pySRURGS - a python package for symbolic regression by uniform random global search

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Summary

Symbolic regression is a regression analysis where we search for the mathematical expression that best describes the relationship between our independent variables and our dependent variable. pySRURGS is a python code for symbolic regression by uniform random global search. Typically, symbolic regression problems are solved using genetic programming (Koza, 1994), but the data demonstrating that genetic programming outperforms random search on symbolic regression problems is lacking. Comparing the performance of an algorithm against that of random search demonstrates the advantage gained by the algorithm’s internal machinery. Our review of the literature found a large study examining the parameter space of genetic programming, which found few patterns with regards to how users should select genetic algorithm hyperparameters (Sipper, Fu, Ahuja, & Moore, 2018). These workers attempt to compare their genetic algorithm’s performance to that of random search on several problems, including a symbolic regression problem. We reproduce their work and find they unfairly disadvantaged the random search by forcing it to only attempt the simplest solutions. There is little evidence that genetic algorithms outperform random search on the symbolic regression problem and the creation of pySRURGS addresses this need.

We use a novel methodology for the enumeration of full binary trees (Tychonievich, 2013) and extend it for the symbolic regression problem. This enumeration allows us to ensure that all equations have an equal probability of being selected. pySRURGS is a command line script, allowing the user to specify the nature and size of the search space and the number of equations that will be attempted by the random search. pySRURGS performs fitting parameter optimization using Levenburg-Marquardt nonlinear optimization (Kommenda, Kronberger, Winkler, Affenzeller, & Wagner, 2013), and leverages a SQLite dictionary along with a symbolic equation simplification scheme to minimize repeating calculations. It receives a comma separated value file and generates a mathematical equation that predicts the output variable.

pySRURGS was designed to be used by researchers and individuals working on applied problems. It allows users to generate benchmark problems in symbolic regression and also to enumerate the problem space. Users are allowed to specify which functions they want permitted and how many fitting parameters they want permitted. The code works very nicely, saving results to a sqlite dictionary file for future review. Though intuitive, uniform random global search is proven to converge on the ideal solution as the number of iterations tends to infinity (Solis & Wets, 1981). In addition, pySRURGS has the capability to perform an exhaustive search, which is useful for simpler symbolic regression problems.
Figure 1: pySRURGS uses a binary tree representation for symbolic regression.

References


