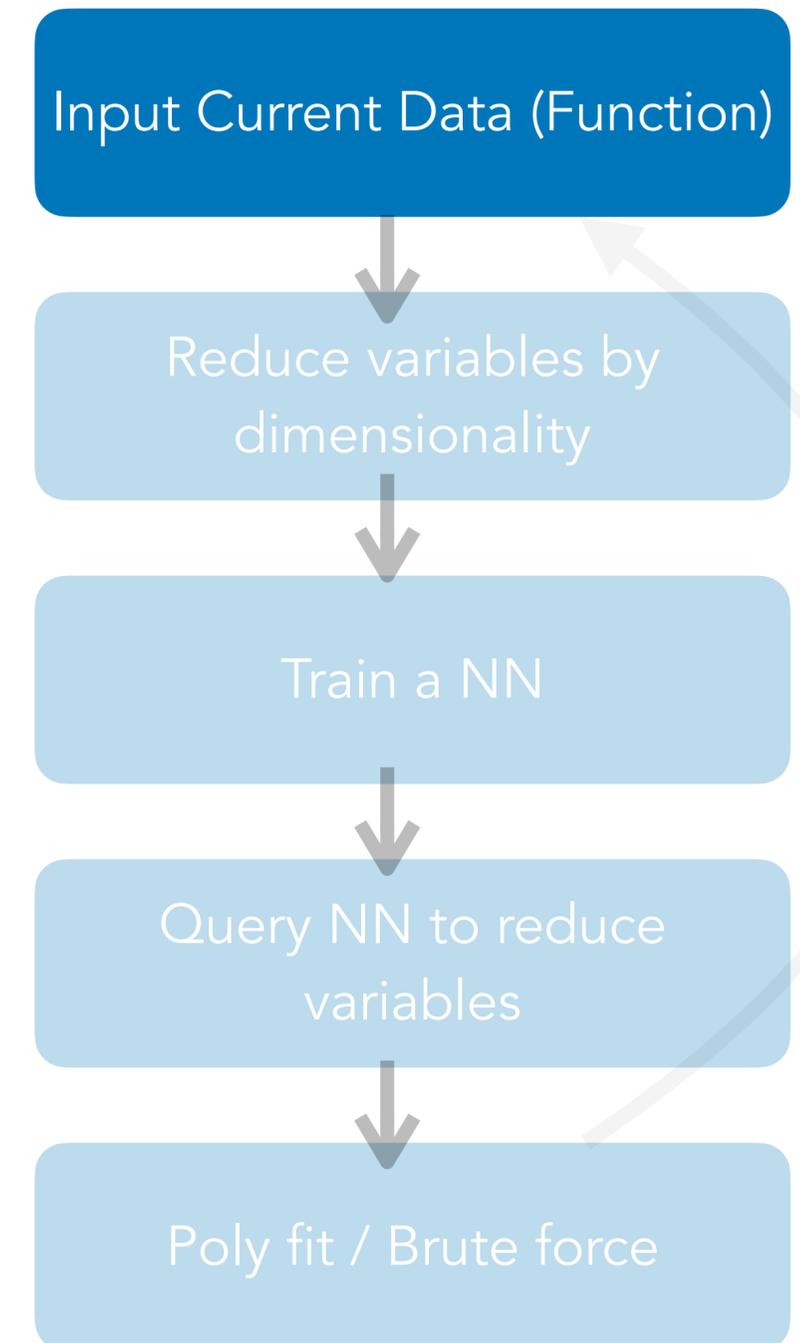


Symbolic Regression - Example

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

```

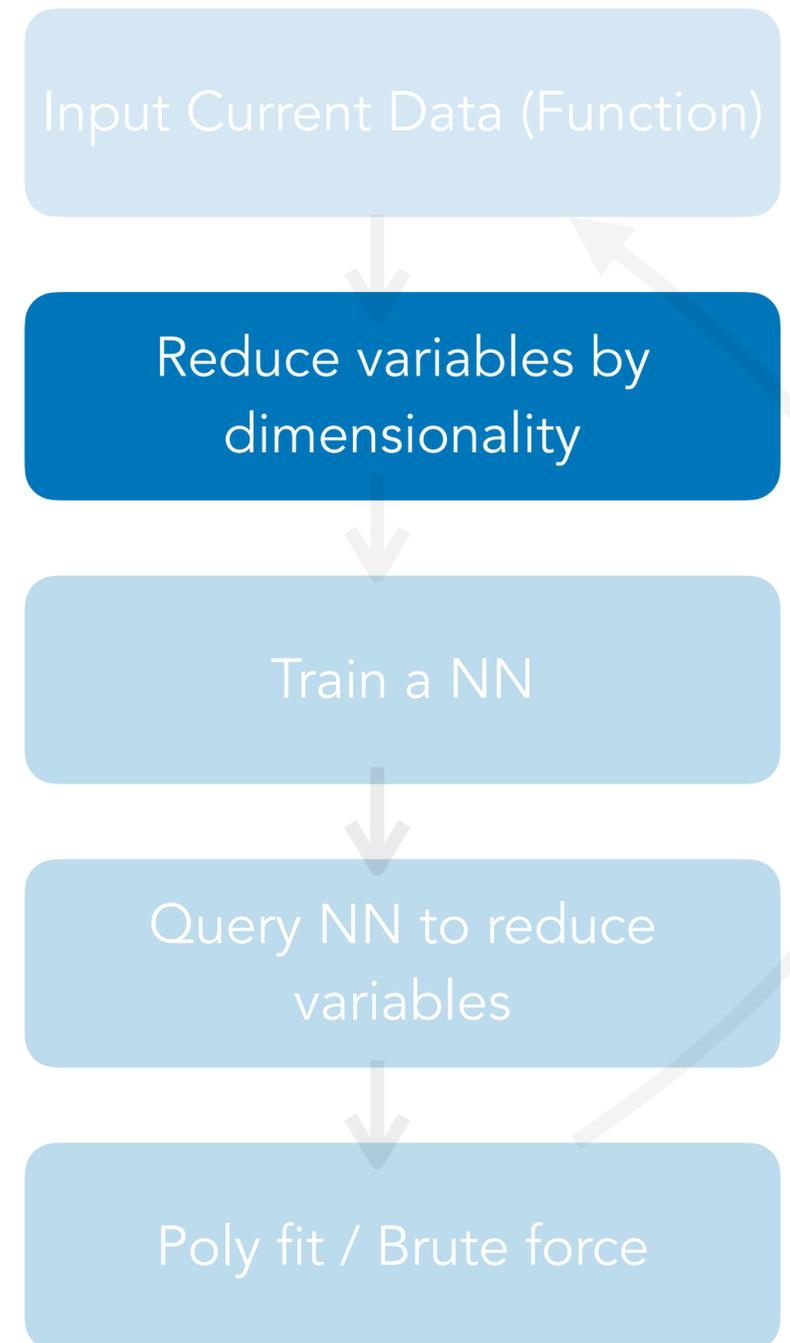
1.1431209959193709 2.7700644791483753 1.7508575540193472 0.23452895063856676
2.4680655653881054 2.2073166947348444 1.7761705838854234 0.15919403345867914
2.7621479700455853 1.4168131204210188 1.5378176974809339 0.14429337334417677
1.9536888384746354 2.7336267945043491 1.2592849110534683 0.15360014539410058
2.1532278876457527 1.5016008010765851 1.4218686278023172 0.18514940761978987
1.9899434091665062 1.4250958039594244 2.5409132056932424 0.17131474581788358
1.2841783534277345 2.5038413591290976 1.2255232096430668 0.18928439532548705
2.3550853261290494 2.2555822345853405 1.4525468706453792 0.15982929556091857
2.7529820467784543 2.6405850369222492 1.6148891450043024 0.13519598787103054
1.2043936184306594 1.4441117081403013 1.4546229392136278 0.33122650381723288
1.3423962980280737 2.0552387587225684 2.8071816262301414 0.25403615776576924
1.4156715177406782 1.0577553334831364 2.5122383795854709 0.16623813635214552
2.0187117984150182 1.0672568295716016 1.4729243386484654 0.19367199411465894
1.5109507435415031 2.5932595628763617 2.9492633493443927 0.25680582940703343
2.5078719313855347 1.0771974670079432 2.7296063077362385 0.12803644285479733
1.4846972064278652 2.7401242687034313 1.3356870260708698 0.17177799061908141
2.1398682204221178 1.5010412666279194 2.0784556152016664 0.17976791449866503
1.7000728811732311 1.5155671571998763 1.5295642030291683 0.23465391617605863
2.3516545980830331 1.0329627134609363 2.4473327905843174 0.14157574334122566
2.6157973581192184 2.0432144044920815 1.4576627239471807 0.14873897153317067
    
```



Symbolic Regression - Example

Idea: Because f is dimensionally consistent, we can factor it into a component that encodes the dimension and a dimensionless term

$$\frac{Gm_1m_2}{(x_2 - x_1)^2 + (y_2 - y_1)^2 + (z_2 - z_1)^2}$$
$$\frac{Gm_1^2}{x_1^2} \cdot \frac{m_2}{\left(\frac{x_2}{x_1} - 1\right)^2 + \left(\frac{y_2}{x_1} - \frac{y_1}{x_1}\right)^2 + \left(\frac{z_2}{x_1} - \frac{z_1}{x_1}\right)^2}$$

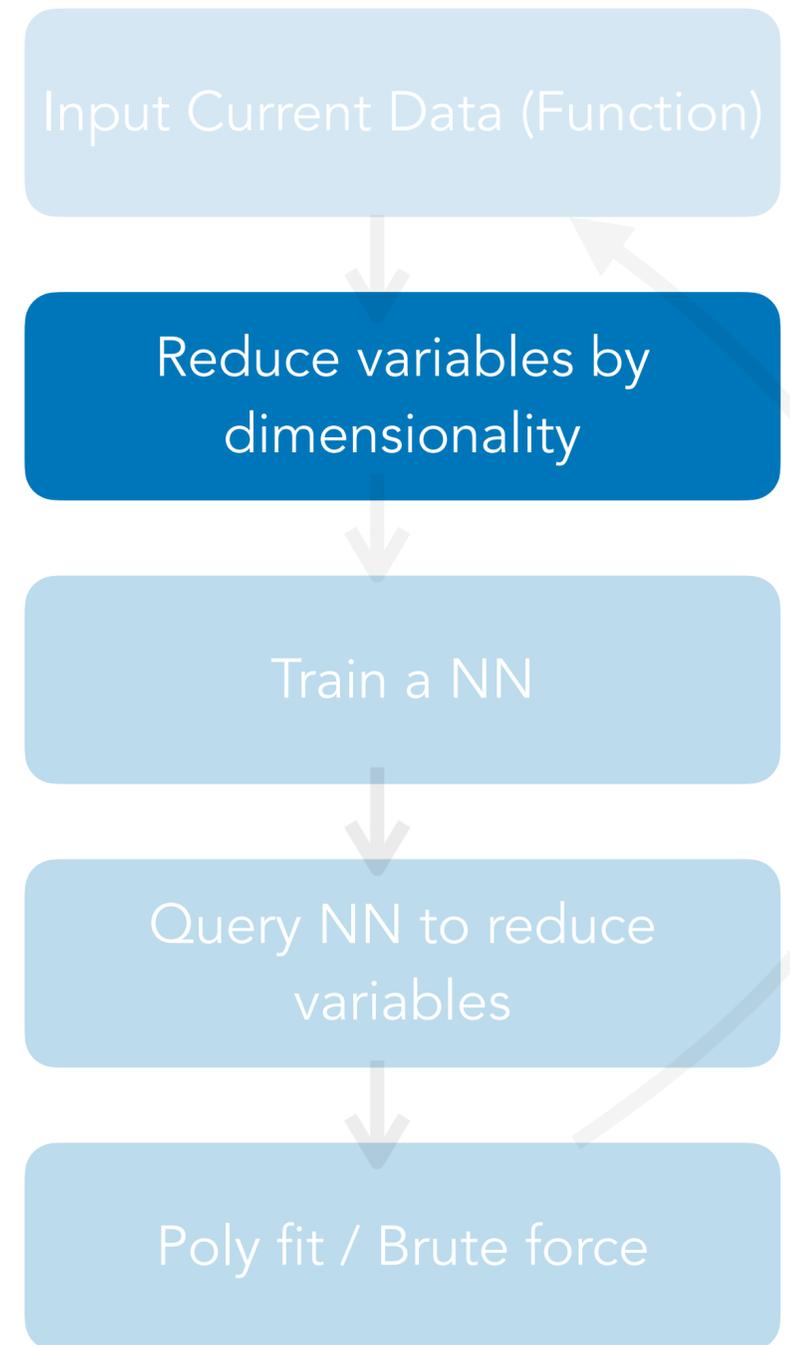


Symbolic Regression - Example

Idea: Because f is dimensionally consistent, we can factor it into a component that encodes the dimension and a dimensionless term

This reduces the number of variables to consider.

$$\frac{Gm_1^2}{x_1^2} = \frac{Gm_1m_2}{(x_2 - x_1)^2 + (y_2 - y_1)^2 + (z_2 - z_1)^2} \cdot a$$
$$a = \frac{a}{(b - 1)^2 + (c - d)^2 + (e - f)^2}$$



Symbolic Regression - Example

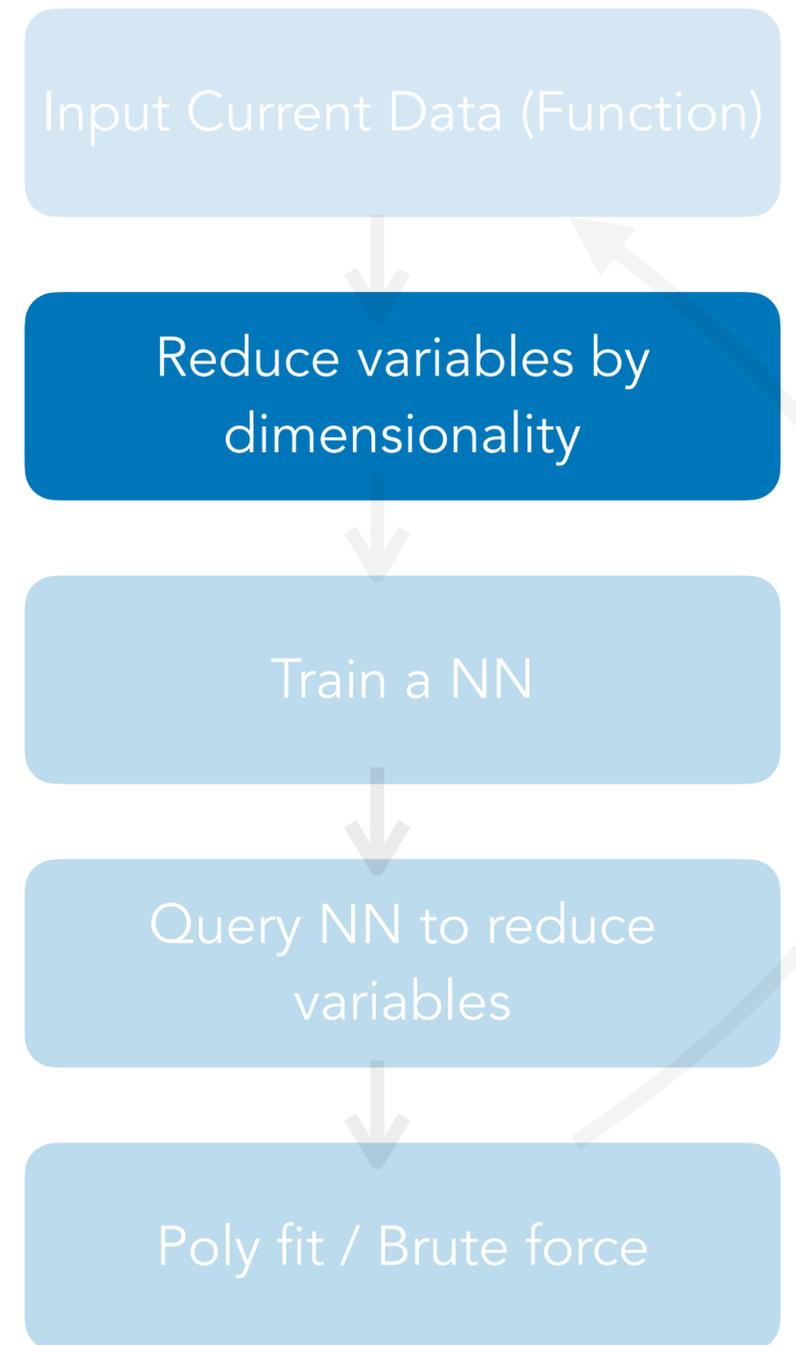
Idea: Because f is dimensionally consistent, we can factor it into a component that encodes the dimension and a dimensionless term

Represent each variable x_i by a 5 integer vector \mathbf{u}_i corresponding to the fundamental units of the vector (being meter, second, kilogram, kelvin, volt). Let \mathbf{M} be a matrix whose i th column is \mathbf{u}_i . Define \mathbf{b} to be the corresponding vector for y .

Let \mathbf{p} be a solution to $\mathbf{M}\mathbf{p} = \mathbf{b}$ and \mathbf{U} be a basis for the null space of \mathbf{M}

Then apply

$$x_i \mapsto \prod_{j=1}^n x_j^{U_{ij}}, y \mapsto \frac{y}{y_*}, \text{ where } y_* = \prod_{i=1}^n x_i^{P_i}$$



Symbolic Regression - Example

Train a NN on the transformed columns. This is a black box oracle that we can query.

$$\frac{a}{(b - 1)^2 + (c - d)^2 + (e - f)^2}$$

Architecture used:

Dimension of layers: (128,128,128,64,64,64)

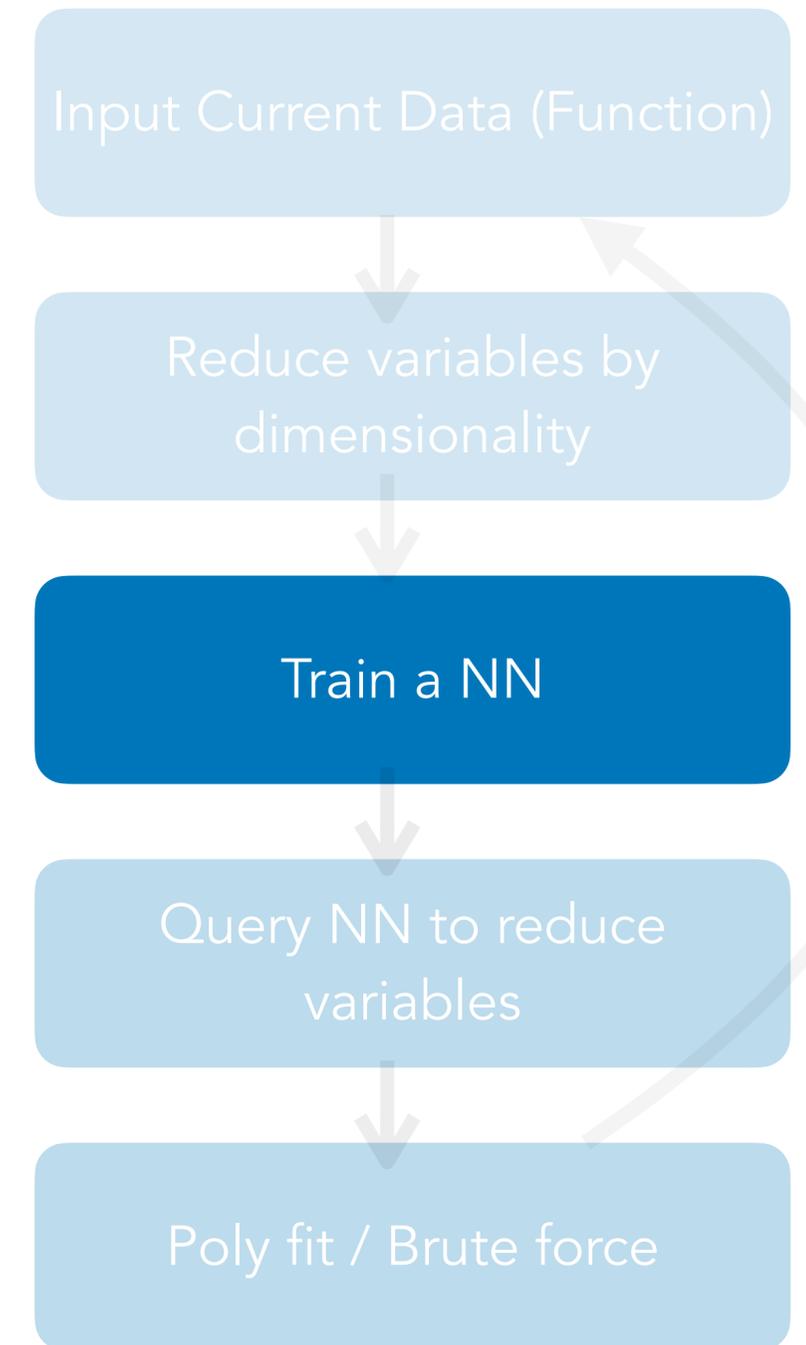
Epochs: 100

Learning rate: 0.005

Batch Size: 2048

Rms loss and Adam optimization

Weight decay: 10^{-2}



Symbolic Regression - Example

Test for symmetry, separability, and other properties and reduce variables accordingly

$$\frac{a}{(b-1)^2 + (c-d)^2 + (e-f)^2}$$

| Translational Symmetry

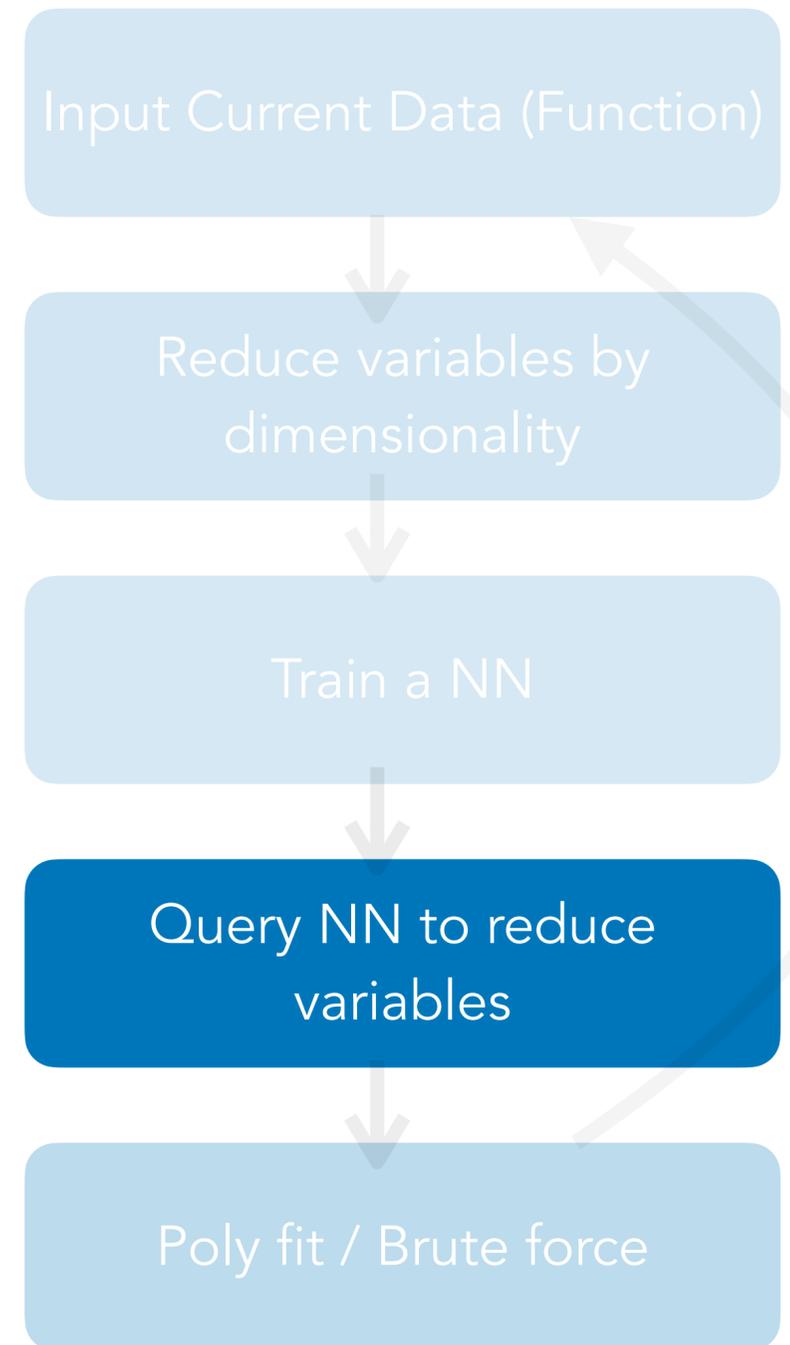
$$\frac{a}{(b-1)^2 + g^2 + (e-f)^2}$$

| Translational Symmetry

$$\frac{a}{(b-1)^2 + g^2 + h^2}$$

| Multiplicative Separability

$$a \cdot \frac{1}{(b-1)^2 + g^2 + h^2}$$



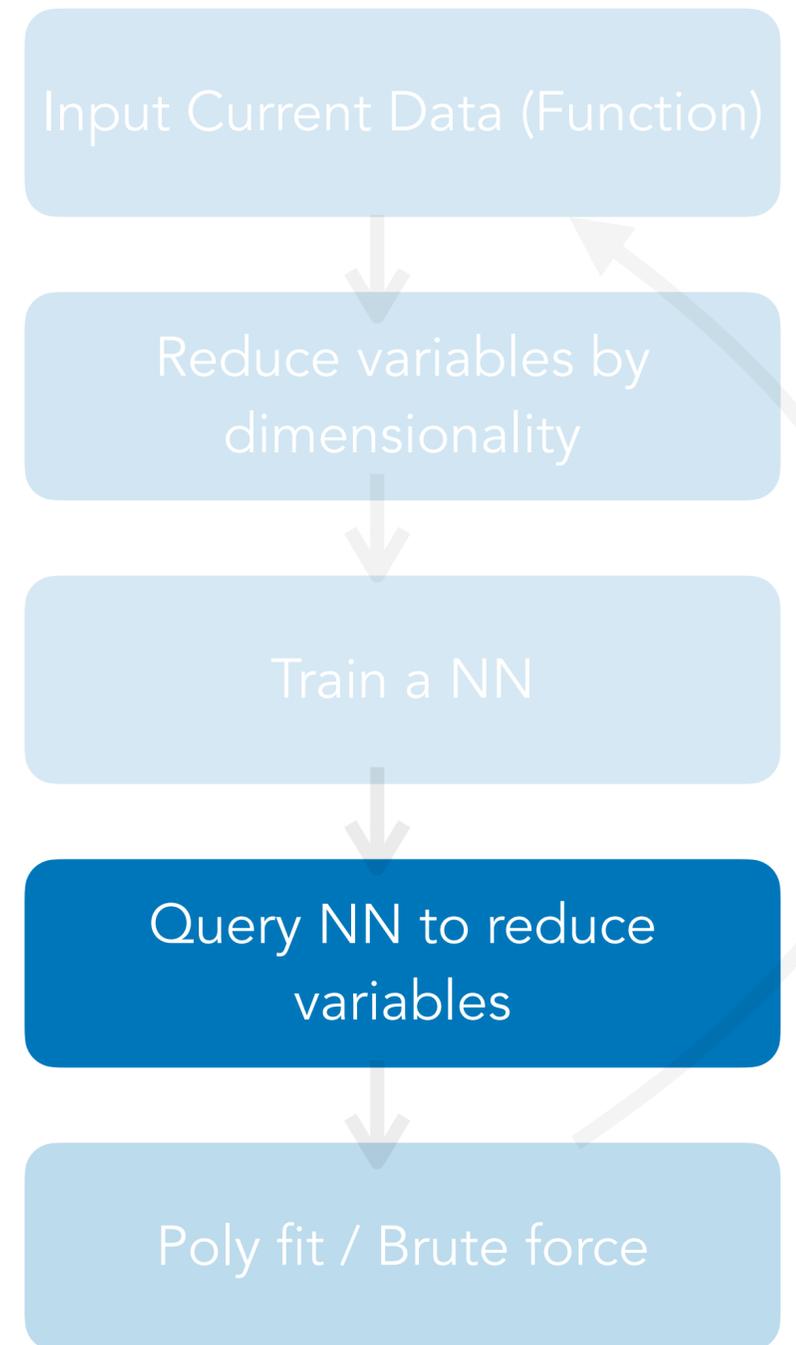
Symbolic Regression - Example

Translational Symmetry

Let $F(x_1, \dots, x_n)$ be the function learned by the neural network. Then translational symmetry with respect to x_1 and x_2 corresponds to

$$F(x_1 + a, x_2 + a, x_3, \dots, x_n) - F(x_1, x_2, \dots, x_n) \approx 0$$

If the difference is $< \epsilon_{\text{sym}}$, then apply $x_1 \mapsto x_2 - x_1$



Symbolic Regression - Example

Multiplicative Separability

f is multiplicatively separable in x_1, x_2 if f can be factored as

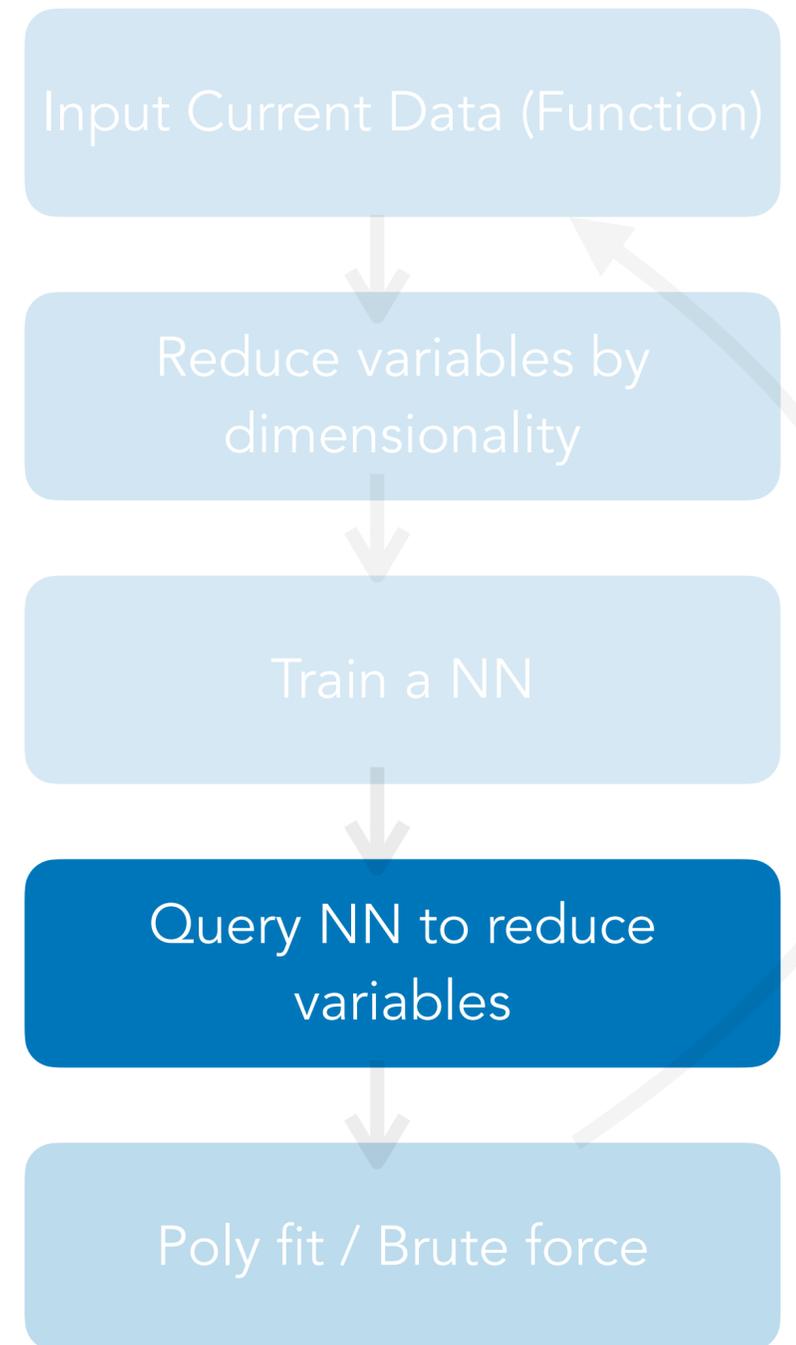
$$f(x_1, x_2) = g(x_1)h(x_2)$$

With no common variables.

To test this, pick constants c_1, c_2 and check if

$$f(x_1, x_2) = \frac{f(x_1, c_2) \cdot f(c_1, x_2)}{f(c_1, c_2)}$$

Up to ϵ_{sep} . If so, then separate the problem of learning f into two subproblems of learning g and h



Symbolic Regression - Example

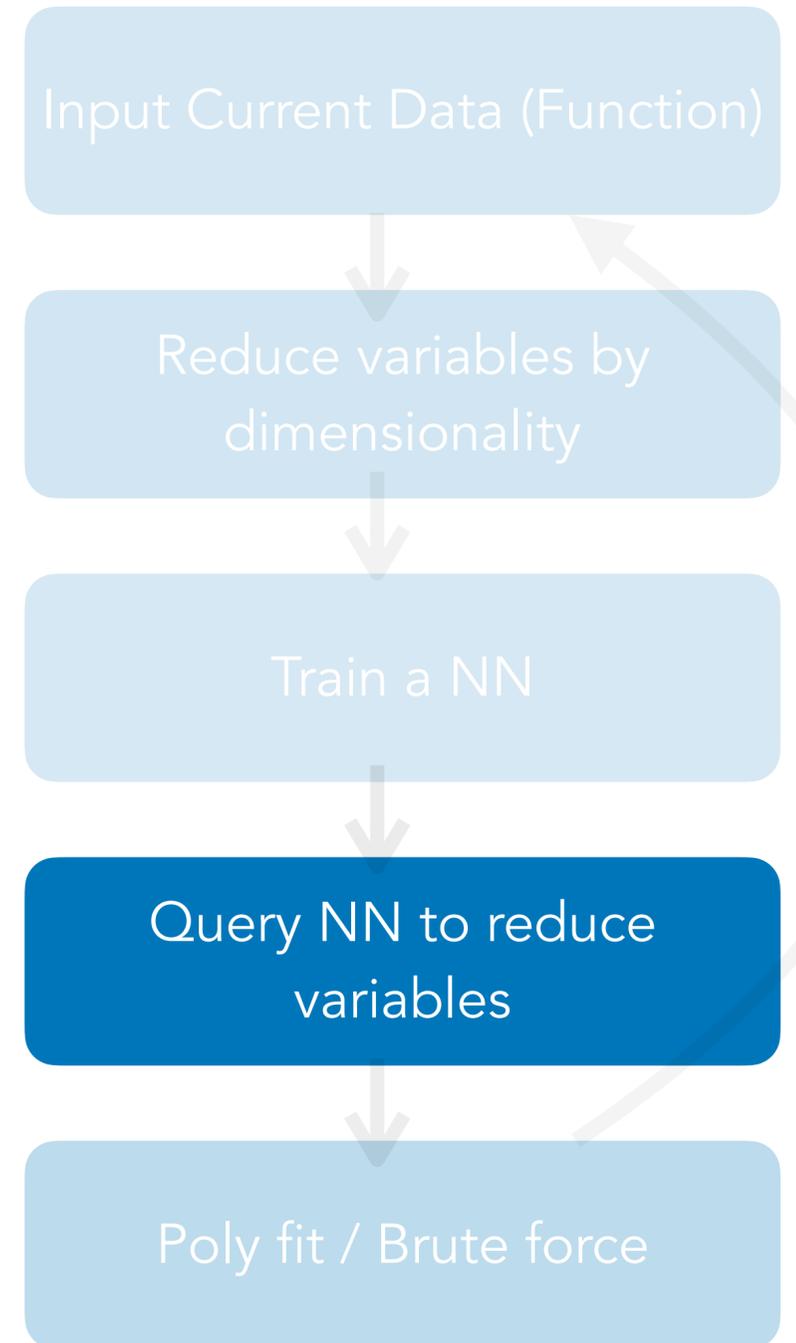
Translational Symmetry

Multiplicative Separability

Rotational Symmetry

Scaling Symmetry

Additive Separability



Symbolic Regression - Example

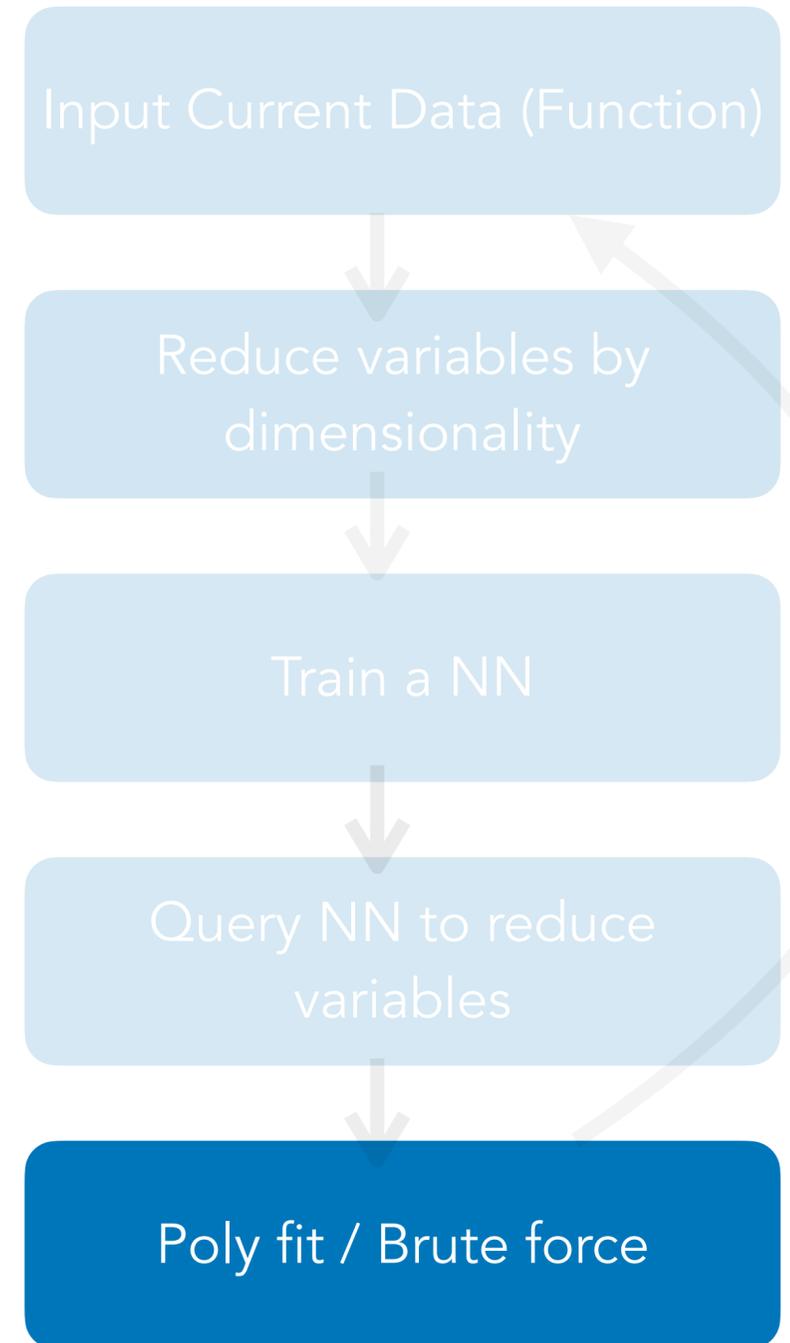
Test brute force / polynomial fit

$$a$$


A green checkmark is positioned below the variable a . A thin black line extends from the top right of a towards the top right of the page.

$$\frac{1}{(b-1)^2 + g^2 + h^2}$$


A green checkmark is positioned below the denominator of the fraction. A thin black line extends from the top left of the fraction towards the top left of the page.



Symbolic Regression - Example

Test brute force / polynomial fit

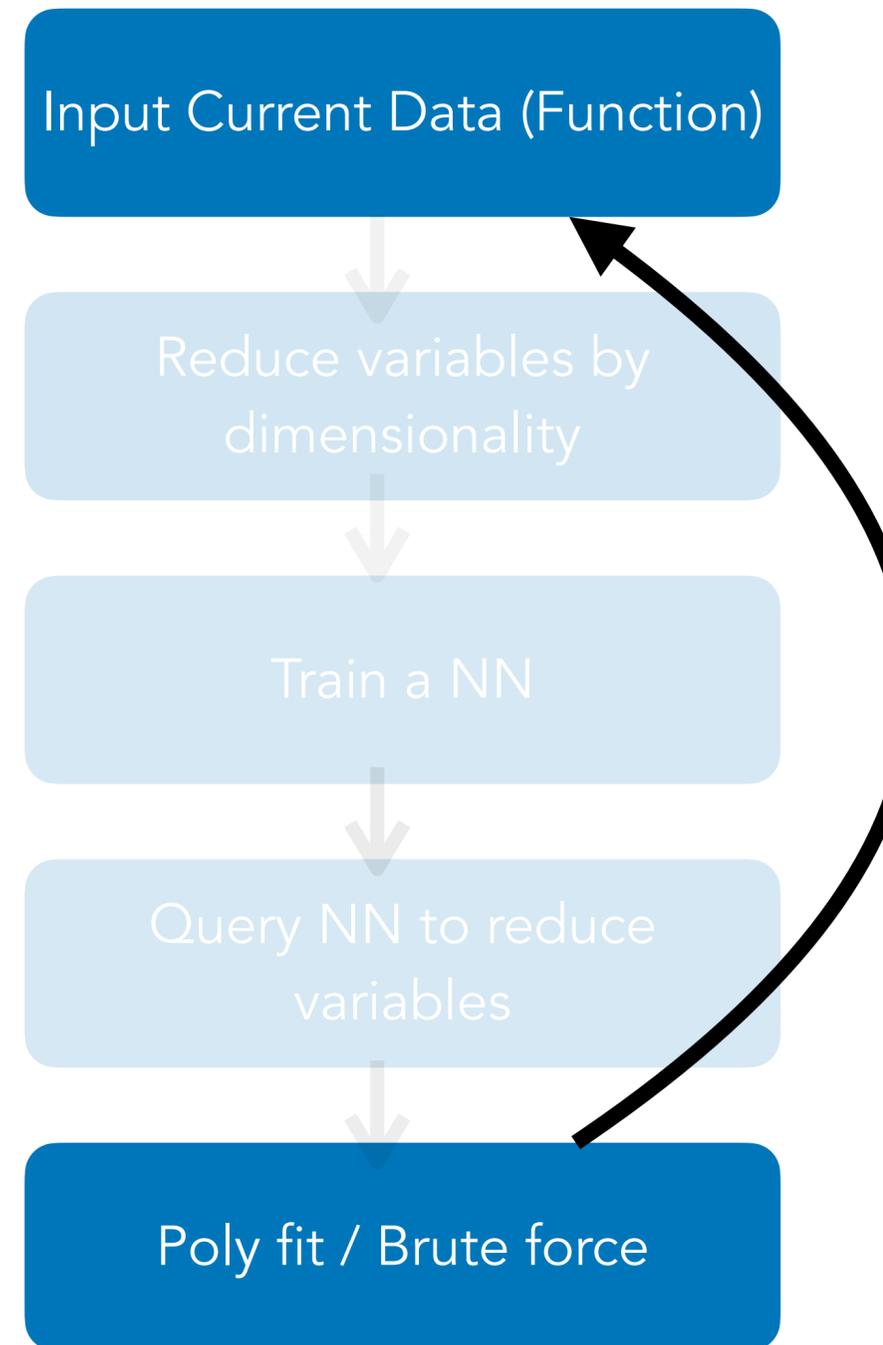
$$a$$

✓

$$\frac{1}{(b-1)^2 + g^2 + h^2}$$

✓

If this fails, then recursively take the smaller problems and rerun



Symbolic Regression - Example

This was tested on 100 equations from Feynman's lecture notes and 20 harder equations

Feynman eq.	Equation	Feynman eq.	Equation	Source	Equation
I.6.20a	$f = e^{-\theta^2/2} / \sqrt{2\pi}$	II.2.42	$P = \frac{\kappa(T_2 - T_1)A}{d}$		
I.6.20	$f = e^{-\frac{\theta^2}{2\sigma^2}} / \sqrt{2\pi\sigma^2}$	II.3.24	$F_E = \frac{P}{4\pi r^2}$	Rutherford Scattering	$A = \left(\frac{Z_1 Z_2 \alpha \hbar c}{4E \sin^2(\frac{\theta}{2})} \right)^2$
I.6.20b	$f = e^{-\frac{(\theta - \theta_1)^2}{2\sigma^2}} / \sqrt{2\pi\sigma^2}$	II.4.23	$V_e = \frac{q}{4\pi\epsilon r}$	Friedman Equation	$H = \sqrt{\frac{8\pi G}{3} \rho - \frac{k_f c^2}{a_f^2}}$
I.8.14	$d = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}$	II.6.11	$V_e = \frac{1}{4\pi\epsilon} \frac{p_d \cos \theta}{r^2}$	Compton Scattering	$U = \frac{E}{1 + \frac{E}{mc^2}(1 - \cos \theta)}$
I.9.18	$F = \frac{Gm_1 m_2}{(x_2 - x_1)^2 + (y_2 - y_1)^2 + (z_2 - z_1)^2}$	II.6.15a	$E_f = \frac{3}{4\pi\epsilon} \frac{p_d z}{r^5} \sqrt{x^2 + y^2}$	Radiated gravitational wave power	$P = -\frac{32}{5} \frac{G^4}{c^5} \frac{(m_1 m_2)^2 (m_1 + m_2)}{r^5}$
I.10.7	$m = \frac{m_0}{\sqrt{1 - \frac{v^2}{c^2}}}$	II.6.15b	$E_f = \frac{3}{4\pi\epsilon} \frac{p_d}{r^3} \cos \theta \sin \theta$	Relativistic aberration	$\theta_1 = \arccos \left(\frac{\cos \theta_2 - \frac{v}{c}}{1 - \frac{v}{c} \cos \theta_2} \right)$
I.11.19	$A = x_1 y_1 + x_2 y_2 + x_3 y_3$	II.8.7	$E = \frac{3}{5} \frac{q^2}{4\pi\epsilon d}$	N-slit diffraction	$I = I_0 \left[\frac{\sin(\alpha/2)}{\alpha/2} \frac{\sin(N\delta/2)}{\sin(\delta/2)} \right]^2$
I.12.1	$F = \mu N_n$	II.8.31	$E_{den} = \frac{\epsilon E_f^2}{2}$	Goldstein 3.16	$v = \sqrt{\frac{2}{m} \left(E - U - \frac{L^2}{2mr^2} \right)}$
I.12.2	$F = \frac{q_1 q_2}{4\pi\epsilon r^2}$	II.10.9	$E_f = \frac{\sigma_{den}}{\epsilon} \frac{1}{1 + \chi}$	Goldstein 3.55	$k = \frac{mk_G}{L^2} \left(1 + \sqrt{1 + \frac{2EL^2}{mk_G^2}} \cos(\theta_1 - \theta_2) \right)$
I.12.4	$E_f = \frac{q_1}{4\pi\epsilon r^2}$	II.11.3	$x = \frac{qE_f}{m(\omega_0^2 - \omega^2)}$	Goldstein 3.64 (ellipse)	$r = \frac{d(1 - \alpha^2)}{1 + \alpha \cos(\theta_1 - \theta_2)}$
I.12.5	$F = q_2 E_f$	II.11.17	$n = n_0 \left(1 + \frac{p_d E_f \cos \theta}{k_b T} \right)$	Goldstein 3.74 (Kepler)	$t = \frac{2\pi d^{3/2}}{\sqrt{G(m_1 + m_2)}}$
I.12.11	$F = q(E_f + Bv \sin \theta)$	II.11.20	$P_* = \frac{n_\rho p_d^2 E_f}{3k_b T}$	Goldstein 3.99	$\alpha = \sqrt{1 + \frac{2\epsilon^2 EL^2}{m(Z_1 Z_2 q^2)^2}}$
I.13.4	$K = \frac{1}{2} m(v^2 + u^2 + w^2)$	II.11.27	$P_* = \frac{n\alpha}{1 - n\alpha/3} \epsilon E_f$	Goldstein 8.56	$E = \sqrt{(p - qA_{vec})^2 c^2 + m^2 c^4} + qV_e$
I.13.12	$U = Gm_1 m_2 \left(\frac{1}{r_2} - \frac{1}{r_1} \right)$	II.11.28	$\theta = 1 + \frac{n\alpha}{1 - (n\alpha/3)}$	Goldstein 12.80	$E = \frac{1}{2m} [p^2 + m^2 \omega^2 x^2 (1 + \alpha \frac{x}{y})]$
I.14.3	$U = mgz$	II.13.17	$B = \frac{1}{4\pi\epsilon c^2} \frac{2I}{r}$	Jackson 2.11	$F = \frac{q}{4\pi\epsilon y^2} \left[4\pi\epsilon V_e d - \frac{qdy^3}{(y^2 - d^2)^2} \right]$
I.14.4	$U = \frac{k_{spring} x^2}{2}$	II.13.23	$\rho_c = \frac{\rho_{c0}}{\sqrt{1 - v^2/c^2}}$		
I.15.3x	$x_1 = \frac{x - ut}{\sqrt{1 - u^2/c^2}}$	II.13.34	$j = \frac{\rho_{c0} v}{\sqrt{1 - v^2/c^2}}$		
I.15.3t	$t_1 = \frac{t - ux/c^2}{\sqrt{1 - u^2/c^2}}$	II.15.4	$E = -\mu_M B \cos \theta$		
I.15.10	$p = \frac{m_0 v}{\sqrt{1 - v^2/c^2}}$	II.15.5	$E = -p_d E_f \cos \theta$		
I.16.6	$v_1 = \frac{u + v}{1 + uv/c^2}$	II.21.32	$V_e = \frac{q}{4\pi\epsilon r(1 - v/c)}$		
I.18.4	$r = \frac{m_1 r_1 + m_2 r_2}{m_1 + m_2}$	II.24.17	$k = \sqrt{\frac{\omega^2}{c^2} - \frac{\pi^2}{d^2}}$		
		II.27.16	$F_E = \epsilon c E_f^2$		
		II.27.18	$E_{den} = \epsilon E_f^2$		
		II.34.2a	$I = \frac{qv}{2\pi r}$		
		II.34.2	$\mu_M = \frac{qvr}{2}$		
		II.34.11	$\omega = \frac{g - q\dot{B}}{2m}$		

Symbolic Regression - Example

This was tested on 100 equations from Feynman's lecture notes and 20 harder equations

The success rate was better than existing state of the art:

Equation Set	Eureqa (Benchmark)	AI Feynman (with DA)	AI Feynman (without DA)
100 Feynman Lecture Equations	68%	100%	93%
20 "Bonus" Equations	15%	90%	?

Symbolic Regression - Example

Couple of interesting notes:

1. Failure cases. For example, the Radiational Gravitational Waves equation:

$$P = -\frac{32 G^4 (m_1 m_2)^2 (m_1 + m_2)}{5 c^5 r^5} \longrightarrow y = -\frac{32 a^2 (1 + a)}{5 b^5}$$

In reverse polish notation, this is the string

$$aaa > ** bbbbb **** */$$

Which would take too long to solve. This is separable, but the 5th power in the denominator cause a wide dynamic range and so it was not detected

Symbolic Regression - Example

Couple of interesting notes:

2. Noise: Performance was consistent up to Gaussian noise levels of $\epsilon = 10^{-4}$ but dropped by 50% with noise around $\epsilon = 10^{-2}$.

The thresholds were not adjusted to each problem so the tolerance can probably be improved.

Symbolic Regression - Example

Couple of interesting notes:

3. Constants: Constants were treated as their own variables and symbols in the data. It's not clear otherwise how we would discover relations such as $G\sqrt{\pi}$, $\frac{G^4}{c^5}$, etc.

But how do we learn these specific relationships with real data?

Symbolic Regression

Problems:

1. Sensitivity to noise
2. Constant Relationships are difficult to detect
3. Require lots of data to train a neural network

Incorporate physics knowledge
into the search

Approach 2: Symbolic Regression
with background knowledge

Approach 2: Symbolic Regression with background knowledge

In particular, we will very briefly look at the approach in this paper:

nature communications



Article

<https://doi.org/10.1038/s41467-023-37236-y>

Combining data and theory for derivable scientific discovery with AI-Descartes

Received: 28 October 2021

Accepted: 8 March 2023

Published online: 12 April 2023

Check for updates

Cristina Cornelio^{1,2} ✉, Sanjeeb Dash¹, Vernon Austel¹, Tyler R. Josephson^{3,4}, Joao Goncalves¹, Kenneth L. Clarkson¹, Nimrod Megiddo¹, Bachir El Khadir¹ & Lior Horesh^{1,5} ✉

Scientists aim to discover meaningful formulae that accurately describe experimental data. Mathematical models of natural phenomena can be manually created from domain knowledge and fitted to data, or, in contrast, created automatically from large datasets with machine-learning algorithms. The problem of incorporating prior knowledge expressed as constraints on the functional form of a learned model has been studied before, while finding models that are consistent with prior knowledge expressed via general logical axioms is an open problem. We develop a method to enable principled derivations of models of natural phenomena from axiomatic knowledge and experimental data by combining logical reasoning with symbolic regression. We demonstrate these concepts for Kepler's third law of planetary motion, Einstein's relativistic time-dilation law, and Langmuir's theory of adsorption. We show we can discover governing laws from few data points when logical reasoning is used to distinguish between candidate formulae having similar error on the data.

Symbolic Regression with Background Knowledge

Key Idea:

Use symbolic regression methods to generate lots of candidates for the formula



Given some background theory B , use an Automated Theorem Prover (ATP) to rank and prove these candidates. Select the

Symbolic Regression with Background Knowledge

Main Contributions:

1. Incorporating a derivability module into the search.

Candidate Formula

$$f = \frac{p}{1.507x_1 + 0.302x_2}$$



Derivability - Prove the Formula

$$B \rightarrow \frac{p}{1.507x_1 + 0.302x_2}$$



Existential Derivability

$$\exists c_1, c_2 \text{ s.t. } B \rightarrow \frac{p}{c_1x_1 + c_2x_2}$$

Confirm Functional Form



Run your favorite method of fitting parameters

Symbolic Regression with Background Knowledge

Main Contributions:

2. If not derivable, then have the theorem proved derive bounds on the error between candidate function and functions derivable from the background theory

Point wise
reasoning error

$$\beta_2^r = \sqrt{\sum_{i=1}^m \frac{f(x_i) - f_{\mathcal{B}}(x_i)}{f_{\mathcal{B}}(x_i)}}$$

Generalized
reasoning error

$$\beta_{\infty}^r = \sqrt{\sum_{i=1}^m \frac{f(x_i) - f_{\mathcal{B}}(x_i)}{f_{\mathcal{B}}(x_i)}}$$

Symbolic Regression with Background Knowledge

Results: Ran this on more problems from the Feynman notes as well as supplementary problems.

Label	Formula	AI-Descartes	AI Feynman	PySR	BMS
Π.11.20	$n_p p_d^2 E_f / (3k_b T)$	✓ ¹	X	X	✓ ²
Π.11.27	$\frac{n\alpha}{1-n\alpha/3} \epsilon E_f$	✓ ¹	X	X	X
Π.11.28	$1 + \frac{n\alpha}{1-n\alpha/3}$	✓ ¹	X	X	X
Π.13.17	$\frac{1}{4\pi\epsilon_0} \frac{2I}{r}$	✓ ¹	X	✓ ¹	X
Π.13.23	$\frac{\rho_{c0}}{\sqrt{1-v^2/c^2}}$	✓ ¹	X	X	X
Π.13.34	$\frac{\rho_{c0} v}{\sqrt{1-v^2/c^2}}$	X	X	X	X
Π.21.32	$\frac{q}{4\pi\epsilon r(1-v/c)}$	X	X	X	X
Π.24.17	$\sqrt{\frac{\omega^2}{c^2} - \frac{\pi^2}{d^2}}$	X	X	X	X
Π.27.16	$\epsilon c E_f^2$	✓	X	✓	✓
Π.27.18	ϵE_f^2	✓ ¹	✓ ¹	✓	✓
Π.34.2a	$qv/(2\pi r)$	✓ ¹	✓ ¹	✓ ¹	✓ ¹
Π.34.2	$qvr/2$	✓ ¹	✓ ¹	✓ ¹	✓ ¹
Π.34.11	$gqB/(2m)$	✓	✓ ¹	✓ ¹	✓ ¹
Π.34.29a	$qh/(4\pi m)$	✓ ¹	✓ ¹	✓ ¹	✓ ¹
Π.34.29b	$g\mu_M B J_z / h$	✓ ²	X	✓ ¹	✓ ¹
Π.35.18	$\frac{n_0}{e^{\frac{mom \times B}{kb \times T}} + e^{\frac{-mom \times B}{(kb \times T)}}}$	X	X	X	X
Π.36.38	$\frac{\mu_m B}{k_b T} + \frac{\mu_m \alpha M}{\epsilon c^2 k_b T}$	X	X	X	X
Π.37.1	$\mu_M(1 + \chi)B$	✓ ¹	X	✓ ¹	✓ ²
Π.38.3	YAx/d	✓ ¹	✓ ²	✓	✓ ²
Π.38.14	$\frac{Y}{2(1+\sigma)}$	✓ ¹	✓ ²	X	✓ ²
	Accuracy	86.67%	80%	73.33%	80%

Symbolic Regression with Background Knowledge

Some Comments:

Failure Cases:

Most of the failure cases came from when the theorem prover could not prove derivability or good bounds on the error.

Approach 3: Polynomial Optimization

Approach 3: Polynomial Optimization

In particular, we will look at the approach in this paper:

nature communications



Article

<https://doi.org/10.1038/s41467-024-50074-w>

Evolving scientific discovery by unifying data and background knowledge with AI Hilbert

Received: 23 September 2023

Accepted: 27 June 2024

Published online: 14 July 2024

Check for updates

Ryan Cory-Wright¹✉, Cristina Cornelio², Sanjeeb Dash³, Bachir El Khadir³ & Lior Horesh³

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. However, this does not include experimental data within the discovery process, which may be inefficient. We propose a solution to this problem when all axioms and scientific laws are expressible as polynomials and argue our approach is widely applicable. We model notions of minimal complexity using binary variables and logical constraints, solve polynomial optimization problems via mixed-integer linear or semidefinite optimization, and prove the validity of our scientific discoveries in a principled manner using Positivstellensatz certificates. We demonstrate that some famous scientific laws, including Kepler's Law of Planetary Motion and the Radiated Gravitational Wave Power equation, can be derived in a principled manner from axioms and experimental data.

Polynomial Optimization

Key Idea: There are a lot of laws in science that can be transformed to polynomial expressions.

Examples:

Kepler's Third Law: $p = \sqrt{\frac{4\pi^2(d_1 + d_2)^3}{G(m_1 + m_2)}} \mapsto p^2 G(m_1 + m_2) - 4\pi^2(d_1 + d_2)^3$

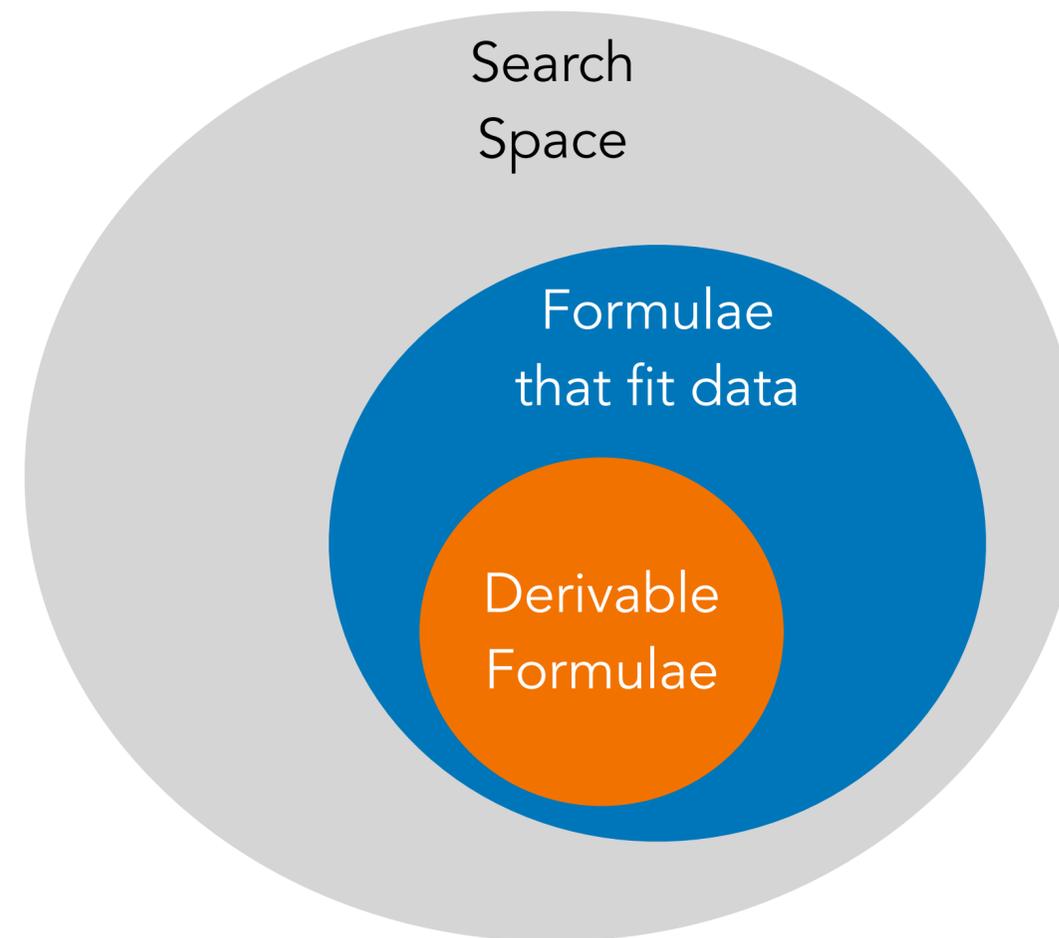
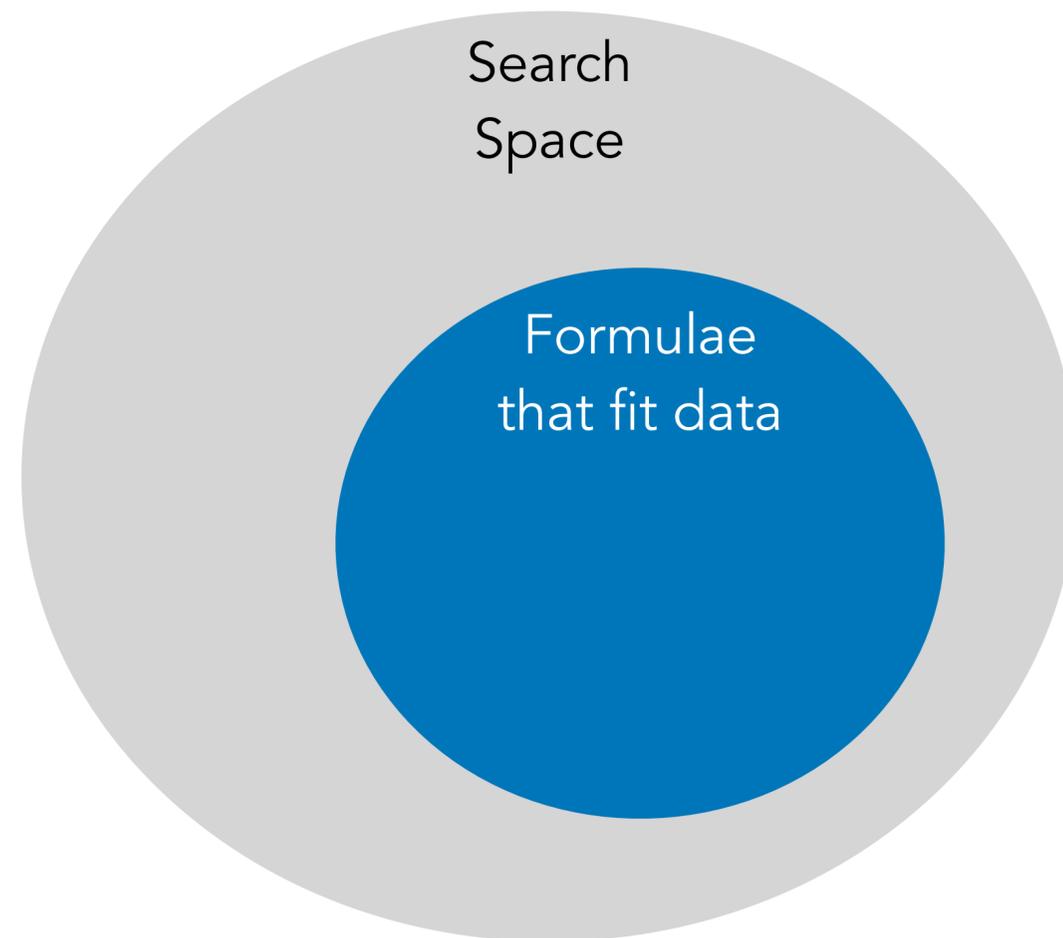
Compton Scattering Equation: $\lambda_2 - \lambda_1 = \frac{h}{m_e c}(1 - \cos \theta) \mapsto (\lambda_2 - \lambda_1) h m_e c^3 (1 + \cos \theta)$

Note: We will model things after polynomials and polynomial inequalities. We will not deal with diffeqs and trig inequalities directly, but we can get some mileage as we will see.

Polynomial Optimization

Key Idea: There are a lot of laws in science that can be transformed to polynomial expressions.

Previous methods:

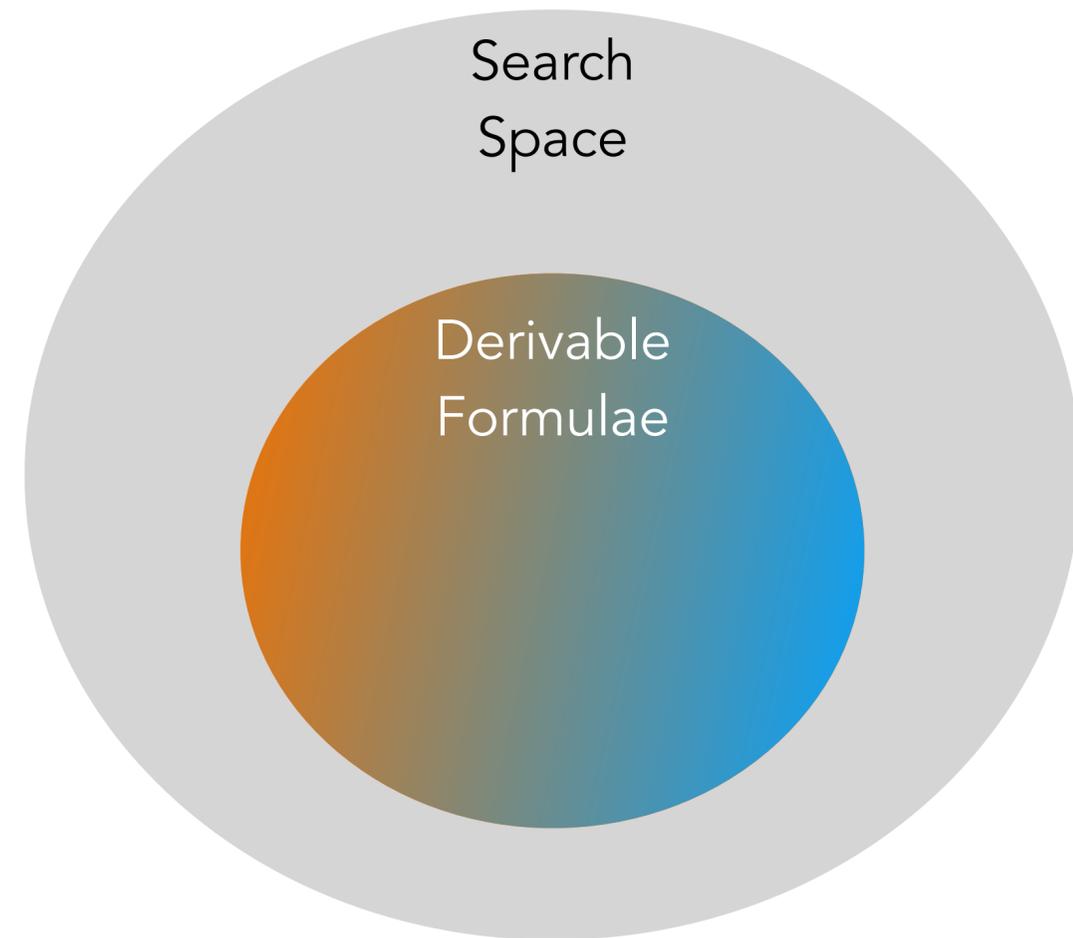


-  Symbolic Regression
-  Theorem Prover

Polynomial Optimization

Key Idea: There are a lot of laws in science that can be transformed to polynomial expressions.

This work:



-  Polynomial Optimization
-  Algebraic Geometry Results

Polynomial Optimization

The idea is to solve the following optimization problem

$$\begin{aligned} \min_{q \in \mathbb{R}_{n,2d}} \quad & \sum_{\bar{\mathbf{x}}_i \in \mathcal{D}} |q(\bar{\mathbf{x}}_i)| + \lambda \cdot d^c(q, \mathcal{G} \cap \mathcal{H}) \\ \text{s.t.} \quad & \sum_{\mu \in \Omega: \mu_1 \geq 1} a_\mu = 1, \\ & a_\mu = 0 \quad \forall \mu \in \Omega: \sum_{j=t+1}^n \mu_j \geq 1, \end{aligned}$$

Polynomial Optimization

The idea is to solve the following optimization problem

$$\begin{aligned} & \min_{q \in \mathbb{R}_{n,2d}} \sum_{\bar{\mathbf{x}}_i \in \mathcal{D}} |q(\bar{\mathbf{x}}_i)| + \lambda \cdot d^c(q, \mathcal{G} \cap \mathcal{H}) \\ & \text{s.t.} \quad \sum_{\mu \in \Omega: \mu_1 \geq 1} a_\mu = 1, \\ & \quad \quad a_\mu = 0 \quad \forall \mu \in \Omega: \sum_{j=t+1}^n \mu_j \geq 1, \end{aligned}$$

Fidelity to data

This can be defined with l_2 or l_∞ loss

Polynomial Optimization

The idea is to solve the following optimization problem

$$\begin{aligned} \min_{q \in \mathbb{R}_{n,2d}} \quad & \sum_{\bar{\mathbf{x}}_i \in \mathcal{D}} |q(\bar{\mathbf{x}}_i)| + \lambda \cdot d^c(q, \mathcal{G} \cap \mathcal{H}) \\ \text{s.t.} \quad & \sum_{\mu \in \Omega: \mu_1 \geq 1} a_\mu = 1, \\ & a_\mu = 0 \quad \forall \mu \in \Omega: \sum_{j=t+1}^n \mu_j \geq 1, \end{aligned}$$

Distance between the discovered q and the background theory $\mathcal{G} \cap \mathcal{H}$

Polynomial Optimization

The idea is to solve the following optimization problem

$$\min_{q \in \mathbb{R}_{n,2d}} \sum_{\bar{x}_i \in \mathcal{D}} |q(\bar{x}_i)| + \lambda \cdot d^c(q, \mathcal{G} \cap \mathcal{H})$$

$$\text{s.t.} \quad \sum_{\mu \in \Omega: \mu_1 \geq 1} a_\mu = 1,$$

$$a_\mu = 0 \quad \forall \mu \in \Omega: \sum_{j=t+1}^n \mu_j \geq 1,$$

Want a
polynomial in x_1

Polynomial Optimization

The idea is to solve the following optimization problem

$$\begin{aligned} \min_{q \in \mathbb{R}_{n,2d}} \quad & \sum_{\bar{\mathbf{x}}_i \in \mathcal{D}} |q(\bar{\mathbf{x}}_i)| + \lambda \cdot d^c(q, \mathcal{G} \cap \mathcal{H}) \\ \text{s.t.} \quad & \sum_{\mu \in \Omega: \mu_1 \geq 1} a_\mu = 1, \\ & a_\mu = 0 \quad \forall \mu \in \Omega: \sum_{j=t+1}^n \mu_j \geq 1, \end{aligned}$$

Bound on the
complexity of the expression

Polynomial Optimization - Distance to Background

Given some axioms $h_1(\mathbf{x}), \dots, h_l(\mathbf{x}) = 0$, inequalities $g_1(\mathbf{x}) \geq 0, \dots, g_k(\mathbf{x}) \geq 0$, where $g_i, h_j \in \mathbb{R}[x_1, \dots, x_n]$ and data \mathcal{D} , define the sets

$$\mathcal{G} = \{x \in \mathbb{R}^n \mid g_i(x) = 0\} \text{ and } \mathcal{H} = \{x \in \mathbb{R}^n \mid h_j(x) \geq 0\}$$

We want to find a polynomial f such that

$$x \in \mathcal{G} \cap \mathcal{H} \implies f(x) \geq 0$$

Theorem: Putinar's Positivestellensatz

If g_i, h_k satisfy the Archimedean property, i.e. there exists R and sum of squares polynomials $\alpha_0, \dots, \alpha_l$ such that

$R - \sum_{i=1}^n x_i^2 = \alpha_0 + \sum_{i=1}^k \alpha_i g_i$, then for any degree d polynomial f , the implication above holds if and only if there exist sum of squares polynomials $\alpha_0, \dots, \alpha_k$ and real polynomials β_1, \dots, β_l such that

$$f = \alpha_0 + \sum_{i=1}^k \alpha_i g_i + \sum_{j=1}^l \beta_j h_j$$

Polynomial Optimization - Distance to Background

Given some axioms $h_1(\mathbf{x}), \dots, h_l(\mathbf{x}) = 0$, inequalities $g_1(\mathbf{x}) \geq 0, \dots, g_k(\mathbf{x}) \geq 0$, where $g_i, h_j \in \mathbb{R}[x_1, \dots, x_n]$ and data \mathcal{D} , define the sets

$$\mathcal{G} = \{x \in \mathbb{R}^n \mid g_i(x) = 0\} \text{ and } \mathcal{H} = \{x \in \mathbb{R}^n \mid h_j(x) \geq 0\}$$

We want to find a polynomial f such that

$$x \in \mathcal{G} \cap \mathcal{H} \implies f(x) \geq 0$$

Case 1: Incomplete background knowledge

$$d(q, \mathcal{G} \cap \mathcal{H}) = \min_{\alpha_i \in \Sigma_{n,2d}, \beta_j \in \mathbb{R}_{n,d}} \|\text{Coeff}(q - \alpha_0 - \sum \alpha_i g_i - \sum \beta_j h_j)\|_2$$

Polynomial Optimization - Distance to Background

Given some axioms $h_1(\mathbf{x}), \dots, h_l(\mathbf{x}) = 0$, inequalities $g_1(\mathbf{x}) \geq 0, \dots, g_k(\mathbf{x}) \geq 0$, where $g_i, h_j \in \mathbb{R}[x_1, \dots, x_n]$ and data \mathcal{D} , define the sets

$$\mathcal{G} = \{x \in \mathbb{R}^n \mid g_i(x) = 0\} \text{ and } \mathcal{H} = \{x \in \mathbb{R}^n \mid h_j(x) \geq 0\}$$

We want to find a polynomial f such that

$$x \in \mathcal{G} \cap \mathcal{H} \implies f(x) \geq 0$$

Case 2: Inconsistent background knowledge

$$d(q, \mathcal{G} \cap \mathcal{H}) = \min_{\alpha_i \in \Sigma_{n,2d}, \beta_j \in \mathbb{R}_{n,d}} \|\text{Coeff}(q - \alpha_0 - \sum \alpha_i g_i - \sum \beta_j h_j)\|_2$$

$$\text{s.t. } \alpha_i = 0 \text{ if } z_i = 0, z_i \in \{0,1\}$$

$$\beta_j = 0 \text{ if } y_j = 0, y_j \in \{0,1\}$$

$$\sum z_i + \sum y_j \leq \tau$$

Polynomial Optimization - Example

Let's say we want to discover Kepler's third law

$$p = \sqrt{\frac{4(d_1 + d_2)^3}{G(m_1 + m_2)}}$$

We have data $\{(d_1, d_2, m_1, m_2, p)_i\}$ as well as some knowledge of physics

$$d_1 m_1 - d_2 m_2 = 0,$$

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

$$F_c - m_2 d_2 \omega^2 = 0,$$

$$F_c - F_g = 0,$$

$$\omega p = 1,$$

Then running solving the optimization problem on a solver gives

$$m_1 m_2 G p^2 - m_1 d_1 d_2^2 - m_2 d_1^2 d_2 - 2 m_2 d_1 d_2^2 = 0$$

Which is the correct expression post-factoring

Polynomial Optimization - Example

Then running solving the optimization problem on a solver gives

$$m_1 m_2 G p^2 - m_1 d_1 d_2^2 - m_2 d_1^2 d_2 - 2 m_2 d_1 d_2^2 = 0$$

Which is the correct expression post-factoring. What's more is that we also get the corresponding α_i :

$$\begin{aligned} & -d_2^2 p^2 w^2, \\ & -p^2, \\ & d_1^2 p^2 + 2d_1 d_2 p^2 + d_2^2 p^2, \\ & d_1^2 p^2 + 2d_1 d_2 p^2 + d_2^2 p^2, \\ & m_1 d_1 d_2^2 p w + m_2 d_1^2 d_2 p w + 2m_2 d_1 d_2^2 p w + m_1 d_1 d_2^2 + m_2 d_1^2 d_2 + 2m_2 d_1 d_2^2, \end{aligned}$$

Polynomial Optimization - Example

Then running solving the optimization problem on a solver gives

$$m_1 m_2 G p^2 - m_1 d_1 d_2^2 - m_2 d_1^2 d_2 - 2 m_2 d_1 d_2^2 = 0$$

Which is the correct expression post-factoring. What's more is that we also get the corresponding α_i :

$$\begin{aligned} & -d_2^2 p^2 w^2, \\ & -p^2, \\ & d_1^2 p^2 + 2d_1 d_2 p^2 + d_2^2 p^2, \\ & d_1^2 p^2 + 2d_1 d_2 p^2 + d_2^2 p^2, \\ & m_1 d_1 d_2^2 p w + m_2 d_1^2 d_2 p w + 2m_2 d_1 d_2^2 p w + m_1 d_1 d_2^2 + m_2 d_1^2 d_2 + 2m_2 d_1 d_2^2, \end{aligned}$$

Polynomial Optimization - Example

Some other examples that were tested:

Radiational Gravitational Wave Power: $P = -\frac{32G^4}{5c^5r^5}(m_1m_2)^2(m_1 + m_2)$ with background

$$\begin{aligned} & \omega^2 r^3 - G(m_1 + m_2) = 0, \\ 5(m_1 + m_2)^2 c^5 P + G \operatorname{tr} & \left(\frac{d^3}{dt^3} \left(m_1 m_2 r^2 \begin{pmatrix} x^2 - \frac{1}{3} & xy & 0 \\ xy & y^2 - \frac{1}{3} & 0 \\ 0 & 0 & -\frac{1}{3} \end{pmatrix} \right) \right)^2 = 0, \\ & x^2 + y^2 = 1, \end{aligned}$$

Hagen-Poiseuille Equation: $u(r) = \frac{-\Delta p}{4L\mu}(r^2 - R^2)$

$$\begin{aligned} u &= c_0 + c_2 r^2, \\ \mu \frac{\partial}{\partial r} \left(r \frac{\partial}{\partial r} u \right) - r \frac{dp}{dx} &= 0, \\ c_0 + c_2 R^2 &= 0, \\ L \frac{dp}{dx} &= -\Delta p, \end{aligned}$$

Polynomial Optimization - Results

Data	AI-Hilbert	AI-Descartes [13]	AI-Feynman [42]	PySR [15]	BMS [24]
S Hagen Poiseuille	✓	✗	✗	✗	✗
S Gravitational Wave Power	✓	✗	✗	✗	✗
R Relat. Time Dilat.	✓	✗	✗	✗	✗
R Kepler's 3 Law	✓	✓*	✗	✓	✗
S Bell inequalities [†]	✓	✗	✗	✗	✗
S [3.1] I.15.10 FSRD	✓	✓*	✗	✗	✗
S [3.1] I.27.6 FSRD	✓▷	✓*	✓*	✓	✗
S [3.1] I.34.8 FSRD	✓▷	✓	✓*	✓	✓*
S [3.1] I.43.16 FSRD	✓	✓*	✓*	✓	✓*
S [3.1] II.10.9 FSRD	✓	✓*	✓*	✓*	✓*
S [3.1] II.34.2 FSRD	✓	✓*	✓*	✓*	✓*
S [3.2] Inelastic Relativ. Collision	✓	✓*	✗	✗	✗
S [3.3] Decay of Pion [◇]	✓	✓*	✗	✗	✓*
S [3.4] Radiation Damping	✓	✗	✗	✓*	✓*
S [3.5] Escape Velocity	✓	✓	✓*	✓*	✓*
S [3.6] Hall Effect	✓	✓*	✗	✓*	✓*
S [3.7] Compton Scattering	✓	✓*	✓*	✓*	✓*

Notation used in table:

✓ denotes the successful recovery of a scientific law.

✗ denotes the failure to recover a scientific law.

✓* denotes recovery up to constants, but not exact recovery.

✓▷ denotes successful recovery when some variables that are potentially not observable are still declared to be observable.

Polynomial Optimization

Some thoughts:

1. Solving the LP can be slow. In the worst case (for gravitational waves)

Ongoing work

Projecting varieties

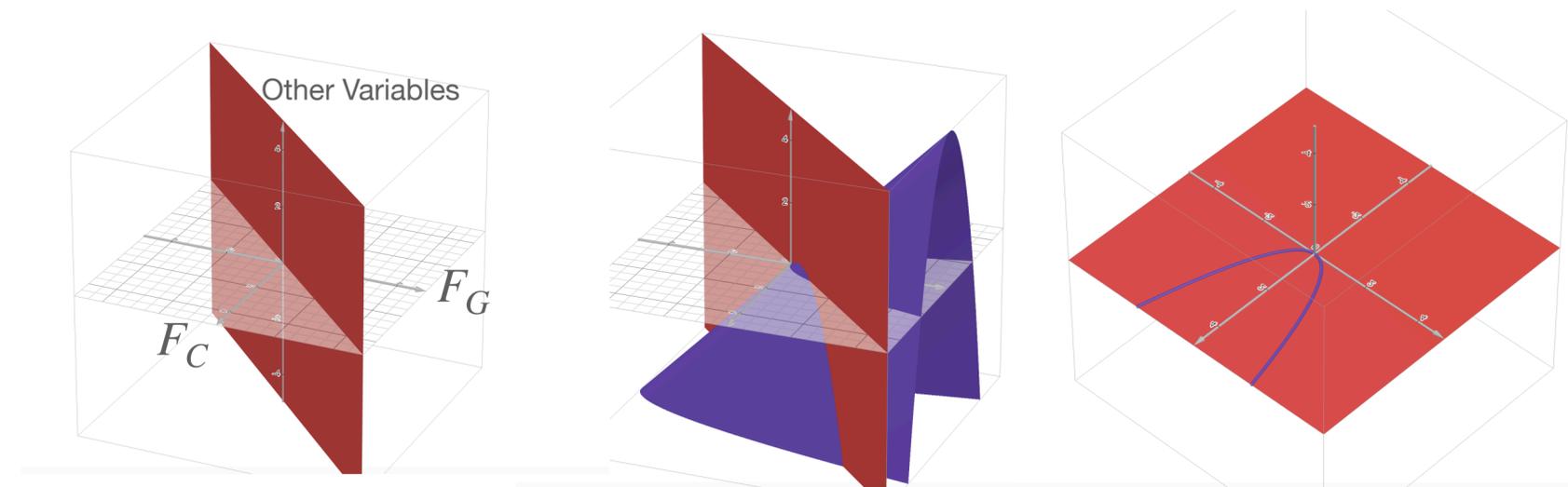
Aim: Discover Kepler's Third Law using just background theory

$$\begin{aligned}
 d_1 m_1 - d_2 m_2 &= 0, \\
 (d_1 + d_2)^2 F_g - G m_1 m_2 &= 0, \\
 F_c - m_2 d_2 w^2 &= 0, \\
 F_c - F_g &= 0, \\
 w p &= 1,
 \end{aligned}
 \implies p = \sqrt{\frac{4\pi^2 (d_1 + d_2)^3}{G(m_1 + m_2)}},$$



$$\pi : V(f_1, f_2, f_3, f_4, f_5) \subseteq \mathbb{R}^8 \longrightarrow \bar{V} \subseteq \mathbb{R}^5$$

This can be done using Groebner bases:



Algebraically: Eliminating Variables

Encode axioms as an ideal: $I = \langle f_1, \dots, f_5 \rangle \subseteq \mathbb{R}[m_1, d_1, m_2, d_2, F_c, F_g, w, p]$

Compute the intersection $I \cap \mathbb{R}[m_1, d_1, m_2, d_2, p]$

Encode axioms as an ideal: $G = \langle g_1, \dots, g_k \rangle = I$

Compute the intersection $G \cap \mathbb{R}[m_1, d_1, m_2, d_2, p]$

Abductive inference

We know we can recover a formula from a complete axiom system

Discovery

$$(d_1 + d_2)^2 F_g - Gm_1 m_2 = 0,$$

$$F_c - m_2 d_2 w^2 = 0,$$

$$F_c - F_g = 0,$$

$$wp = 1,$$

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

Abductive inference

In practice, axiom systems can be incomplete. Can we rediscover a missing axiom in the discovery process?

Abductive inference

Discovery

$$\begin{aligned}(d_1 + d_2)^2 F_g - Gm_1 m_2 &= 0, \\ F_c - m_2 d_2 w^2 &= 0, \\ F_c - F_g &= 0, \\ \cancel{wp = 1},\end{aligned}$$

$$p = \sqrt{\frac{4\pi^2(d_1 + d_2)^3}{G(m_1 + m_2)'}}$$

?

$$wp = 1,$$

Abductive inference

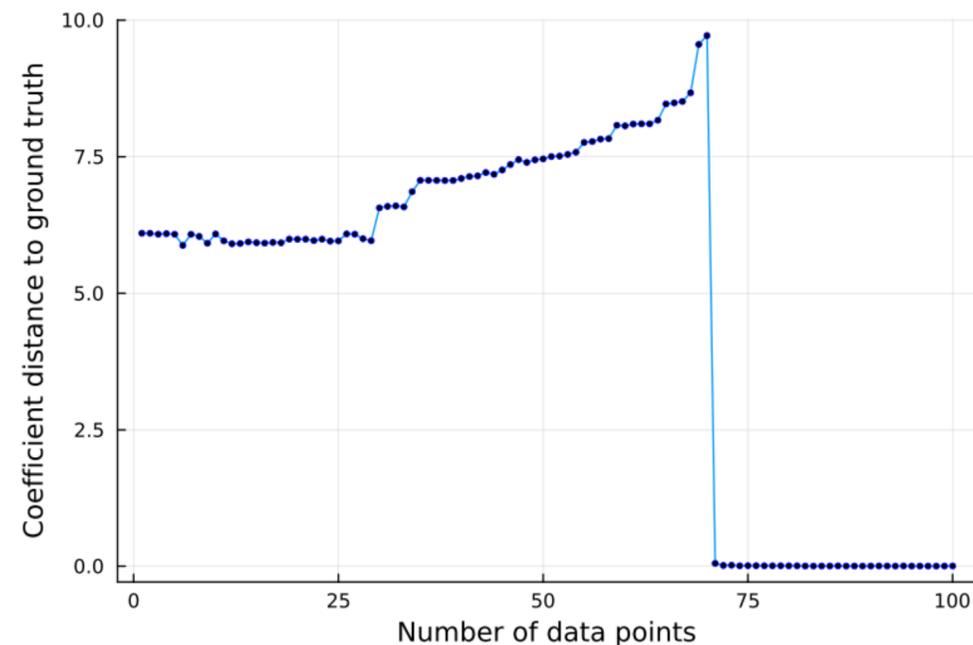
Key idea: Using data and variable elimination, we can still discover formulae with AI Hilbert

Assumption: The discovered formula q can be proven if we had an additional axiom.

$$\text{i.e. } q = \alpha_1 f_1 + \alpha_2 f_2 + \alpha_3 f_3 + \alpha_4 F_4$$

Where $\alpha_4 F_4$ is unknown.

Then $\langle f_1, f_2, f_3, q \rangle = \langle f_1, f_2, f_3, \alpha_4 F_4 \rangle$.



Rediscover Kepler with 70 data points if we omit $wp - 1$

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

Take the new “discovered” surface and break it into its irreducible components

$$V(f_1, f_2, f_3, q) = \bigcup V(p_i)$$

Where each $V(p_i)$ is irreducible. This is known as “primary decomposition” in commutative algebra.

Abductive inference

For Kepler's third law with $wp - 1$ missing, we get the following primary decomposition:

$$\langle f_1, f_2, f_3, q \rangle = \langle m_2, F_g, F_c \rangle \cap \langle d_2, m_1, F_g, F_c \rangle \cap \langle d_1 + d_2, m_1, F_c - F_g, w^2 m_2 d_2 - F_g \rangle \cap \langle F_g - F_c, (wp - 1), m_1 p^2 - d_1^2 d_2 - 2d_1 d_2^2 - d_2^3, F_g (d_1 + d_2)^2 - m_1 m_2, w m_2 d_2 - F_g p \rangle \cap \langle F_g - F_c, (wp + 1), m_1 p^2 - d_1^2 d_2 - 2d_1 d_2^2 - d_2^3, F_g (d_1 + d_2)^2 - m_1 m_2, w m_2 d_2 + F_g p \rangle$$

$$f_1 \quad (d_1 + d_2)^2 F_g - G m_1 m_2 = 0,$$

$$f_2 \quad F_c - m_2 d_2 w^2 = 0,$$

$$f_3 \quad F_c - F_g = 0,$$

$$q \quad p^2 m_1 m_2 - d_1^2 d_2 m_2 - 2d_1 d_2^2 m_2 - d_2^3 m_2$$

Abductive inference results

Problem & Axiom #	Axiom	Recovered*			
Kepler 1	$(d_1 + d_2)^2 F_g - m_1 m_2$	✓	Light Damping 1	$Sr^2 - q_c^2 a_p^2 \sin^2 \theta$	✓
Kepler 2	$F_c - m_2 d_2 w^2$	✓	Light Damping 2	$dA - 2\pi r^2 \sin \theta d\theta$	✓
Kepler 3	$F_c - F_g$	✓	Light Damping 3	$P - \int_0^\pi S dA$	✓
Kepler 4	$wp - 1$	✓	Light Damping 4	$\frac{4}{3} - \int_0^\pi \sin^3 \theta d\theta$	✓
Compton 1	$E_1 + Ee_1 - E_2 - Ee_2$	✓	Light Damping 5	$a_p^2 - \frac{1}{2} w^4 x_0^2$	✓
Compton 2	$E_1 - hf_1$	✓	Hagen Poiseuille 1	$u - c_0 - c_2 r^2$	✓
Compton 3	$E_2 - hf_2$	✓	Hagen Poiseuille 2	$\mu \frac{\partial}{\partial r} (r \frac{\partial}{\partial r} u) - r \frac{dp}{dx}$	✓
Compton 4	$p_1 c - hf_1$	✓	Hagen Poiseuille 3	$c_0 + c_2 R^2$	✓
Compton 5	$p_2 c - hf_2$	✓	Hagen Poiseuille 4	$L \frac{dp}{dx} = -\Delta p$	✓
Compton 6	$\lambda_2 f_1 - c$	✓	Neutrino Decay 1	$p_\nu - p_\mu$	✓
Compton 7	$\lambda_2 f_2 - c$	✓	Neutrino Decay 2	$E_\pi - m_\pi$	✓
Compton 8	$Ee_1 - m_c^2$	✓	Neutrino Decay 3	$E_\nu - p_\nu$	✓
Compton 9	$Ee_2^2 - c^2 p e_2^2 - m e^2 c^4$	X ⁺	Neutrino Decay 4	$E_\pi - E_\mu - E_\nu$	✓
Compton 10	$p e_2^2 - p_2^2 - p_1^2 + 2p_1 p_2 \cos$	X ⁺	Neutrino Decay 5	$E_\mu^2 - p_\mu^2 - m_\mu^2$	X ⁺
Einstein 1	$cdt_0 - 2 * d$	✓	Hall Effect 1	$F_m - q_e v B$	✓
Einstein 2	$4L^2 - 4d^2 - v^2 dt^2$	✓	Hall Effect 2	$F_e - q_e E$	✓
Einstein 3	$f_0 dt_0 - 1$	✓	Hall Effect 3	$F_m - F_e$	✓
Einstein 4	$f dt - 1$	✓	Hall Effect 4	$Eh - U_H$	✓
Einstein 5	$c * dt - 2L$	✓	Hall Effect 5	$v dt - L^{19}$	✓
Escape Velocity 1	$K_i - \frac{1}{2} m v_e^2$	✓	Hall Effect 6	$I dt - Q$	✓
Escape Velocity 2	$K_f = 0$	✓	Hall Effect 7	$Q - N q_e$	✓
Escape Velocity 3	$U_i r + GMm$	✓	Hall Effect 8	$nV - N$	X
Escape Velocity 4	$U_f = 0$	✓	Hall Effect 9	$V - Lhd$	X
Escape Velocity 5	$K_i + U_i - (K_f + U_f)$	✓			

Other goings on

Dataset and Benchmarking

Aim: Creating a synthetic dataset of polynomial axioms, data, and discovered formulae for benchmarking progress in the field

New Discoveries

Aim: Apply the tools developed to research problems in physics to discover new scientific facts. Current work ongoing in cosmology.

Non-polynomial Systems

Aim: Extending the current framework to systems involving differential equations, black box axioms, and trig functions

THANKS A BUNCH!



Karan Srivastava
ksrivastava4@wisc.edu