Form 2A - Research Master's Psychology: Research Internship Research Proposal

1 General Information

1.1 Student information

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1.2 Supervisor information

Supervisor (eligible for the ResMas): Eric-Jan Wagenmakers

Specialization: Psychological Methods

1.3 Other information

Date: 25.03.2021

Number of ECs for the research internship: 18EC

Ethics Review Board (ERB) code: -

2 Title and Summary of the Research Project

2.1 Title: Bayesian Symbolic Regression

2.2 Summary of proposal

Symbolic regression is a machine learning method that generates explicit mathematical expressions by composing basic functions. Since the models are just mathematical expressions they are fully interpretable, unlike most other machine learning techniques.

The goal of this project is to develop and test a general Bayesian symbolic regression framework. The current state of the art in symbolic regression are methods that are able to include information about the structure of the target system they are trying to model. However, they use an approach with neural networks that is convoluted and hard to generalize. We believe that Bayesian methods could be a straightforward alternative to incorporate prior knowledge.

Word count: 107/150

3 Project description

Symbolic regression is a machine learning technique that attempts to find a mathematical expression that describes relationships between features of the data. The

mathematical expressions can be arbitrarily complex and are constructed from a prespecified set of features and operators (e.g. addition, multiplication, trigonometric functions, etc.). The main advantage of symbolic regression over other machine learning techniques is that the resulting models are explicit and interpretable. This lack of interpretability is one of the biggest barriers to the use machine learning methods for basic scientific research, but symbolic regression avoids this issue. The goal of this research is to implement an easy to use Bayesian Symbolic Regression framework and to compare its performance with other methods.

The space of possible mathematical expressions is infinitely large, and therefore it is not viable to explore it exhaustively. The most common approach to perform symbolic regression is to do a targeted search using evolutionary algorithms, which work by mimicking the evolution of a population of candidate expressions. An example of this approach is the widely used software Eureqa[1] (Schmidt & Lipson, 2009). More recently, some researchers have explored the use of neural networks to assist in the search of expressions. Udrescu and Tegmark (2020) use a neural network to discover hidden structure that is common in physical formulas (e.g. coherent units, symmetry), and they outperform by large margins the previous best efforts. On the other hand, Cranmer et al. (2020) fit neural networks that induce bias about the structure of the target system, and then they recover a mathematical expression with evolutionary algorithms from the networks instead of directly from the target system. This approach has better generalizability and predictive performance than just the neural networks or evolutionary algorithms on their own. The key aspect of these methods is that the neural networks encode prior information about the structure of the target mathematical expression, and therefore encourage a low-dimensional representation. These methods are the current state of the art when it comes to recovering or discovering new mathematical expressions.

A different approach to perform symbolic regression is the use of Bayesian methods. The main feature of these models are the Markov chain Monte Carlo samplers that explore the space of possible mathematical expressions. One of the disadvantages of having to sample from a multidimensional space is that Bayesian methods are usually

[1] https://www.creativemachineslab.com/eureqa.html

more computationally demanding than alternative techniques, but in this case they are not necessarily more demanding than their evolutionary or machine learning counterparts. Furthermore, an advantage of Bayesian methods is that we can encode prior information about the components and the structure of mathematical expressions. Guimerà et al. (2020) use the possibilities of Bayesian modelling to incorporate prior information about the frequency of mathematical operators, while Jin et al. (2019) specify a model that is constrained to a linear combination of mathematical expressions. However, as long as we assume a distribution over the residuals, we can specify models with other structures. In this way, we could encode prior information about the structure of the target system that matches our knowledge about how the system behaves, similarly to how Cranmer et al. (2020) do with neural networks. And that is the key of this research. We aim to develop a general way to specify Bayesian symbolic regression models.

Word count: 531/1200

4 Procedure

The first step will be to implement Jin et al. (2019) Bayesian symbolic regression algorithm. Their algorithm is constrained to a linear combination of mathematical expressions represented as symbolic trees:

$$y = \beta_0 + \beta_1 \Psi_1(x) + \cdots + \beta_K \Psi_K(x) \ ,$$

where Ψ_i is the ith symbolic tree that represents a function of the features x, y is the outcome variable and β are the linear coefficients.. We want to test two possible modifications to their algorithm. First, since a single symbolic tree can capture the default linear combination of tress we want to explore the differences between using K trees versus only using 1 tree. And second, their algorithm generates possible movements for the MCMC sampler from the prior distribution of the parameters. We want to test if there is a computational advantage if we generate proposals from a distribution centered around the current values of the parameters.

We will compare the original algorithm's performance against the performance of the modifications and the performance of a standard evolutionary symbolic regression algorithm.[2] To assess the predictive performance of the different models we will use the variance of the residuals. We will also look at the complexity of the models measured as the number of nodes, the speed to convergence and the stability of the solutions. We will perform the comparisons with data generated from a standard set of functions (Expression 1) that have been used to benchmark other symbolic regression algorithms. Additionally, we plan on using a publicly available data set[3] that we could use to evaluate the interpretability of the expressions produced by the model.

$$
\begin{aligned}
f_1(x_0, x_1) &= 2.5x_0^4 - 1.3x_0^3 + 0.5x_1^2 - 1.7x_1 \\
f_2(x_0, x_1) &= 8x_0^2 + 8x_1^3 - 15 \\
f_3(x_0, x_1) &= 0.2x_0^3 + 0.5x_1^3 - 1.2x_1 - 0.5x_0 \\
f_4(x_0, x_1) &= 1.5\exp(x_0) + 5\cos(x_1) \\
f_5(x_0, x_1) &= 6.0\sin(x_0)\cos(x_1) \\
f_6(x_0, x_1) &= 1.35x_0x_1 + 5.5\sin\left[(x_0 - 1)(x_1 - 1)\right]
\end{aligned} \tag{1}
$$

The last step will be to implement a Bayesian symbolic regression algorithm that incorporates information about the structure of the Newtonian Dynamics system described in Cranmer et al. (2020). They use graphical neural networks to encode prior information about the shape of the target mathematical expression. For example, in a model of particles attached to each other by springs, the acceleration that a particle experiences is proportional to the sum of forces between that particle and all other particles in the system. Moreover, the mathematical expression that describes every force should be the same for any pair of particles. In a Bayesian symbolic regression approach we can encode this structure in the following model

$$
\vec{a}_i \propto \sum_{\forall j \neq i} F_{ij} \approx \sum_{\forall j \neq i} \Psi_F(x_i, x_j) \ ,
$$

[2]There are two main evolutionary algorithms we could choose. ExprOptimization.jl, which is based on the same tooling that we have chosen to use, and SymbolicRegression.jl, which is the one developed by the authors of Cranmer et al. (2020).

[3]Possibly a psychological data set instead of one of the examples used in the referenced literature.

where Ψ_F denotes the mathematical expression that the algorithm needs to estimate and x_i is the set of features corresponding to the ith particle. To compare the performance of the Bayesian algorithm versus their approach we plan on using the same system that they use and measure the predictive performance and speed of both methods.

Word count: 465/1000

5 Intended results

Symbolic regression algorithms perform best when the relationships they are trying to capture can be represented by a sparse mathematical expression. Including prior knowledge about the properties of a system in the model is a way of encouraging such sparsity, reducing the amount of relationships that the algorithm needs to capture on its own. The main advantages we see of using a Bayesian approach is that it is a general framework that could be used in a multitude in contexts. If the Bayesian models end up performing better than the alternatives, they will be a straightforward alternative that avoids formulating neural networks to incorporating prior knowledge.

Word count: 106/250

6 Work plan

6.1 Time schedule

This internship project consists of 18EC which corresponds to 504 hours of work. Over a period of 21 weeks it averages to 24 hours of work per week.

- February/March: During these months we have reviewed the relevant literature, selected and learned the tooling we are going to use, and designed the structure of the project.

- April: We plan to implement a simple Bayesian symbolic regression algorithm and evaluate its performance.
- May: We plan to implement and evaluate a Bayesian symbolic regression model equivalent to Cranmer et al. (2020) Newtonian Dynamics case.
- June: I will write my internship report. I intend to present the final draft of my internship report on the 18th of June.

If we encounter delays in our planning we could cut down on the number of models to which we compare the performance of the Bayesian symbolic regression algorithm at any step. If it were necessary we could cut the whole comparison with the Newtonian Dynamics case too.

6.2 Data storage

We plan on only using either synthetic or publicly available datasets. We are keeping and will keep all project files under version control, with physical and remote daily backups.

Word count: 192/500

7 References

Cranmer, M., Sanchez-Gonzalez, A., Battaglia, P., Xu, R., Cranmer, K., Spergel, D., & Ho, S. (2020). Discovering symbolic models from deep learning with inductive biases. CoRR. http://arxiv.org/abs/2006.11287v2

Guimerà, R., Reichardt, I., Aguilar-Mogas, A., Massucci, F. A., Miranda, M., Pallarès, J., & Sales-Pardo, M. (2020). A bayesian machine scientist to aid in the solution of challenging scientific problems. Science Advances, 6(5), eaav6971. https://doi.org/10.1126/sciadv.aav6971

Jin, Y., Fu, W., Kang, J., Guo, J., & Guo, J. (2019). Bayesian symbolic regression. CoRR. http://arxiv.org/abs/1910.08892v3

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

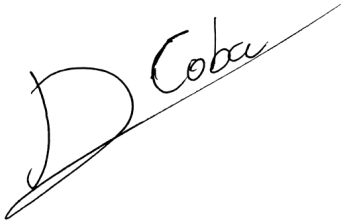
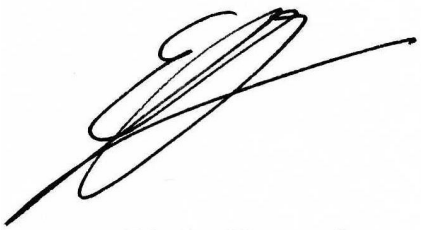
Udrescu, S.-M., & Tegmark, M. (2020). Ai feynman: A physics-inspired method for symbolic regression. Science Advances, 6(16). https://doi.org/10.1126/sciadv.aay2631

8 Further steps

Make sure your supervisor submits an Ethics Checklist for your intended research to the Ethics Review Board of the Department of Psychology at https://www.lab.uva.nl/lab/ethics/ .

9 Signatures

- ☐ I hereby declare that both this proposal, and its resulting internship, will only contain original material and is free of plagiarism (cf. Teaching and Examination Regulation in the research master's course catalogue).
- ☐ I hereby declare that the results section of the internship report will consist of two subsections, one entitled "confirmatory analyses" and one entitled "exploratory analyses" (one of the two subsections may be empty):
    1. The confirmatory analysis section reports exactly the analyses proposed in Section 4 of this proposal
    2. The exploratory analysis section contains not previously specified, and thus exploratory, analyses.

Location:	Student's signature:	Supervisor's signature:
Amsterdam		

Form 2b – Research Master's Psychology: Peer Review Form
Research Internship Proposal

Title of research project: Bayesian Symbolic Regression

Author name: David Coba

Peer reviewer name: Maximilian Maier

Date: 25.03.2021

Write a *one page* review about the project-proposal of your fellow student. At least include the following points in your peer-review:

(1) Summary of project
This needs to be only 1-3 sentences, but it demonstrates that you understand the project-proposal and, moreover, can summarize it more concisely than the author in his abstract.

The author aims to develop a Bayesian symbolic regression, which will allow researchers to find mathematical expressions that describe the data. Unlike other machine learning techniques, this symbolic regression is highly interpretable. However, it can not yet take advantage of the benefits of Bayesian statistics (e.g., incorporating prior information). Therefore, the author's proposal seems highly relevant.

(2) Good things about the proposal (one paragraph)
This is not always necessary, especially when the review is generally favorable. However, it is strongly recommended if the review is critical. Such introductions are good psychology if you think the author needs to drastically revise the proposal.

The purpose of the proposal is clear and seems important. In addition, the proposal is very well written and, in most parts, easy to understand.

(3) Major comments
Discuss the author's assumptions, technical approach, procedure, reference, etc. Be constructive, if possible, by suggesting improvements.

No major comments.

(4) Minor comments
This section contains comments on style, grammar, etc. If any of these are especially poor and detract from the overall presentation, then they might escalate to the 'major comments' section. It is acceptable to write these comments in list (or bullet) form.

- The concept of symbolic trees requires a more detailed explanation. Are these just classification trees, or other kinds of trees?
- I am not familiar with the amount of literature on symbolic regression; therefore, this advice should be taken with skepticism, but I believe the proposal could benefit from incorporating somewhat more literature. For example, the statement "Bayesian methods are not necessarily more demanding than their evolutionary machine learning counterparts" is not supported by any literature.
- I think it would be good to have one expression set to test and try out modifications of the algorithm (like Expression 1) and another applied example to use once the algorithm is finished to avoid overfitting to Expression 1. For example, the Statistical Rethinking book has several nice mathematical models in chapter 16 that could maybe be used for this purpose.

(5) Recommendations
Provide the author with some useful recommendations that you seem fit.

I would add a more detailed explanation of symbolic trees, take another look at the literature to be sure nothing has been missed, and add a mathematical model from Statistical Rethinking chapter 16. All other aspects of the proposal are already of very high quality.

Form 2b – Research Master's Psychology: Peer Review Form
Research Internship Proposal

Title of research project:	Bayesian Symbolic Regression
Author name:	David Coba Castellano
Peer reviewer name:	Leonhard Volz
Date:	24th March 2021

Summary of project
The internship project concerns a Bayesian implementation of symbolic regression. For this purpose, the plan is to first implement and then adapt a previously proposed algorithm and benchmark these with other existing approaches to symbolic regression. If successful, the further aim is to implement this approach as easily usable software.

The proposal is rather concisely written, but get across the idea of symbolic regression, current and proposed approaches and their relative strengths pretty well. Moreover, the subsequent steps to be taken are presented quite clearly.

Major comments
- if I am not mistaken, the proposal should include a project summary (i.e., abstract)
- Rather remove the square brackets and phrase it within the text. Especially at the end of the project description, you could add a paragraph that expands on why this general way to specify Bayesian symbolic regression is relevant / sketch out your aims
- Generally, since you refer to very few papers as you underpinning, you could expand on what their approaches in more detail (e.g., describe the Newtonian Dynamics system if you plan to go through with that step)

Procedure
- Standard: evolutionary algorithm: the footnote implies you made the decision already, the main text however not – try to clarify
- Do you have any considerations regarding assessing overfitting of your modifications? Seems like a general issue to be aware of in symbolic regression
- I wonder about the computational feasibility – possibly explain the environment in which simulations will be conducted

Intended results:
- What you currently describe is more of a rationale that would suit the project description section more than here. I would suggest making a summary of what your tangible outcomes would be (e.g., working algorithms, performance results comparisons, possible package)

Minor comments
Project description:
- ad advantage of SR: compared to specifically fully data-driven machine learning techniques, right?

- in which sense do neural networks encode “prior information”? A bit confusing when you then go on with Bayesian alternatives later, try to make that a bit more clear

Procedure:

- What software do you plan to work with? Julia?

Work plan:

- seems rather optimistic to me, given the necessary steps within each point of the plan. Maybe expand on the individual steps necessary, might give yourself a better overview of the project as well

Recommendations

So far, the proposal is rather short, so it would be good to extend it with a bit more detail on the rationale and the background of the different approaches. Similarly, the procedure is rather vague (but that is more of an outcome given the exploratory nature of such a project). Specific recommendations or points that could be expanded upon are mentioned above.