Analyzing the influence of Selection on Genetic Programming's Generalization ability in Symbolic Regression

A comparison of epsilon-lexicase Selection and Tournament Selection

Roman Hoehn, B.Sc. Wirtschaftspaedagogik

2022-06-29

Introduction

Research Question

- Does the usage of ϵ-lexicase parent selection influence the generalization behaviour of genetic programming in symbolic regression if compared to tournament selection?

Genetic Programming

- A metaheuristic that searches for computer programs that solve a given problem
- Inventor: John R. Koza [1]
- Evolutionary algorithm that simulates the process of Darwinian evolution:
  1. Population based
  2. The quality of solutions is evaluated by a fitness function
  3. Selection: Solutions are selected based on their individual fitness
  4. Variation: Mutation and recombination of solutions
- Unique Features:
  - Evolve solutions of variable length and structure
  - Solutions are typically represented by recursive tree structures

[1] Koza (1992)

Parent Selection

- Operator that selects individual solutions from the population for reproduction and mutation
- Most commonly used selection operator in Genetic Programming (GP): Tournament selection[2]
- Intuition: High chance for "generalist" solutions to be selected since it is based on aggregated fitness scores

[2] Fang and Li (2010), p.181

epsilon-Lexicase Selection

- Recent alternative: Lexicase Selection and it's variation ϵ-lexicase selection
- Idea: Selection method for uncompromising, continous-valued symbolic regression problems [3]
- Increases genetic diversity inside the population[4]
- Higher chance for "specialist" solutions to be selected since it is decided on a per case basis
- Performance increases have been demonstrated in many benchmarking problems [5]

[3] Helmuth, Spector and Matheson (2015), p.12

[4] Helmuth, Spector and Matheson (2015), p.1

[5] La Cava, Spector and Danai (2016), p.744-745

Symbolic Regression

- Task: Find a mathematical model that fits a given set of datapoints
- One of the first applications of GP described by Koza (1992)
- High relevance: GP can outperform state-of-the-art machine learning algorithms like gradient boosting [6]

[6] Orzechowski, Cava and Moore (2018)

Generalization

- The ability of a model to perform well on previously unseen fitness cases
- Main objective in most supervised machine learning problems
- Challenge: Avoid overfitting to training data

Motivation

- Little attention has been paid to generalization in GP [7]
- High practical relevance of symbolic regression in many fields, e.g. financial forecasting

[7] O'Neill *et al.* (2010), Kushchu (2002)

Experimental Study

Benchmark problem

UC Irvine Machine Learning Repository: Prediction of energy efficiency in buildings [8]

Table 1: Overview - Energy Heating data set

Variable	Description
X1	Relative Compactness
X2	Surface Area
X3	Wall Area
X4	Roof Area
X5	Overall Height
X6	Orientation
X7	Glazing Area
X8	Glazing Area Distribution
y1	Heating Load
y2	Cooling Load

[8] Dua and Graff (2017)

Experiment

Single run

- Total dataset ($N = 768$) is randomly split into a training and testing dataset (50:50)
- Fitness metric: Mean squared Error (MSE)
- Train two models using GP with the training dataset only, one using tournament selection and the other ϵ-lexicase selection
- For each generation: Select elite model and compute its fitness for the testing dataset

Full experiment

- Stochastic algorithm: Repeat the basic experiment for 50 total runs
- Collect and aggregate results for training error, testing error and program length

Evolutionary Parameters

Table 2: Evolutionary Parameters

Parameter	Value
Population Size	500
Number of Generations	100
Mutation Rate	20%
Crossover Rate	80%
Tournament Size	3
Epsilon selection	automatic
Elite Size	0

Function Set

Function	Arity
Addition	2
Subtraction	2
Multiplication	2
Negation	1
Sine	1
Cosine	1
Protected Division	2
Protected Natural Logarithm	1
Protected Square Root	1

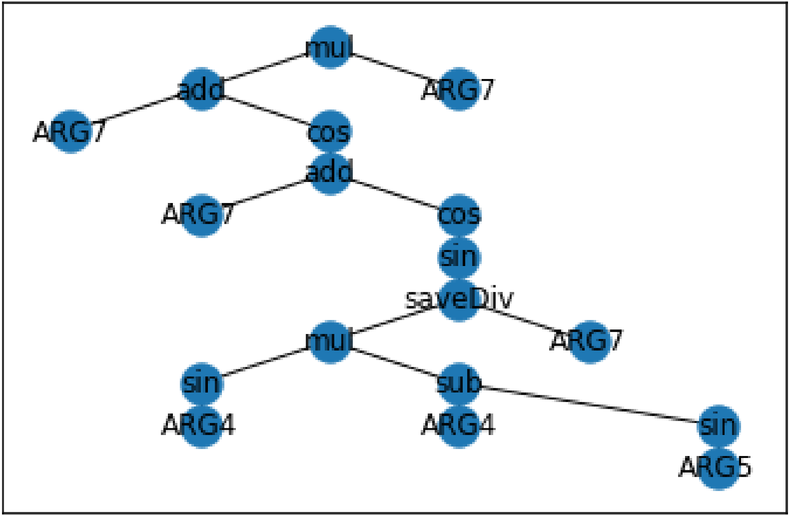
Terminal Set

Terminal	Description
X1	Relative Compactness
X2	Surface Area
X3	Wall Area
X4	Roof Area
X5	Overall Height
X6	Orientation
X7	Glazing Area
X8	Glazing Area Distribution
random_int	Ephemeral Constant (integer)
random_float	Ephemeral Constant(float)

Example

Model evolved by tournament selection after 100 generations:

Best Solution



Research Question

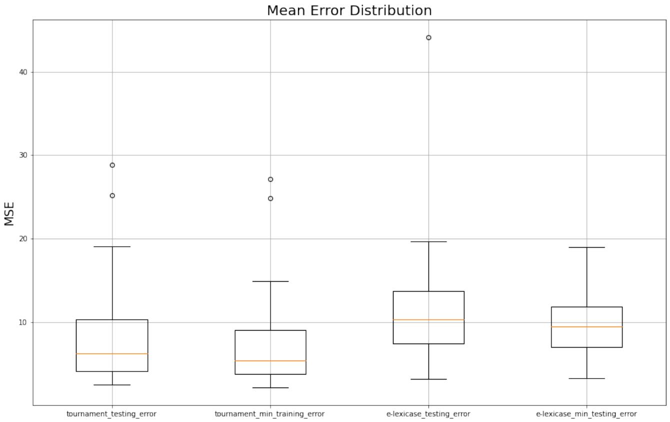
- Does the usage of ϵ-lexicase parent selection influence the generalization behavior of genetic programming in symbolic regression if compared to tournament selection?

3 Questions

1. Differences in average fitness for both algorithms?
2. Differences in fitness for training and testing data?
3. Differences in program size?

Results

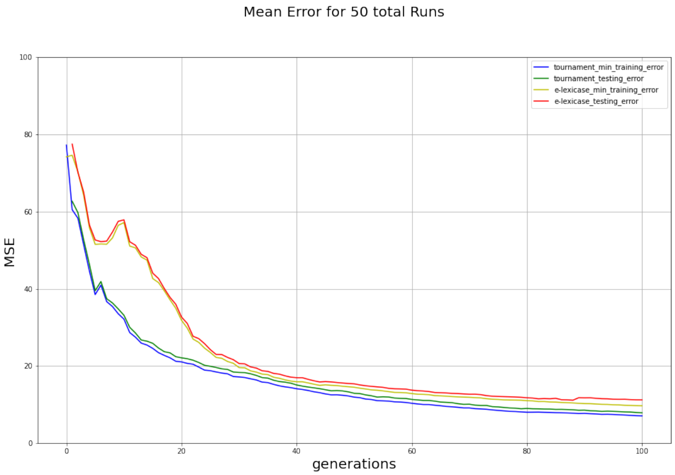
Distribution of Fitness



Finding 1

- The differences in average fitness of the final solutions between tournament selection and ϵ-lexicase selection are highly statistical significant ($\alpha = 0.01$)
- Tournament selection-based GP achieves a higher fitness for both training and testing data
- Unexpected results based on the reviewed literature (La Cava, Spector and Danai, 2016), (La Cava *et al.*, 2017)

Evolution of Fitness



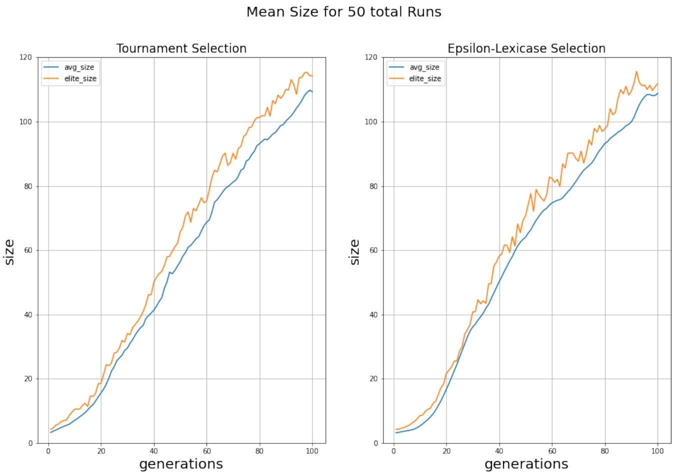
Finding 2

- The gap between training and testing error is not statistically significant for both selection algorithms
- Both algorithms achieve a slightly better performance for the training data
- No proof for overfitting

Statistical Test

```
##                             tournament_training_errors to
## tournament_training_errors                1.000000e+00
## tournament_testing_errors                 3.092303e-01
## elexicase_training_errors                 1.180222e-04
## elexicase_testing_errors                  4.192079e-06
##                             elexicase_training_errors ele
## tournament_training_errors               0.0001180222
## tournament_testing_errors                0.0024468832
## elexicase_training_errors                1.0000000000
## elexicase_testing_errors                 0.2567805508
```

Evolution of Size



Finding 3

...

Conclusions

Conclusions

. . .

Limitations and open Questions

Limitations and open Questions

...

Dua, D. and Graff, C. (2017) "UCI machine learning repository." University of California, Irvine, School of Information; Computer Sciences. Available at: http://archive.ics.uci.edu/ml.

Fang, Y. and Li, J. (2010) "A review of tournament selection in genetic programming," in Cai, Z. et al. (eds.) *Advances in computation and intelligence*. Berlin, Heidelberg: Springer Berlin Heidelberg, pp. 181–192.

Helmuth, T., Spector, L. and Matheson, J. (2015) "Solving uncompromising problems with lexicase selection," *IEEE Transactions on Evolutionary Computation*, 19(5), pp. 630–643. doi:10.1109/TEVC.2014.2362729.

Koza, J.R. (1992) *Genetic programming: On the programming of computers by means of natural selection*. Cambridge, MA, USA: MIT Press. Available at: http://mitpress.mit.edu/books/genetic-programming.

Kushchu, I. (2002) "An evaluation of EvolutionaryGeneralisation in genetic programming," *Artificial Intelligence Review - AIR*, 18, pp.