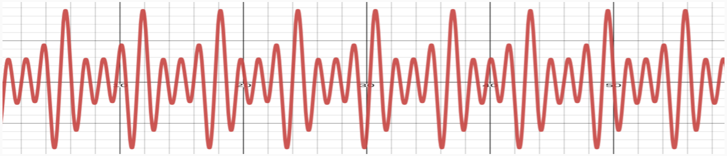
Symbolic Regression Toolbox



Prof. Fabrício Olivetti de França

Federal University of ABC

05 Februrary, 2024

SRBench: A Living Benchmark for Symbolic Regression

SRBench: A Living Benchmark for Symbolic Regression

For a long time, the SR community relied on toy problems and artificial datasets to benchmark new approaches.

Often, new SR algorithms were compared solely to other SR algorithms.

This eventually created some myths:

- SR will return simple expressions but less accurate than opaque models (both statements can be false :-))
- SR is too impractical and it takes a long time to return a model
- Using SR requires complicated installation procedures and fine-tuning many hyperparameters

SRBench: A Living Benchmark for Symbolic Regression

SRBench[1] was created with the objective of reporting the curren state of SR when facing traditional regression algorithms.

The three main goals were:

- Stimulate cross-pollination between SR and ML communities
- Propose a large benchmark set with varying challenges
- Standardize the SR implementations with a common framework

[1] La Cava, William, et al. "Contemporary symbolic regression methods and their relative performance." arXiv preprint arXiv:2107.14351 (2021).

SRBench: A Living Benchmark for Symbolic Regression

The lack of cross-pollination is being addressed by keeping the benchmark open-source[2] and easily reproducible for anyone to verify the current results or add new results.

[2]https://github.com/cavalab/srbench/releases/tag/v2.0

SRBench: A Living Benchmark for Symbolic Regression

The datasets were taken from the PMLB[3] that contains 252 datasets for regression comprehending synthetic and real-world data with different characteristics.

[3] Romano, Joseph D., et al. “PMLB v1. 0: an open-source dataset collection for benchmarking machine learning methods.” Bioinformatics 38.3 (2022): 878-880.

SRBench: A Living Benchmark for Symbolic Regression

The first set of benchmark are termed **black-box regression problems** and were taken from different public sources:

- 122 datasets
- No known generator function, but…
- 62 are generated from the Friedman benchmark with varying degree of noise and correlated features
- The Friedman sets have known generator function but cannot be identified by the benchmark names.

more on that later

SRBench: A Living Benchmark for Symbolic Regression

The second set of benchmark are termed **ground-truth regression problems** and inclued data from two sources:

- Feynman Symbolic Regression dataset: 116 datasets
- ODE-Strogatz database: 14 datasets
- We know the generator function for all of them

SRBench: A Living Benchmark for Symbolic Regression

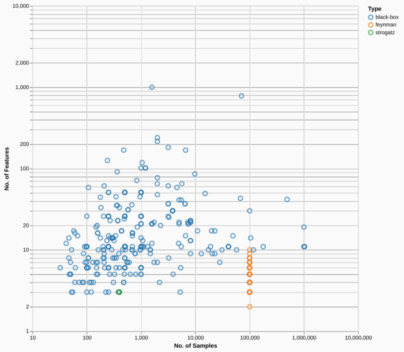


Figure 1: https://cavalab.org/srbench/datasets/

SRBench: A Living Benchmark for Symbolic Regression

To address the lack of an unified framework, the benchmark required the implementation of a common API compatible with the well known *scikit-learn*.

SRBench: A Living Benchmark for Symbolic Regression

Requirements for a competitor:

- scikit-learn compatible API (https://scikit-learn.org/stable/developers/develop.html)[https://scikit-learn.org/stable/developers/develop.html]
- Compatible with Python 3.7 or higher
- If your method uses a random seed, support a `random_state` attribute
- The method should have the requirements and installation script at the algorithms folder (upload through a pull request)

SRBench: A Living Benchmark for Symbolic Regression

The algorithm folder should have:

- `metadata.yml` describing the algorithm
- `regressor.py` a Python script with instructions on how to benchmark the method
- `LICENSE` with the license information
- `environment.yml` a conda environment file with additional requirements
- `requirements.txt` a `pypi` file with additional requirements
- `install.sh` a script that copies the source-code or package from an external source (e.g., github repo) and installs the method.

SRBench: A Living Benchmark for Symbolic Regression

Example of `install.sh`:

```
# remove directory if it exists
if [ -d tir ]; then
    rm -rf tir
fi

git clone https://github.com/folivetti/tir.git
cd tir
export BOOTSTRAP_HASKELL_NONINTERACTIVE=1
curl --proto '=https' --tlsv1.2 -sSf
       https://get-ghcup.haskell.org | bash
export PATH=$PATH:~/.ghcup/bin:~/.cabal/bin
cabal install --overwrite-policy=always
       --installdir=./python
cd python
pip install .
```

SRBench: A Living Benchmark for Symbolic Regression

Example of `regressor.py`:

```python
import sys
import os
import pyTIR as tir
from itertools import product
os.environ["LD_LIBRARY_PATH"] = os.environ["CONDA_PREFIX"] + "/lib"

hyper_params = [
    {
        'transfunctions' : ('Id,Tanh,Sin,Cos,Log,Exp,Sqrt',),
        'ytransfunctions' : ('Id,Sqrt,Exp,Log,ATan,Tan,Tanh',),
        'exponents' : ((-5,5),)
    },
    {
        'transfunctions' : ('Id,Tanh,Sin,Cos,Log,Exp,Sqrt',),
        'ytransfunctions' : ('Id,Sqrt,Exp,Log,ATan,Tan,Tanh',),
        'exponents' : ((-2,2),)
    },
]
```

SRBench: A Living Benchmark for Symbolic Regression

The `regressor.py` file should contain a function `model` that returns a sympy compatible model.

```python
# Create the pipeline for the model
eval_kwargs = {'scale_x': False, 'scale_y': False}
est = tir.TIRRegressor(npop=1000, ngens=500, pc=0.3, pm=0.7,
       exponents=(-5,5), error="R^2", alg="MOO")

def pre_train(est, X, y):
    """Adjust settings based on data before training"""
    if X.shape[0]*X.shape[1] <= 1000:
        est.penalty = 0.01

def complexity(e):
    return e.len

def model(e, X):
    new_model = e.sympy.replace("^","**")
    for i,f in reversed(list(enumerate(X.columns))):
        new_model = new_model.replace(f'x{i}',f)
    return new_model
```

SRBench: A Living Benchmark for Symbolic Regression

- You can install SRBench together with all supported algorithms using `conda` or `docker`
- You can either run the entire benchmark, or just selected algorithm or selected dataset
- You can also run for new datasets provided they are compatible with PMLB format

See: https://cavalab.org/srbench/user-guide/

SRBench: A Living Benchmark for Symbolic Regression

Evaluated methods:

- Age-Fitness Pareto Optimization (Schmidt and Lipson 2009)
- Age-Fitness Pareto Optimization with Co-evolved Fitness Predictors (Schmidt and Lipson 2009)
- AIFeynman 2.0 (Udrescu et al. 2020)
- Bayesian Symbolic Regression (Jin et al. 2020)
- Deep Symbolic Regression (Petersen et al. 2020)
- Fast Function Extraction (McConaghy 2011)
- Feature Engineering Automation Tool (La Cava et al. 2017)

SRBench: A Living Benchmark for Symbolic Regression

Evaluated methods (cont.):

- epsilon-Lexicase Selection (La Cava et al. 2016)
- GP-based Gene-pool Optimal Mixing Evolutionary Algorithm (Virgolin et al. 2017)
- gplearn (Stephens)
- Interaction-Transformation Evolutionary Algorithm (de Franca and Aldeia, 2020)
- Multiple Regression GP (Arnaldo et al. 2014)
- Operon (Burlacu et al. 2020)
- Semantic Backpropagation GP (Virgolin et al. 2019)

SRBench: A Living Benchmark for Symbolic Regression

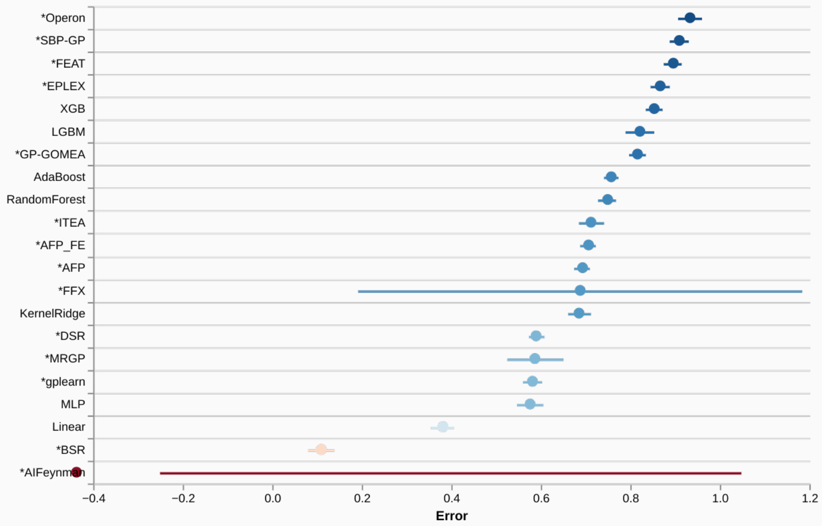


Figure 2: https://cavalab.org/srbench/results/

SRBench: A Living Benchmark for Symbolic Regression

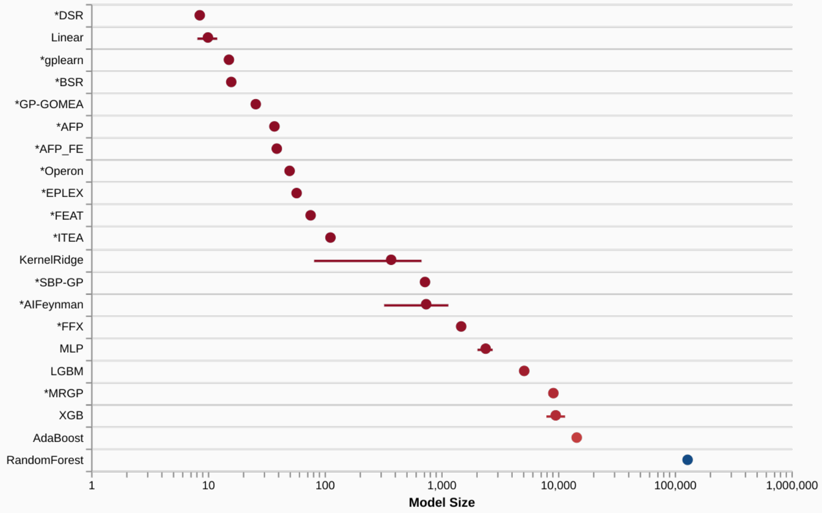


Figure 3: https://cavalab.org/srbench/results/

SRBench: A Living Benchmark for Symbolic Regression

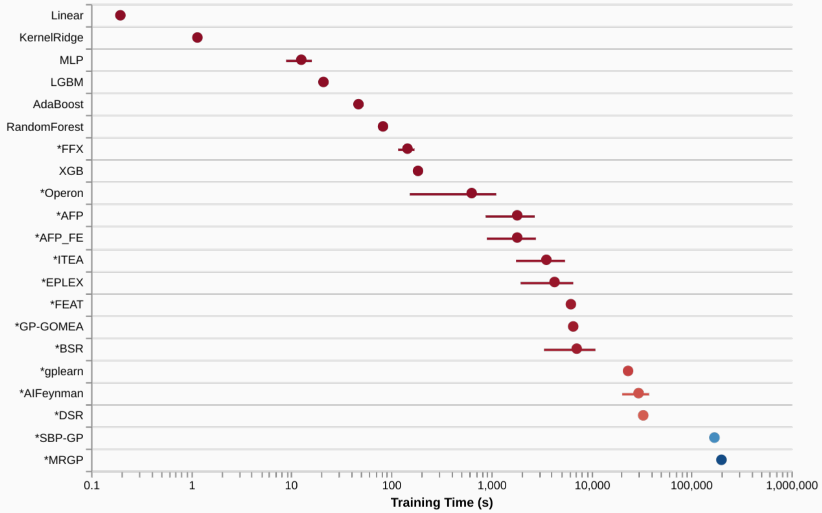


Figure 4: https://cavalab.org/srbench/results/

SRBench: A Living Benchmark for Symbolic Regression

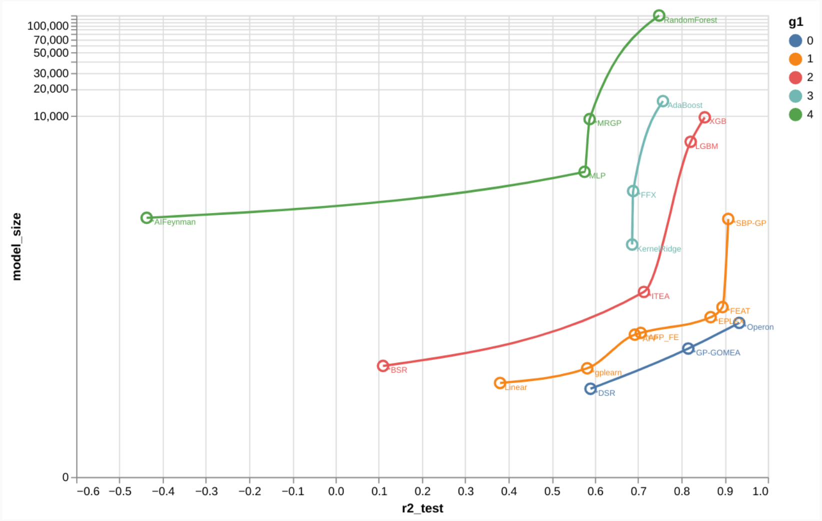


Figure 5: https://cavalab.org/srbench/results/

SRBench: A Living Benchmark for Symbolic Regression

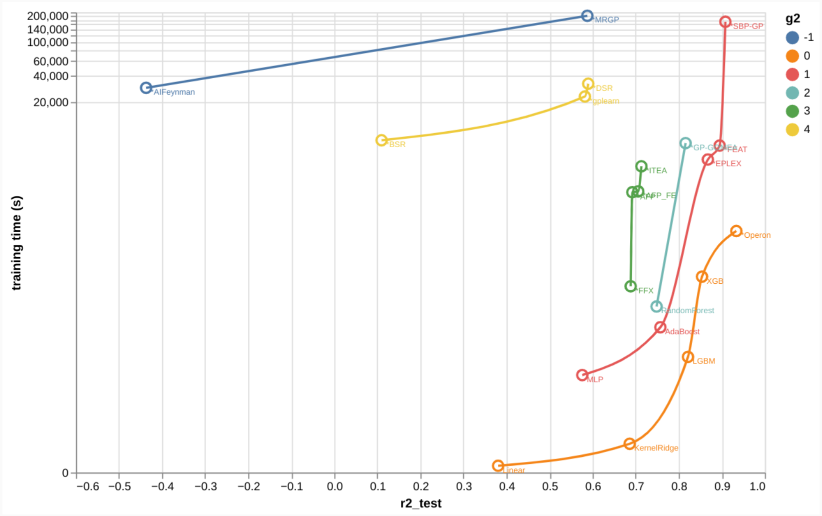


Figure 6: https://cavalab.org/srbench/results/

SRBench 1st Competition

A competition based on SRBench was hosted in GECCO 2022[4] and it was divided into two tracks:

- synthetic track: composed of different challenges provided by artificial datasets
- real-world track: real-world data where the models were judged by an expert in the field

[4] https://cavalab.org/srbench/competition-2022/

SRBench 1st Competition

The synthetic track was composed of:

- **rediscovery of the exact expression:** where the exact expression of the generating function should be returned.
- **selection of relevant features:** the models must use only relevant features.
- **escaping local optima:** the models should not use imperfect *shortcuts* of the true expression.
- **extrapolation accuracy:** the models should behave correctly outside the training boundary.
- **sensitivity to noise:** the models should be robust against added noise.

SRBench 1st Competition

The real-world track was composed of time-series of case, hospitalization, and death during the covid pandemic.

This dataset was processed to become a tabular data compatible with most SR methods.

The main goal of this track was to find a model that was easy to interpret with accurate predictions.

SRBench 1st Competition

We got some new participants on-board:

- Bingo
- E2ET
- PS-Tree
- QLattice
- TaylorGP
- EQL
- GeneticEngine
- Operon
- PySR
- uDSR
- GP_{ZGD}
- NSGA-DCGP

SRBench 1st Competition

- Varying degree of difficulties by introducing noise to the target variable.
- Evaluated in two or three criteria: R^2 on a noiselees data, log of tree length, property score.
- Property score depends on the task: feature absence score and exact expression.

SRBench 1st Competition

- Recovery of true expression:

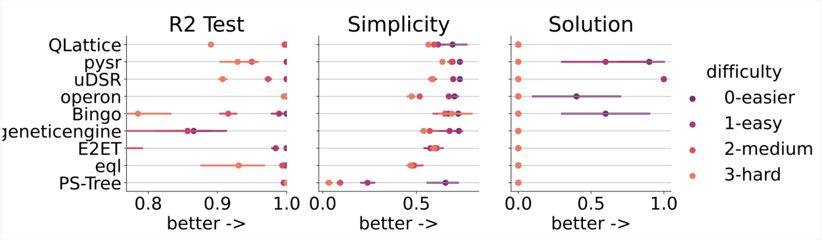


Figure 7: de Franca, F. O., et al. “Interpretable Symbolic Regression for Data Science: Analysis of the 2022 Competition.” arXiv preprint arXiv:2304.01117 (2023).

SRBench 1st Competition

$$f(x) = \frac{-1.66x_1 + (-0.02x_1 - 0.15)(-16.15x_2 - 6.46)}{(0.2x_1^2 + 1)\left(\frac{0.19x_2^2}{0.2x_1^2+1} + 1\right)^{0.5}\left(\frac{0.21x_2^2}{0.2x_1^2+1} + 1\right)^{0.5}} \tag{6}$$

Figure 8: de Franca, F. O., et al. “Interpretable Symbolic Regression for Data Science: Analysis of the 2022 Competition.” arXiv preprint arXiv:2304.01117 (2023).

SRBench 1st Competition

- Feature Selection:

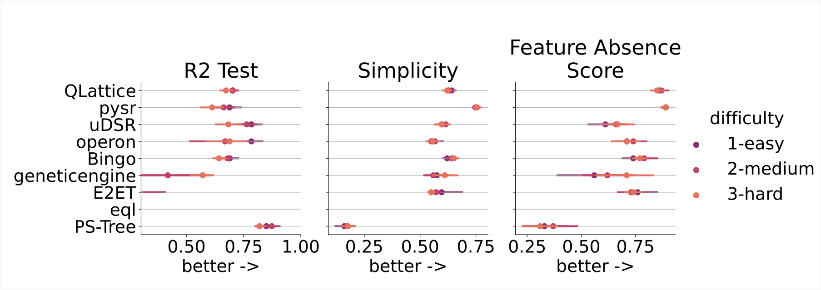


Figure 9: de Franca, F. O., et al. “Interpretable Symbolic Regression for Data Science: Analysis of the 2022 Competition.” arXiv preprint arXiv:2304.01117 (2023).

SRBench 1st Competition

- Local optima:

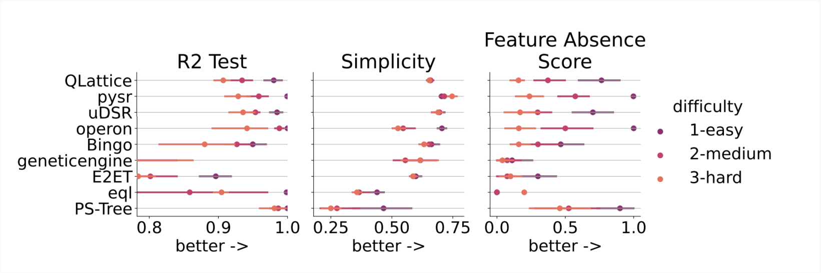


Figure 10: de Franca, F. O., et al. “Interpretable Symbolic Regression for Data Science: Analysis of the 2022 Competition.” arXiv preprint arXiv:2304.01117 (2023).

SRBench 1st Competition

- Extrapolation:

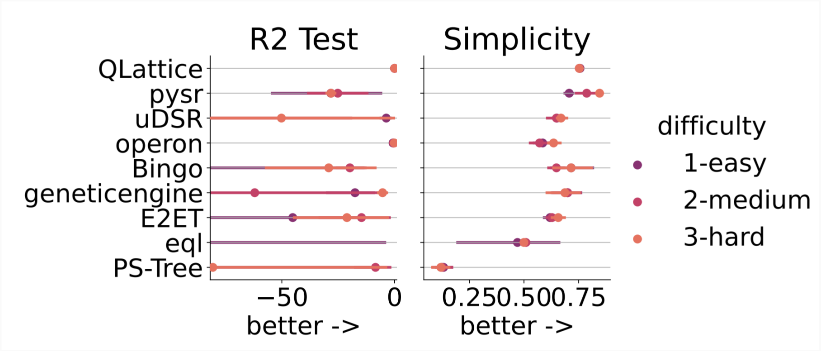


Figure 11: de Franca, F. O., et al. “Interpretable Symbolic Regression for Data Science: Analysis of the 2022 Competition.” arXiv preprint arXiv:2304.01117 (2023).

SRBench 1st Competition

- Extrapolation:

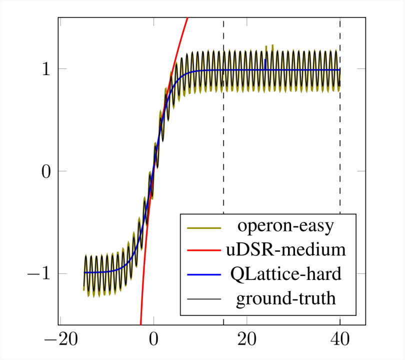


Figure 12: de Franca, F. O., et al. “Interpretable Symbolic Regression for Data Science: Analysis of the 2022 Competition.” arXiv preprint arXiv:2304.01117 (2023).

SRBench 1st Competition

- Noise:

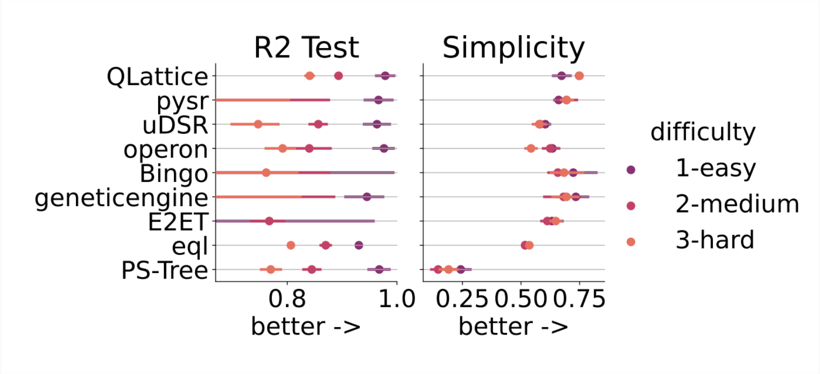


Figure 13: de Franca, F. O., et al. "Interpretable Symbolic Regression for Data Science: Analysis of the 2022 Competition." arXiv preprint arXiv:2304.01117 (2023).

SRBench 1st Competition

This competition brought to light many aspects of the current state-of-the-art in SR[5]:

- **No free lunch and the need for finetuning:** as expected there is no dominating method in this competition, each method favored one aspect of regression analysis. Besides, for many reasons, some of these methods may not have been correctly fine-tuned for the competition.
- **Simplicity measure is too simple:** using only the length hides some undesired constructs such as the chaining of nonlinear functions.

[5]de Franca, F. O., et al. “Interpretable Symbolic Regression for Data Science: Analysis of the 2022 Competition.” arXiv preprint arXiv:2304.01117 (2023).

SRBench 1st Competition

This competition brought to light many aspects of the current state-of-the-art in SR[6]:

- **Few repetitions x computational budget:** having a limited computational budget allowed for only a few repetitions which can increase the uncertainties of the results.
- **Interpretable:** judging whether a model is interpretable or not is too subjective and error prone.

[6] de Franca, F. O., et al. “Interpretable Symbolic Regression for Data Science: Analysis of the 2022 Competition.” arXiv preprint arXiv:2304.01117 (2023).

SRBench 1st Competition

This competition brought to light many aspects of the current state-of-the-art in SR[7]:

- Most implementations lack a post-analysis tool that provides: a set of alternative models, algebraic simplification of the expressions, uncertainty measures, visual inspection tools, general customizations.

[7] de Franca, F. O., et al. “Interpretable Symbolic Regression for Data Science: Analysis of the 2022 Competition.” arXiv preprint arXiv:2304.01117 (2023).

SRBench 2nd Competition

A second competition was hosted in GECCO 2023[8] where the competitors could play with a training data for a period of time and submit a single model to be evaluated.

[8]https://cavalab.org/srbench/competition-2023/

SRBench 2nd Competition

- SRBench Competition 2023
- https://cavalab.org/srbench/competition-2023/

- Two tracks:
    - Performance
    - Interpretability

SRBench 2nd Competition

- Github Classroom: participants can form teams and play with the datasets until the deadline
- Enjoying more freedom to perform regression analysis, can the participants succeed?
    - More about the use of the SR tools rather than comparing algorithms

Europain Secret

Europain created by GitHub Classroom - Edit

1 member

SRBench 2nd Competition

- 3 datasets:
  - Shubert function
  - NASA dataset (black-box)
  - Vincent function

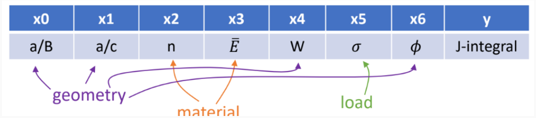
$$f_1 = \prod_{i=1}^{n} \sum_{j=1} 3j * cos((j+1) * x_i + j)$$

$$f_2 = ??$$

$$f_3 = \frac{1}{8} \sum_{i=1}^{8} 10 \log(x_i)$$

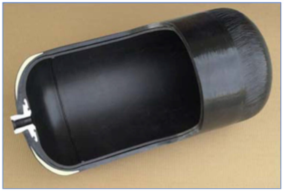
SRBench 2nd Competition (NASA dataset)

- Based on 600 3-D simulations of cracks in flat plates under loading
  - Goal: to predict the growth of cracks in thin metal layers
- A closed form expression has a profound impact on material characterization, structural design, and failure analysis at NASA and beyond



x0	x1	x2	x3	x4	x5	x6	y
a/B	a/c	n	$\bar{E}$	W	σ	ϕ	J-integral

geometry
material
load



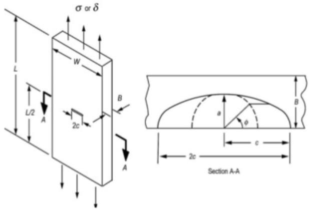


Illustration of a semi-elliptical surface crack in a flat plate.

Figure from: Allen, Phillip A., and Douglas N. Wells. "Interpolation methodology for elastic–plastic J-integral solutions for surface cracked plates in tension." *Engineering Fracture Mechanics* 119 (2014): 173-201.

SRBench 2nd Competition

- We added a little spice to these datasets:
  - Gaussian noise
  - Noisy and irrelevant features
  - Colinear features

SRBench 2nd Competition

$$\text{tot-score} = \frac{6}{\sum_{i=1}^{3} \frac{1}{acc_i} + \frac{1}{simpl_i}}$$

$$acc_i = N - k + 1$$

$$simpl_i = N - k + 1$$

where N is the number of participants and k is the rank w.r.t. R^2 or expression length.

SRBench 2nd Competition

- Montreal Bike Lane: predict the number of bikes crossing a bike lane in Montreal
    - contains additional info about the weather of any given day
- Participants must explore the dataset, apply one or more SR algorithms, and extract interesting findings

SRBench 2nd Competition

- Level of details in the pipeline
- Readability of the model
- Interestingness of the pre and post analysis process
- Analysis of interpretation (with special points for analysis that can only be made using SR models)
- Average of organizers grading.

SRBench 2nd Competition

Team	Participants	method	score	rank	src
pksm	Parshin Shojaee Kazem Meidan	TPSR	6.307885	1	N
newton-sr	Nicolas Lassabe Paul Gersberg	NewTonSR++	6.224784	2	Y
sarma	Aleksandar Kartelj Marko Djukanovic	RILS	6.136364	3	Y
player	Lianjie Zhong Jinghui Zhong Dongjunlan Nikola Gligorovski	PFGP	5.448649	4	Y
stackgp	Nathan Haut	stackgp	5.130641	5	Y
university-of-wellington	Hengzhe Zhang Qi Chen Bing Xue Mengjie Zhang	SR-Forest	4.251969	6	Y
wonderful-time	Hai Minh Nguyen	SymMFEA	3.440273	7	Y
his_jsr	Gurushant Gurushant Jatinkumar Nakrani Rajni Maandi	LR + gplearn	3.43949	8	Y
tontakt	Andrzej Odrzywołek	enumeration, PySR, rational poly	2.855524	9	Y
amir	Mohammad Amirul Islam	PySR	1.788926	10	Y

SRBench 2nd Competition

Team	Participants	method	score	rank	src
university-of-wellington	Hengzhe Zhang Qi Chen Bing Xue Mengjie Zhang	SR-Forest	3.25	1	Y
player	Lianjie Zhong Jinghui Zhong Dongjunlan Nikola Gligorovski	PFGP	2.83	2	Y
his_jsr	Gurushant Gurushant Jatinkumar Nakrani Rajni Maandi	gplearn	2.25	3	Y
c-bio-ufpr	Adriel Macena Falcão Martins Aurora Trinidad Ramirez Pozo	PySR	1.75	4	Y

SRBench 2nd Competition

- Additional freedom stimulated creativity and hybrid approaches
- Evaluation of SR under a practical point of view
- Not to be used to compare average performance of SR algorithms
- Making new datasets is still hard
- SR can generate accurate and interpretable models, this should be explored more!

srtree-opt

srtree-opt

srtree-opt[9] is a command line tool to parse and post-process symbolic regression models.

It was created as a support library for ITEA and TIR algorithms and changed into a CLI tool for convenience.

It currently support expressions generated by: TIR, HeuristicLab, Operon, BINGO, GP-GOMEA, PySR, SBP, and EPLEX.

[9] https://github.com/folivetti/srtree-opt

srtree-opt

It supports two modes: csv and detailed report.

- CSV report: stores the main properties and different quality measures of the parsed expression.
- Detailed report: shows the same information as the CSV report but as a prettyfied format and it shows the confidence intervals for the parameters and predictions.

It also supports to refit the parameters and simplification of the expressions using equality saturation.

srtree-opt

The CSV report shows:

- Expression in a standard format
- Number of nodes of the expression
- Number of parameters
- Parameters values
- Iterations to converge to local optima (if asked to optimize)

srtree-opt

Error and accuracy measures for the training, validation, test sets and for the original and refitted expression:

- Sum of Squared Error (SSE)
- Bayesian Information Criteria
- Akaike Information Criteria
- Minimum Description Length (and variations)
- Evidence
- Negative Log-Likelihood
- Log-Functional
- Log-Parameters
- Fisher Information Matrix

srtree-opt

In report mode it also shows the confidence interval for the parameters and predictions using either Laplace approximation or Profile Likelihood

srtree-opt

Available options:

```
  -f,--from ['tir'|'hl'|'operon'|'bingo'|'gomea'|'pysr'|'sbp'|'eplex']
                           Input expression format
  -i,--input INPUT-FILE    Input file containing expressions.
                           Empty string gets expression from stdin.
  -o,--output OUTPUT-FILE  Output file to store the stats. Empty
                           string prints expressions to stdout.
  -d,--dataset DATASET-FILENAME
                           Filename of the dataset used for optimizing
                           the parameters.
                           Empty string omits stats that make use of
                           the training data.
```

srtree-opt

Available options (cont.):

```
  --test TEST                Filename of the test dataset.
  --hasheader                Uses the first row of the csv
                             file as header.
  --simplify                 Apply basic simplification.
```

srtree-opt

Available options (cont.):

```
  --niter NITER              Number of iterations for the
                             optimization algorithm.
                             Set 0 for no optimization.

  --distribution ['gaussian'|'bernoulli'|'poisson']
                             Minimize negative log-likelihood
                             following one of the
                             avaliable distributions.
                             The default will use least
                             squares to optimize the model.
  --sErr Serr                Estimated standard error of the data.
                             Defaults to model MSE.
  --restart                  If set, it samples the initial values
                             of the parameters using a Gaussian
                             distribution N(0, 1),
                             otherwise it uses the original values of the
                             expression.
  --seed SEED                Random seed to parameter initialization.
```

srtree-opt

Available options (cont.):

```
  --report                     If set, reports the analysis in
                               a user-friendly format instead of csv.
                               It will also include
                               confidence interval for the parameters and
                               predictions
  --profile                    If set, it will use profile likelihood
                               to calculate CIs.
  --alpha ALPHA                Significance level for confidence intervals.
                               (default: 5.0e-2)
```

srtree-opt

This tool will automatically handle gzipped datasets if the last extension is `.gz`. It will auto-detected the delimiter.

The filename can include additional information in the format:

`filename.csv:start:end:target:vars`

where `start` and `end` corresponds to the range of rows that should be used for training, the other rows will be used for validation.

`target` is the column index or name of the target variable, and `vars` is a comma separated list of column indices or variable names to use as predictors.

srtree-opt

If our dataset `data.csv` has the header row with the following information:

```
var1,var2,var3,target1,target2
```

we can load it by passing `data.csv`, where it will use every row for training and every column as a predictor, except for the last one that will be the target.

srtree-opt

If we pass `data.csv:0:10:target1:var1,var3,var2`, it will use the first 10 rows for training, the remainder for validation, the taget variable will be the column named `target1`, and `x0,x1,x2` will be `var1,var3,var2`, respectivelly.

We can also use index values such as `data.csv:0:10:3:0,2,1` and we can mix both names and indices. The values can be omitted to use the defaults.

srtree-opt

Example usage:

```
srtree-opt -f operon -i expression_file
   -d data.csv::99:target_noise --sErr 7.2659 --hasheader
   --niter 100 --distribution gaussian
   --restart --simplify
```

srtree-opt

Example report output:

```
=================== EXPR 0 ===================
(Sqrt((Abs((x3 + 0.6699816344531162)) / x1))
   - (393.7006500300653 / (x4 + (9.51898304028687 * x5))))

---------General stats:---------

Number of nodes: 15
Number of params: 3
theta = [0.6699816344531162,393.7006500300653,9.51898304028687]

----------Performance:--------

SSE (train.): 5258.3653
SSE (val.): 0.0
SSE (test): 0.0
NegLogLiklihood (train.): 1187.4301
NegLogLiklihood (val.): 0.0
NegLogLiklihood (test): 0.0
```

srtree-opt

Example report output (cont.):

```
------Selection criteria:-----

BIC: 2397.8578
AIC: 2382.8603
MDL: 1229.8937
MDL (freq.): 1229.663
Functional complexity: 35.9684
Parameter complexity: 6.4951

---------Uncertainties:----------

Correlation of parameters:
3x3
 1.00  0.17  -0.04
 0.17  1.00   0.97
-0.04  0.97   1.00

Std. Err.: [0.2737,137.6956,3.724]
```

srtree-opt

Example report output (cont.):

```
Confidence intervals:

lower <= val <= upper
0.1315 <= 0.67 <= 1.2085
122.768 <= 393.7007 <= 664.6333
2.1916 <= 9.519 <= 16.8464

Confidence intervals (predictions training):

lower <= val <= upper
2.9795 <= 3.0478 <= 3.1161
2.3457 <= 2.422 <= 2.4983
4.0335 <= 4.151 <= 4.2684
2.9836 <= 3.0796 <= 3.1755
2.5375 <= 2.6771 <= 2.8167
```

SR Implementations Highlights

PyOperon

Operon[10] is a modern C++ implementation of a GP algorithm for SR created with the objective of being performant and offering a wide range of customizations.

It uses vectorized evaluations, a cutting edge library for linear algebra, and concurrency to achive high performance and be one of the fastest SR implementations.

[10]Burlacu, Bogdan, Gabriel Kronberger, and Michael Kommenda. “Operon C++ an efficient genetic programming framework for symbolic regression.” Proceedings of the 2020 Genetic and Evolutionary Computation Conference Companion. 2020.

PyOperon

PyOperon[11] is a Python binding for the C++ implementation offering easy-to-install and easy-to-use access to Operon.

This implementation offer a scikit-learn compatible library, for easy of use, and a direct binding to the C++ implementation, offering a more customized experience.

[11]Burlacu, Bogdan, Gabriel Kronberger, and Michael Kommenda. “Operon C++ an efficient genetic programming framework for symbolic regression.” Proceedings of the 2020 Genetic and Evolutionary Computation Conference Companion. 2020.

PyOperon - scikit-learn interface

```python
from pyoperon.sklearn import SymbolicRegressor
reg = SymbolicRegressor(
        allowed_symbols= "add,sub,mul,div,constant,variable",
        brood_size= 10,
        comparison_factor= 0,
        crossover_internal_probability= 0.9,
        crossover_probability= 1.0,
        epsilon= 1e-05,
        female_selector= "tournament",
        generations= 1000,
        pool_size= 1000,
        population_size= 1000,
        random_state= None,
        reinserter= "keep-best",
        time_limit= 900,
        tournament_size= 3,
        uncertainty= [sErr]
        )
reg.fit(x, y)
reg.score(x,y)
res = [(s['objective_values'], s['tree'],
          s['minimum_description_length']) for s in reg.pareto_front_]
for obj, expr, mdl in res:
    print(obj, mdl, reg.get_model_string(expr, 16))
```

PyOperon - scikit-learn interface

Main arguments:

- `allowed_symbols`: a comma separated list of operators (add,sub,mul,div,constant,variable, aq, pow, exp, log, sin, cos, tan, tanh, sqrt, cbrt, square, dyn)
- `crossover_probability`: probability of applying crossover
- `mutation_probability`: probability of applying mutation
- `mutation:` prob. distribution of each mutation (onepoint, discretepoint, changevar, changefunc, insertsubtree, replacesubtree, removesubtree)
- `offspring_generator`: basic, offspring, brood, polygenic
- `reinserter`: keepbest, replaceworst
- `objectives`: a list of objectives (r2,c2,mse,rmse,mae)
- `optimizer`: lm, lbgs, sgd

PyOperon - scikit-learn interface

Main arguments (cont.):

- `optimizer_likelihood`: gaussian, poisson
- `initialization_method`: grow, ptc, btc
- `population_size`: an integer of the population size
- `generations`: the number of generations
- `max_evaluations`: maximum number of evaluations
- `model_selection_criterion`: mdl, bic, aik

PyOperon - binding

(from https://github.com/heal-research/pyoperon/blob/main/example/operon-bindings.py):

```
import random, time, sys, os, json
import numpy as np
import pandas as pd
from scipy import stats

import pyoperon as Operon
from pmlb import fetch_data

# get some training data - see https://epistasislab.github.io/pmlb/
D = fetch_data('1027_ESL', return_X_y=False, local_cache_dir='./dataset

# initialize a dataset from a numpy array
ds             = Operon.Dataset(D)

# define the training and test ranges
training_range = Operon.Range(0, ds.Rows // 2)
test_range     = Operon.Range(ds.Rows // 2, ds.Rows)
```

PyOperon - binding

```
# define the regression target
target          = ds.Variables[-1] # take the last column in the dataset
                                                                                                                          
# take all other variables as inputs
inputs          = [ h for h in ds.VariableHashes if h != target.Hash ]

# initialize a rng
rng             = Operon.RomuTrio(random.randint(1, 1000000))

# initialize a problem object which encapsulates the data,input,target
problem         = Operon.Problem(ds, training_range, test_range)
problem.Target = target
problem.InputHashes = inputs
```

PyOperon - binding

```
# initialize an algorithm configuration
config = Operon.GeneticAlgorithmConfig(generations=1000,
             max_evaluations=1000000, local_iterations=0,
             population_size=1000, pool_size=1000
             p_crossover=1.0, p_mutation=0.25
             epsilon=1e-5, seed=1, time_limit=86400)

selector        = Operon.TournamentSelector(objective_index=0)
selector.TournamentSize = 5

problem.ConfigurePrimitiveSet(Operon.PrimitiveSet.Arithmetic
          | Operon.NodeType.Exp | Operon.NodeType.Log |
          Operon.NodeType.Sin | Operon.NodeType.Cos)
pset = problem.PrimitiveSet

minL, maxL      = 1, 50
maxD            = 10

btc             = Operon.BalancedTreeCreator(pset,
                  problem.InputHashes, bias=0.0)
tree_initializer = Operon.UniformLengthTreeInitializer(btc)
tree_initializer.ParameterizeDistribution(minL, maxL)
tree_initializer.MaxDepth = maxD
```

PyOperon - binding

```python
coeff_initializer = Operon.NormalCoefficientInitializer()
coeff_initializer.ParameterizeDistribution(0, 1)

mut_onepoint   = Operon.NormalOnePointMutation()
mut_changeVar  = Operon.ChangeVariableMutation(inputs)
mut_changeFunc = Operon.ChangeFunctionMutation(pset)
mut_replace    = Operon.ReplaceSubtreeMutation(btc,
                       coeff_initializer, maxD, maxL)

mutation       = Operon.MultiMutation()
mutation.Add(mut_onepoint, 1)
mutation.Add(mut_changeVar, 1)
mutation.Add(mut_changeFunc, 1)
mutation.Add(mut_replace, 1)

# define crossover
crossover_internal_probability = 0.9
crossover = Operon.SubtreeCrossover(crossover_internal_probability,
                   maxD, maxL)
```

PyOperon - binding

```
dtable           = Operon.DispatchTable()
error_metric     = Operon.R2()
evaluator        = Operon.Evaluator(problem, dtable, error_metric, True)
evaluator.Budget = 1000 * 1000

optimizer        = Operon.LMOptimizer(dtable, problem, max_iter=10)

generator        = Operon.BasicOffspringGenerator(evaluator,
                         crossover, mutation, selector, selector)

reinserter       = Operon.ReplaceWorstReinserter(objective_index=0)
gp               = Operon.GeneticProgrammingAlgorithm(problem,
                      config, tree_initializer, coeff_initializer,
                      generator, reinserter)

gen = 0
max_ticks = 50
interval = 1 if config.Generations < max_ticks
             else int(np.round(config.Generations / max_ticks, 0))
t0 = time.time()
```

PyOperon - binding

```python
def report():
    global gen
    best = gp.BestModel
    bestfit = best.GetFitness(0)
    sys.stdout.write('\r')
    cursor = int(np.round(gen / config.Generations * max_ticks))
    for i in range(cursor):
        sys.stdout.write('\u2588')
    sys.stdout.write(' ' * (max_ticks-cursor))
    sys.stdout.write(f'{100 * gen/config.Generations:.1f}%,
                     generation {gen}/{config.Generations},
                     train quality: {-bestfit:.6f},
                     elapsed: {time.time()-t0:.2f}s')
    sys.stdout.flush()
    gen += 1

# run the algorithm
gp.Run(rng, report, threads=0)

# get the best solution and print it
best = gp.BestModel
model_string = Operon.InfixFormatter.Format(best.Genotype, ds, 6)
print(f'\n{model_string}')
```

PySR

PySR[12] is a python binding for a high-performance SR implementation in Julia.

The main focus of this implementation is to enable SR as an automatic tool to discover science laws from data.

[12]https://github.com/MilesCranmer/PySR

PySR

As such, this SR tool was engineered to be high-performant, customizable, and easy to use.

It is multi-objective by default and it returns a selection of expressions with the tradeoff of accuracy and simplicity.

PySR

This implementation differs from traditional GP by introducing some novelties[13]:

- It applies a simulated annealing strategy to accept or reject a mutated solution, alternating between high and low temperature (to promote either a local search or diversity).
- It envelopes the evolution into a evolve-simplify-optimize loop, where the population is evolved (through mutation and crossover) for a number of iterations and then they go through algebraic simplification (to remove some redundancies) and nonlinear optimization of the parameters.
- It introduces an adaptive parsimony control that enables the population to keep individuals of different complexity levels.

[13]Cranmer, Miles. “Interpretable machine learning for science with PySR and SymbolicRegression. jl.” arXiv preprint arXiv:2305.01582 (2023).

PySR

Besides that, it provdes several additional features to help mitigate some common problems:

- Denoising the dataset using a Gaussian process to predict denoised target values.
- Specifying weights for each data point.
- Custom loss function: it is possible to pass a python or julia function to be used as a loss function.
- Custom operators: it is also possible to pass custom operators.
- Feature selection by applying a gradient boosting tree to select the n most important features
- Operators constraints: we can specify functional constraints such as maximum size of the expression, maximum deph, maximum size following a certain operator, maximum nestedness of operators.

PySR

```python
from pysr import PySRRegressor

model = PySRRegressor(
    niterations=40,  # < Increase me for better results
    binary_operators=["+", "*"],
    unary_operators=[
        "cos",
        "exp",
        "sin",
        "inv(x) = 1/x",
        # ^ Custom operator (julia syntax)
    ],
    extra_sympy_mappings={"inv": lambda x: 1 / x},
    # ^ Define operator for SymPy as well
    loss="loss(prediction,target) = (prediction - target)^2",
    # ^ Custom loss function (julia syntax)
)
```

PySR

Main arguments:

- `model_selection`: how to pick the best model (accuracy, best, score)
- `binary_operators`: a list of binary operators (see the operators page)
- `unary_operators`: a list of unary operators
- `niterations`: number of iterations
- `populations`: number of populations for island model
- `population_size`: size of each populaton
- `max_evals`: maximum evaluation count
- `maxsize`: maximum complexity of an equation

PySR

Main arguments (cont.):

- `constraints`: enforces maxsize for the children of operators (`pow : (-1, 1)` leave the left child unconstrained and allows only subtrees of size 1 for the right child).
- `nested_constraints`: nested constraints (`{"sin": {"cos": 0}}` means that cosine cannot be applied after sine).
- `loss`: the loss function (`LPDistLoss{P}()`, `L1DistLoss()`, `L2DistLoss()` (mean square), `LogitDistLoss()`, `HuberLoss(d)`, `L1EpsilonInsLoss( )`, `L2EpsilonInsLoss( )`, `PeriodicLoss(c)`, `QuantileLoss( )`, `ZeroOneLoss()`, `PerceptronLoss()`, `L1HingeLoss()`, `SmoothedL1HingeLoss( )`, `ModifiedHuberLoss()`, `L2MarginLoss()`, `ExpLoss()`, `SigmoidLoss()`, `DWDMarginLoss(q)`)

TIR

Transformation-Interaction-Rational SR[14] extends the IT representation to support a rational of two IT expressions:

invertible function

$$f_{TIR}(\mathbf{x}, \mathbf{w_p}, \mathbf{w_q}) = \boxed{g}\left(\frac{\boxed{p(\mathbf{x}, \mathbf{w_p})}}{1 + \boxed{q(\mathbf{x}, \mathbf{w_q})}}\right)$$

IT expressions

linear coefficient

$$f_{IT}(\mathbf{x}, \mathbf{w}) = w_0 + \sum_{j=1}^{m} \boxed{w_j} \cdot (\boxed{f_j} \circ \boxed{r_j})(\mathbf{x})$$

transformation function

interaction function

$$r_j(\mathbf{x}) = \prod_{i=1}^{d} x_i^{\boxed{k_{ij}}}$$

strength of interaction

[14] de França, Fabrício Olivetti. “Transformation-interaction-rational representation for symbolic regression.” Proceedings of the Genetic and Evolutionary Computation

TIR

The main implementation is written in Haskell[15] with support to a Python wrapper following the scikit-learn API.

Besides the Python wrapper it has a command line interface that requires a configuration file that specifies the main options of the algorithm

[15] https://github.com/folivetti/tir

TIR

The main configuration file is split into sections regarding each aspect of the algorithm:

```
[IO]
train = path and name of the training set
test  = path and name of the test set
log   = PartialLog "path and name of the output file"

[Mutation]
krange      = (-3, 3)
transfunctions = [Id, Sin, Cos, Tanh, SqrtAbs, Log, Exp]
ytransfunctions  = [Id, Exp, Sin]
```

TIR

The algorithm option specifies the different supported variants: GPTIR, SCTIR, MOO, FS.

```
[Algorithm]
npop      = 1000
ngens     = 500
algorithm = GPTIR
measures  = ["RMSE", "NMSE", "MAE", "R^2"]
task      = Regression
probmut   = 0.8
probcx    = 0.8
seed      = Nothing
```

TIR

- GPTIR: vanilla genetic programming.
- SCTIR: genetic programming with shape-constraints
- MOO[16]: Multi-objective with the first objective being the first measure in the list of measures and the second is the model size.
- FS[17]: Finess sharing version that returns a set of expressions that behave similarly in the training data but it behaves differently outside the predictors domain range.

[16] de França, Fabrício Olivetti. “Alleviating overfitting in transformation-interaction-rational symbolic regression with multi-objective optimization.” Genetic Programming and Evolvable Machines 24.2 (2023): 13.

[17] de França, Fabrício Olivetti. “Transformation-Interaction-Rational representation for Symbolic Regression: a detailed analysis of SRBench results.” ACM Transactions on Evolutionary Learning (2023).

TIR

This implementation also supports shape-constraints that constrains the generated model to specific properties.

The `penalty` argument can be `NoPenalty`, `Len Double`, or `Shape Double` to penalize the length of the model or the shape property, respectivelly. `Double` is a floating point value representing the penalization factor.

```
[Constraints]
penalty = NoPenalty
shapes  = []
domains = []
evaluator = Nothing
```

TIR

The argument `shapes` is a list of shape constraints involving a variable (specified by an `Int` index) and the range of the constraint:

```haskell
data Shape    = Range (Double, Double)
                 -- ^ f(x) \in [a,b]
              | DiffRng Int (Double, Double)
                 -- ^ d f(x) / dx \in [a,b]
              | NonIncreasing Int
                 -- ^ d f(x) / dx \in [-inf,0]
              | NonDecreasing Int
                 -- ^ d f(x) / dx \in [0,inf]
              | PartialNonIncreasing Int (Double, Double)
                 -- ^ d f(x) / dx \in [-inf,0],a <= x <= b
              | PartialNonDecreasing Int (Double, Double)
                 -- ^ d f(x) / dx \in [0,inf],a <= x <= b
              | Inflection Int Int
                 -- ^ d^2 f(x)/dx^2 == 0
              | Convex Int Int
                 -- ^ d^2 f(x)/dx^2 \in (0,Infinity)
              | Concave Int Int
                 -- ^ d^2 f(x)/dx^2 \in (-Infinitiy,0)
```

TIR

The argument `domains` is just a list of tuples specifying the domain range of each variable that must be evaluated.

The final argument, `evalutor`, specifies how to evaluate the constraints:

```
data Evaluator = InnerInterval
               | OuterInterval
               | Kaucher
               | Sampling Int
               | Hybrid Double
               | Bisection Int
```

HeuristicLab

HerusiticLab[18] is a framework supporting a large variaty of heuristics and evolutionary algorithms for different problems.

It has an intuitive Graphical User Interface and can also be used programmaticaly as a C# library.

[18]https://dev.heuristiclab.com/

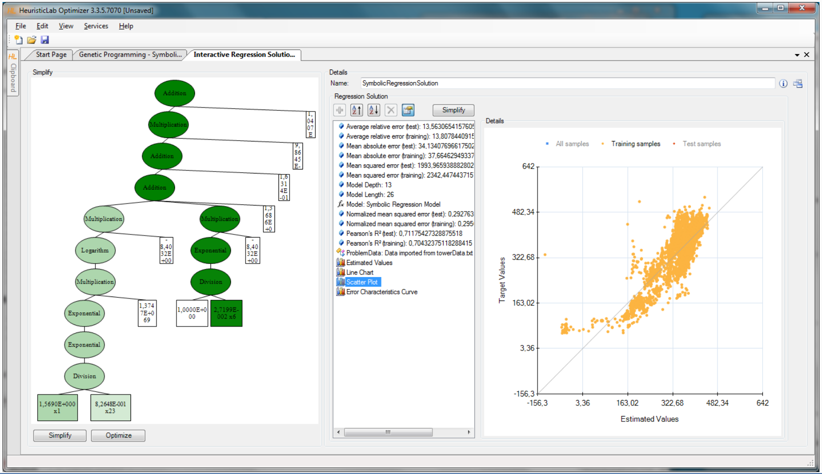
HeuristicLab

Specific to Genetic Programming it supports:

- Artificial Ant
- Lawn Mower
- Even Parity
- Multiplexer
- Robocode
- Trading
- Symbolic Classification
- Symbolic Regression
- Koza-style Symbolic Regression
- Symbolic Time-Series Prognosis
- Grammatical Evolution

HeuristicLab

Another outstanding fetaure is the post-processing plots and reports that helps the practitioner to debug the model and have some insights about the data.



Name: SymbolicRegressionSolution

Average relative error (test): 13,563065415760
Average relative error (training): 13,8078440915
Mean absolute error (test): 34,13407696617502
Mean absolute error (training): 37,66462949337
Mean squared error (test): 1993,965938882802
Mean squared error (training): 2342,447443715
Model Depth: 13
Model Length: 26
Model: Symbolic Regression Model
Normalized mean squared error (test): 0,292763
Normalized mean squared error (training): 0,295
Pearson's R² (test): 0,71175427328875518
Pearson's R² (training): 0,70432375118288415
ProblemData: Data imported from towerData.txt
Estimated Values
Line Chart
Scatter Plot
Error Characteristics Curve

HeuristicLab

A brief usage introduction: https://dev.heuristiclab.com/trac.fcgi/export/HEAD/misc/documentation/Tutorials/Algorithm%20and%20Experiment%20Design%20with%20HeuristicLab.pdf

Next lecture

- Likelihood Functions

Acknowledgments