Federal State Autonomous Educational Institution
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Machine Learning Approach to Search for Patterns in Physical Phenomena

Project Proposal

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Abstract

This work is an overview of several existing machine learning methods that aim at extracting knowledge from empirical data, and an attempt to create a new method. Most existing methods suffer from a disadvantage that there is no interaction between an algorithm and an environment. Although the new algorithm that is proposed in this work also has this disadvantage, the goal is to overcome it.

1 Introduction

Our goal is to model the way humans investigate and understand the physical laws of nature and create an AI agent that would be able to behave like a scientist, devising hypotheses and performing experiments. We are aiming at creating a system that would be able to discover regularities in data and present them in human-interpretable forms, such as a symbolic formula.

There has been huge progress in the field of Machine Learning in recent years. However, how most modern ML algorithms work can be described as recovering deep correlations between the data and the target variable. This is unlike the way human scientists investigate the world - they often try to use a short symbolic expression

This work is done together with Julia Semavina (3rd-year graduate student at Faculty of Computer Science, HSE) under the supervision of Vladislav Belavin (Research Assistant, Postgraduate Student at the Laboratory of Methods for Big Data Analysis, Faculty of Computer Science, HSE)

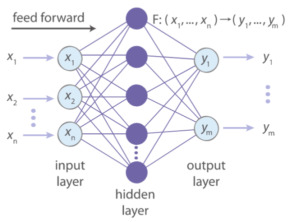
The work is primarily based on the model proposed in [1], which is capable of recovering simple equations that govern a movement of a particle in certain environments.

2 Preliminaries

This work belongs to the field of Machine Learning, therefore, I will provide here some basic definitions that we will need.

Machine Learning algorithm is a family of functions $f(x, \theta) : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}^k$, where θ are called parameters of the model. During the learning process, the parameters are changed using the optimization algorithm.

Multilayer perceptron is a Machine Learning algorithm which is defined as a composition of functions $f_n \circ f_{n-1} \circ \dots f_1(x)$, where function f_k is called a layer of Multilayer perceptron and has the form $f_k(x) = \sigma_k(W_k x + b_k)$, where W_k is a matrix, b_k is a vector.



A *regression problem* is a problem where we are given a training dataset $\{(X_i, y_i)\}, i = 1..N$, where $X_i \in \mathbb{R}^n, y_i \in \mathbb{R}$, and the goal is to learn to predict values of y that correspond to values of X that are not present in the dataset.

A *symbolic regression problem* is a regression problem, where we also want to explicitly understand the formula that maps X to y.

3 Main Results

3.1 Literature review

The key question of this research is the following: is artificial intelligence capable of discovering physical laws from observations? In the following papers AI is used as follows: data is somehow gathered and given to the algorithm, which uses some assumptions on what formulas look like. The problem is that the agent itself does not interact with the environment.

Let us see what progress has already been done in the field.

3.1.1 AI Physicist

Roughly speaking, a scientific theory might be viewed as a formula that can be used for prediction, and an area of space where this theory is applicable.

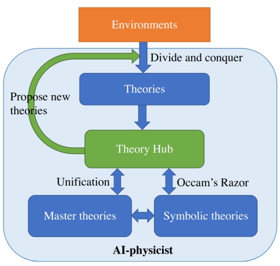
In this paper authors propose an algorithm, which observes movements of a particle in the environment and tries to learn the physical laws, that govern the environment.

More formally, let us define a theory as a tuple (f, c), where $f : \mathbb{R}^{n \times m} \to \mathbb{R}^n$ is a function that maps m previously observed coordinates of the particle to its coordinate in the next time step, and $c : \mathbb{R}^n \to \{0, 1\}$ is a classifier of whether this theory is applicable at the current point.

Machine Learning methods can be used to estimate these functions.

The algorithm that is proposed in this paper has the following key components:

- *Divide and conquer* Learn multiple theories each of which specializes to fit part of the data very well
- *Occam's Razor* Avoid overfitting by minimizing description length, which can include replacing fitted constants by simple integers or fractions
- *Unification* Try unifying learned theories by introducing parameters
- *Lifelong Learning* Remember learned solutions and try them on future problems



The algorithm of exploration of the new environment has the following steps:

Propose theories from the Theory Hub and some randomly initialized theories, fit them with data, add new theories that are good enough to the theory hub, perform unification and simplification.

The quality of the theory is measured as the sum of its descriptive length and the value of loss function. The descriptive length of a theory is the sum of descriptive lengths of its coefficients.

The number of binary digits required to specify a natural number $n = 1, 2, 3, \ldots$ is approximately $\log_2 n$, so we define $\mathrm{DL}(n) \equiv \log_2 n$ for natural numbers.

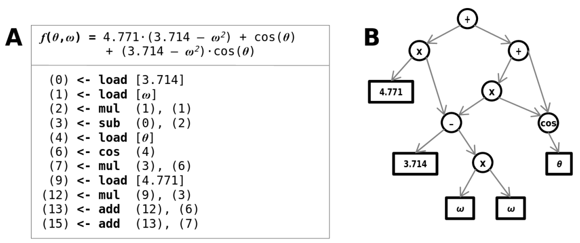
For an integer m, we define $\mathrm{DL}(m) \equiv \log_2(1 + |m|)$

For a rational number $q = m/n$, the description length is the sum of that for its integer numerator and (natural number) denominator $\mathrm{DL}\left(\frac{m}{n}\right) = \log_2[(1 + |m|)n]$

For a real number r and a numerical precision floor ϵ, we define $\mathrm{DL}(r) = \log_+\left(\frac{r}{\epsilon}\right)$ where $\log_+(x) \equiv \frac{1}{2}\log_2\left(1 + x^2\right)$

Testing it on a suite of mystery worlds involving random combinations of gravity, electromagnetism, harmonic motion, and elastic bounces, authors found that its divide-and-conquer and Occam's razor strategies effectively identified domains with different laws of motion and reduced the mean-squared prediction error billion-fold, typically recovering integer and rational theory parameters exactly.

3.1.2 Genetic Algorithm



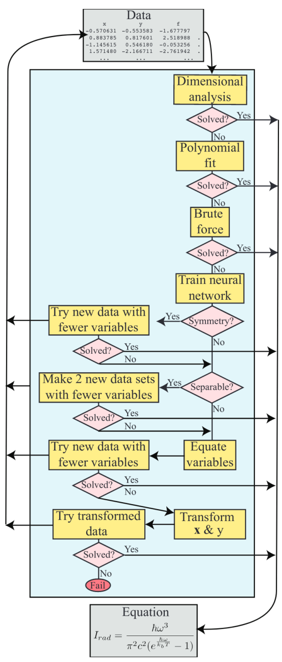
Another method of symbolic regression is genetic algorithm, which does not involve machine learning, but mimics biological evolution.

In this paper, authors represent a formula as a tree, in which each node is one of the operations $(+, \cdot, \sin, \cos, \div)$, a variable, or a number.

The algorithm repeats the following two steps until reasonable quality is reached:

1. Random changes in the structure of a tree and/or merging different trees
2. Selection of the best models using the following function:
$-\frac{1}{N}\sum_{i=1}^{N}\log\left(1+abs\left(\frac{\Delta x_i}{\Delta y_i}-\frac{\delta x_i}{\delta y_i}\right)\right)$, where $\frac{\Delta x}{\Delta y}\approx\frac{dx}{dt}\Big/\frac{dy}{dt}$, $\frac{\delta x}{\delta y}=\frac{\delta f}{\delta y}\Big/\frac{\delta f}{\delta x}$

3.1.3 AI Feynman



This algorithm sequentially applies several strategies based on the following assumptions about the formula

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

3.2 New algorithm

The idea of this algorithm is to provide a general model for many possible scientific laws and recover them using the optimization of the model parameters.

Let us define a *nested formula* of depth 0 as a constant number:

$\varphi_0(x_1, \dots x_n) = \lambda_0$

The *nested formula* of depth k + 1 is defined inductively as follows:

$$\varphi_{k+1}(x_1, \dots x_n) = \varphi_k(x_1, \dots x_n) + \sum_{i=1}^{n} (\lambda_{k+1,i,0} x_i^{\alpha_{k+1,i}} \varphi_{k,i,0}(x_1, \dots x_n) + \lambda_{k+1,i,1} \sin(\varphi_{k,i,1}(x_1, \dots x_n)) + \lambda_{k+1,i,2} \cos(\varphi_{k,i,2}(x_1, \dots x_n))$$

Examples: $Gm_1^1 m_2^1 r^{-2} + kq_1^1 q_2^1 r^{-2} - m_1 a_1$ (depth 3)
$cmT_2 - cmT_1 - \frac{1}{\pi} I^2 l^1 t^1 r^{-2}$ (depth 4)
$T - \frac{2\pi}{\sqrt{G}} RM^{-0.5} l^{0.5} - \frac{2\pi}{\sqrt{G}} RM^{-0.5} hl^{0.5}$ (depth 2),
$qvB\sin(\alpha) - ma$ (depth 4)

Note that this object can be viewed as a Machine Learning algorithm with parameters $\lambda_{i,j}, \alpha_{i,j}$.

3.3 Possible future work directions

Gain a better understanding of which types of formulas my algorithm can discover, which it cannot discover and why. Add an algorithm that could simplify the resulting formulas. Cover existing methods in more detail.

Design an environment and an agent that could interact with it. To be more specific, it would be desirable if an agent could estimate its uncertainty of predictions and pick the point of the environment where this uncertainty is the biggest so that the experiment would be as informative as possible.

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