Electronics and Computer Science
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An AI Approach to Chaotic Physicl Systems:

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Abstract

Physical laws are generalisation established through empirical observations of the physical world. It has taken humans centuries to discover, requires huge amounts of research, repeated experiments and plenty of scientists to produce an universally accepted law in the scientific community. Thanks to recent advances in neural networks and increased computational power, we can now train models to replicate and fasten our discovery of physical laws such as the laws of motion,also including chaotic systems such as the double pendulum, drastically shortening the time required to find new physical laws. Furthermore human's have a cognitive bias when looking at data, find it difficult to spot patterns in chaotic systems. This report explores how an AI without any bias or prior knowledge views the physical world, how it is capable of spotting chaotic patterns and how it is a tool that can reduce the time taken to make new discoveries.

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ECS Statement of Originality Template, updated August 2018, Alex Weddell aiofficer@ecs.soton.ac.uk

Contents

1 Introduction:

1.1 Goals:

It took humans centuries to derivie physical laws, can this process be sped up through AI, by feeding it data and letting the model derive complex laws for us. I aim to derive physical laws, from experimental data. I will explore deriving simpler physical laws such as acceleration without air resistance, and move onto to complex chaotic systems such as pendulums, and explore how an unbiased AI views the physical world, compared to humans who's views of physical systems are naturally biased through systematic learning.
Can this lead to perhaps different prespectives of viewing the physical world around us, allowing for further progress?

1.2 Scope:

- Aim to derive simple laws of motions (ie acceleration) through AI frameworks.

- Move onto more complex systems such as pendulums, and initially explore smaller initial values, moving onto larger initial values, thereby increasing the chaos, and difficulty of spotting patterns.

- To explore using various AI techniques, (Graph Neural Networks, Deep learning, Neural Networks) in combination with no prior knowledge and observe how and in what form the physical laws are derived.
- Simulate physical data required using pymunk, and perhaps use real world data from physics labs.

2 Literature Review:

2.1 Introduction:

Humans have spent millennia observing the world around us, creating concepts that describe the variables in the physical world, such as mass and force, to derive the laws of motion. In physics, like with all human endeavours, new discoveries and ways of thought are based upon previous works, creating a natural bias in the way we humans approach new problems. All existing theories, are therefore somewhat biased, this combined with our pre-existing bias in our biological brains, can introduce some hurdles in our future progress [1,2].

In the 17th Century, Kepler had gotten his hands on the word's most precise data tables on the orbits on planets, using this and his intellect, he spent close to half a decade, and after numerous unsuccessful attempts, he had began a scientific revolution at the time, describing Mar's orbit to be an ellipse [3]. In essence, scientists throughout history, much like Kepler, have spent a great deal of time, discovering the right expressions to match the relevant data they have, this at it's core is symbolic regression. Now, a few centuries later, with exponential increases in orders of magnitude in our capability to perform calculations through computers, the process of discovering natural laws and the way to express them, has to some extent resisted automation.

One of the core challenges of physics and artificial intelligence, is finding analytical relations automatically, discovering a symbolic expression that accurately matches the data from an unknown function. This problem, due to it's nature, is most certainly NP-hard [4] in principle. The vastness of the space of mathematical constants, further adds to the difficulty. This literature review aims to present the recent advances in deriving expressions and laws through data, how we can avoid human bias by seeking solutions without prior assumptions and describing the various tools and techniques used to achieve this. Then it will introduce the 3-body problem and explore how artificial intelligence is being used to

6find faster and more efficient solutions.

2.2 Symbolic Regression:

Symbolic regression, is a technique that analyses and searches over the space of traceable mathematical expressions to find the best fit for a data set. By not requiring prior information about the model, it is unbiased. There are a plethora of various strategies that have been implemented in solving for empirical laws [5], we will explore some of them below. It is also worth mentioning, that unlike other well-known techniques for regression, (eg: neural networks), that are essentially black boxes, symbolic regression, aims to extract white-box models and is easy to analyse.

Brute Force:

Symbolic Regression (SR), is interpretable [6], unlike Neural Networks (NN), which are often considered more explainable. The difference is interpretability allows us to comprehend how the model works, like observing how gears move in a glass box, while explainable means you get an overview of why a certain output was achieved, even without knowing the full nuances of it's inner workings.

There however, are some challenges associated with SR, in comparison to function fitting (NN). SR, starts with nothing, a blank slate, and it has to learn the entire expression [7], unlike function fitting which just tweaks an already existing function. The exponential search space [8] , causes it to be extremely computationally expensive to explore all possibilities. This combined with the face that, most optimisation algorithms expect a smooth search space [9], however SR lack's smooth interpolation, small changes in the potential solutions (expression), ie: $x3andx3 + 0.1$ can significantly alter the the output. Finally, if the nature of the problem is badly posed [10], there might potentially be multiple solutions to the same data. Imagine trying to find a single polynomial equation with only two points of data, the need to balance finding accurate expressions with finding the most simplistic and generalisable fit, is sometimes troublesome.

The brute force approach of simply trying all possible combinations of symbolic expressions within some defined space. The model will subsequently increase the complexity over time, and will stop when either the fitting errors lowers below some defined limit or exceeds the upper limit of runtime. While in theory can solve all of our problems, in practise takes longer than the age of our universe to finish. In essence it's like searching for a singular drop in the ocean. Thankfully, there are some ways of pruning the search space, and drastically reducing the time taken to solve for the most accurate expression.

Partial Derivatives:

Partial derivatives, of some function f, with multiple variables such as x and y, is it's dervative with respect to one of those two variables, while the other variables in the function are kept constant. Formally, given a function with two or more variables, $f(x_1, x_2, \ldots, x_n)$, the partial derivative of f with respect to x_i, where x_i is some value x in $(x_1, x_2, \ldots, x_i, \ldots, x_n)$, gives the rate of change of f with respect to x_i. It is calculated by taking the ith derivative of f with respect to x_i, whilst holding the other variables fixed. [11]

The partial derivative of a function $f(x, y)$ with respect to x is denoted $\frac{\partial f}{\partial x}$ [12] and is defined:

$$\frac{\partial f}{\partial x} = \lim_{h \to 0} \left[\frac{f(x+h,y) - f(x,y)}{h} \right]$$

Once you pass in the experimental data, you can pre-process the data, using calculated partial derivatives, for every pair of existing variables. Many physical laws, involve rates of change, and partial derivatives help us represent them. Furthermore it also guides the search process, as the algorithm can use the derivative to accurately represent the underlying laws involved. Through comparing how well the partial derivatives derived through the experimental data compared to the potential expression, the algorithm can assess the accuracy and feasibility of the expressions involved. This strategy can even be extended to prune the search space further, this could be achieved through incorporating knowledge of physics into the constraints for the partial derivatives. These concepts will be illustrated with an example below.

Consider a iron rod, that has been heated up, such that it is hotter on one side than the other. Now it is intuitive to say that closer to the heat source, the temperature will be higher than further along the rod, where it will be colder. We can illustrate this temperature distribution with a function:

$$T(x, y, z)$$

where T is the temperature at a point in the rod, and (x,y,z) are the coordinates along the axis in 3 dimensions. This leads to these 3 partial derivatives:

$$\frac{\partial T}{\partial x}, \frac{\partial T}{\partial y}, \frac{\partial T}{\partial z}$$

These partial derivatives, gives us information about the direction and magnitude of heat flow at various points on the rod. The algorithm then searches for an equation T(x,y,z), that sufficiently predicts the observed temperature distribution and it's partial derivatives, deriving laws such as the heat transfer equations, or elasticity relationships.

$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T$$

Through using partial derivatives, we have in essence redefined the search criteria for the algorithm, through it's measure of the accuracy in comparison of potential solutions over the invariants represented in the experimental data. This also leads to the pleasant finding, that it can additionally capture relationships that represent other identities of the system, beyond invariants and heat transfer equations.

You can subtly guide the type of laws that such an algorithm finds, by selectively picking the variables to input into the algorithm,. For example providing velocities and force to find laws of motion.

Dimensional Analysis:

Dimensional Analysis is a method of solving problems usually in maths and physics, where we analyse the relationships between different physical quantities, by comparing their "units." It is a powerful method of reducing the complexity of systems, enabling engineers and scientists to analyse problems that we can't even pose, much less solve the equations of [13].

Using the fact that numerous questions in science can be simplified by requiring the dimensions/units of the right and left hand side of the expression to be equal, we can transform the question into a smaller number of variables, which all have no dimension. It has been automated to find the integer powers of expressions and has proven to be useful especially when the power is an irrational number.

Here is a general strategy that showcases how dimensional analysis can be used:

Let's say we have a variable in an equation that can be broken down into it's fundamental units, such as (second, kilograms, ampere ...) to various powers. We can then take this, and represent each of the units as vectors, such that each of the fundamental units, is assigned a dimension, and it's important to note, this then allows us to represent any physical quantity as a product of these units, so let us construct a vector v, with 3 integers, where each corresponding integer represents the power of each of the fundamental units.

Given that we want to derive an expression, such as $y = f(x_1, \ldots, x_n)$ we can then create some matrix M. Each of the columns of the given matrix, is the unit vector v of the corresponding variable x_i. We then need to define another vector to represent the units of y, which will be called z. If we let the solution be some vector s, solving $Ms = z$, this then lets us raise the powers on both sides, to elevate the independent variables, to make this equation dimensionally consistent.

Taking the null space of the matrix M, where $MV = 0$, allows us a basis to create a dimensionless group, allows for a simplification of the problem.

This is also more intuitive to understand physical phenomena, the nature of physics comprehension, making this vital in further understanding derived laws, making the process easier to explain and understand [14,15]. Therefore, this is a crucial tool, for cultivating a deeper understanding of physics effectively [16].

Genetic Programming:

Genetic programming (GP), is a special evolutionary algorithmic technique, where the individuals are seen as programs that evolve, starting for a population, is iteratively "evolved," transforming the populations of individual programs, intro other populations. This new generation of programs are created using some genetic operations or survival criteria, mimicking natural evolutionary condition on earth.

A very basic overview, shows that genetic programming algorithms, consists of initializing the population, then evaluation of the said population through some predefined metrics and functions, followed by selection of the fittest programs based on the score given by the metric, and "genetic operation," such as reproduction, mutation and cross-over. The algorithm then iterates these steps thousands of times, through many generations, and finally terminates once the desired result has been achieved.

We can use genetic programming, and tweak the algorithm, and combine it with symbolic regression, to help us derive laws.

Consider modelling the various potential formulas as a tree, which is composed of various functions in the nodes. These functions can vary from arithmetic operations, mathematical functions, or defined unique operators. Then we can program the fitness function, and use it to measure how well the given potential expression in the population compares with the given databases, and given the nature of genetic programming, the better performing functions are more likely to be passed down into the next generation. Then after many iterations, we can give the solution with the best performance.

There are various ways to implement the fitness function, and for example we can use a criteria like this, along with mean squared error:

$$V = 2X + N \cdot ln(M/N)$$

Here M is the mean squared error, and N is the number of data points, X is the number of parameters used on the genetic programming algorithm. The lower the value of V is, the better the model performs. The performance of this stratergy can then be evaluated with various other metrics, to judge how well the algorithm performs.

2.3 Conclusion:

These are some of the methods, that can be utilised to reduce the search space, and an algorithm, that combines these strategies is theoretically efficient at solving for derived laws, while maintaing some generality. In the following section, the aim is to explore various ways, to design and fine tune these methods, along with black box models, such as neural networks, and potentially transformers, to derive laws.

3 Progress:

placeholder

4 Project Planning:

placeholder

5 Project Management:

5.1 Risk Assessment:

Issue	Impact	Prob	Risk	Mitigation
Unexpected delays and accidents	3	3	7	Include contingency plans and a 3 week break between major stages of the project, to allow for unexpected incidents.of the project, to allow for unexpected incidents.
Unable to generate enough experimental data due to lack of computational power.	4	1	14	Explore alternate more efficient ways of simulating data, consider using cloud infrastructure or potentially the Universities HPC facilities.
Challenges learning the double pendulum laws and the derivation.	2	4	5	Seek other resources from the Physics Department to learn the Physics required. Look up explanations online to learn.
Interpretability Challenges	3	2	10	Challenges in interpreting how the model works, can be mitigated through visualising the data, plotting results and through seeking ways to explain the model.

5.2 Project Planning:

A Gantt chart along with a rough outline of the relevent dates for various submission was made towards the beginning of this project, this alose included contengency planning and short yet frequent breaks every couple weeks.

blah blah

5.3 Gantt Chart:

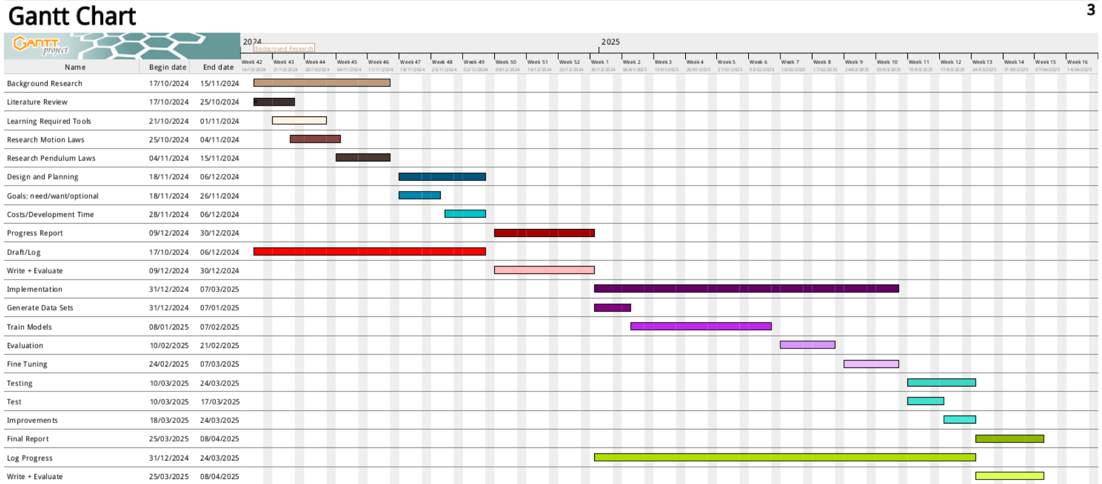
Part3Project 20 Oct 2024

Tasks 2

Name	Begin date	End date
Background Research	17/10/2024	15/11/2024
Literature Review	17/10/2024	25/10/2024
Learning Required Tools	21/10/2024	01/11/2024
Research Motion Laws	25/10/2024	04/11/2024
Research Pendulum Laws	04/11/2024	15/11/2024
Design and Planning	18/11/2024	06/12/2024
Goals: need/want/optional	18/11/2024	26/11/2024
Costs/Development Time	28/11/2024	06/12/2024
Progress Report	09/12/2024	30/12/2024
Draft/Log	17/10/2024	06/12/2024
Write + Evaluate	09/12/2024	30/12/2024
Implementation	31/12/2024	07/03/2025
Generate Data Sets	31/12/2024	07/01/2025
Train Models	08/01/2025	07/02/2025
Evaluation	10/02/2025	21/02/2025
Fine Tuning	24/02/2025	07/03/2025
Testing	10/03/2025	24/03/2025
Test	10/03/2025	17/03/2025
Improvements	18/03/2025	24/03/2025
Final Report	25/03/2025	08/04/2025
Log Progress	31/12/2024	24/03/2025
Write + Evaluate	25/03/2025	08/04/2025

Part3Project 20 Oct 2024

Gantt Chart 3



6 Bibliography:

[1] C. Wood Powerful ‘Machine Scientists’ Distill the Laws of Physics From Raw Data. Quanta Magazine, 2022.

[2] M. Schmidt and H. Lipson, Distilling Free-Form Natural Laws from Experimental Data. Science, 324, 5923, 2009.

[3] A. Koyr´e, The Astronomical Revolution: Copernicus- Kepler-Borelli (Routledge, 2013).

[4] A Computational Inflection for Scientific Discovery by Hope, Tom and Downey, Doug and Weld, Daniel S. and Etzioni, Oren and Horvitz, Eric

[5] Schmidt M, Lipson H (2009) Distilling free-form natural laws from experimental data. Science 324(5923):81–85.

[6] Interpretability in symbolic regression: a benchmark of explanatory methods using the Feynman data set, Aldeia, Guilherme Seidyo Imai and de França, Fabrício Olivetti, 2022

[7] "Discovering Symbolic Models from Deep Learning with Inductive Biases" by Miles Cranmer et al. (2020)

[8] "Scaling Up Symbolic Regression with Operator Grammars" by Michael O'Neill et al. (2020)

[9] "A Survey of Symbolic Regression Methods" by Bogdan Burlacu et al. (2020)

[10] "Regularized Evolution for Symbolic Regression" by Nguyen Quang Uy et al. (2011)

[11] Calculus: Early Transcendentals" by James Stewart

[12] Partial Differential Equations for Scientists and Engineers" by Stanley J. Farlow:

[13] A first course in Dimensional Analysis by Juan G Santiago

[14] W. Blasiak, M. Godlewska, R. Rosiek, and D. Wcislo, "Spectrum of physics comprehension," European Journal of Physics, vol. 33, p. 565, 2012. [Online]. Available: https://www.researchgate.net/publication/254496494 Spectrum of physics comprehension

[15] K. S. Taber, "Maths should be the last thing we teach," Physics Education, vol. 44, no. 4, p. 336, jul 2009. [Online]. Available: https://dx.doi.org/10.1088/0031-9120/44/4/F01

[16] Y. Zhu, Z. -Y. Khoo, J. S. Choong Low and S. Bressan, "A Personalised Learning Tool for Physics Undergraduate Students Built On a Large Language Model for Symbolic Regression," 2024 IEEE Conference on Artificial Intelligence (CAI), Singapore, Singapore, 2024, pp. 38-43, doi: 10.1109/CAI59869.2024.00017. keywords: Knowledge engineering;Systematics;Large language models;Learning (artificial intelligence);Mathematical models;Physics education;Problem-solving;AI and Education;Symbolic Regression;Large Language Models;Physics Education;Prompt Engineering;Undergraduate Learning,