



HeuristicLab

A Paradigm-Independent and Extensible
Environment for Heuristic Optimization

Algorithm and Experiment Design with HeuristicLab

An Open Source Optimization Environment for
Research and Education

S. Wagner, G. Kronberger

Heuristic and Evolutionary Algorithms Laboratory (HEAL)

School of Informatics/Communications/Media, Campus Hagenberg

University of Applied Sciences Upper Austria



HEAL

Heuristic and Evolutionary
Algorithms Laboratory



**Heuristic
Optimization in
Production and
Logistics**

Instructor Biographies

- Stefan Wagner
 - Full professor for complex software systems (since 2009)
University of Applied Sciences Upper Austria
 - Co-founder of the HEAL research group
 - Project manager and chief architect of HeuristicLab
 - PhD in technical sciences (2009)
Johannes Kepler University Linz, Austria
 - Associate professor (2005 – 2009)
University of Applied Sciences Upper Austria
 - <http://heal.heuristiclab.com/team/wagner>
- Gabriel Kronberger
 - Full professor for business intelligence (since 2011)
University of Applied Sciences Upper Austria
 - Member of the HEAL research group
 - Architect of HeuristicLab
 - PhD in technical sciences (2010)
Johannes Kepler University Linz, Austria
 - Research assistant (2005 – 2011)
University of Applied Sciences Upper Austria
 - <http://heal.heuristiclab.com/team/kronberger>



Agenda



- Objectives of the Tutorial
- Introduction
- Where to get HeuristicLab?
- Plugin Infrastructure
- Graphical User Interface
- Available Algorithms & Problems
- **Demonstration Part I: Working with HeuristicLab**
- **Demonstration Part II: Data-based Modeling**
- Some Additional Features
- Planned Features
- Team
- Suggested Readings
- Bibliography
- Questions & Answers

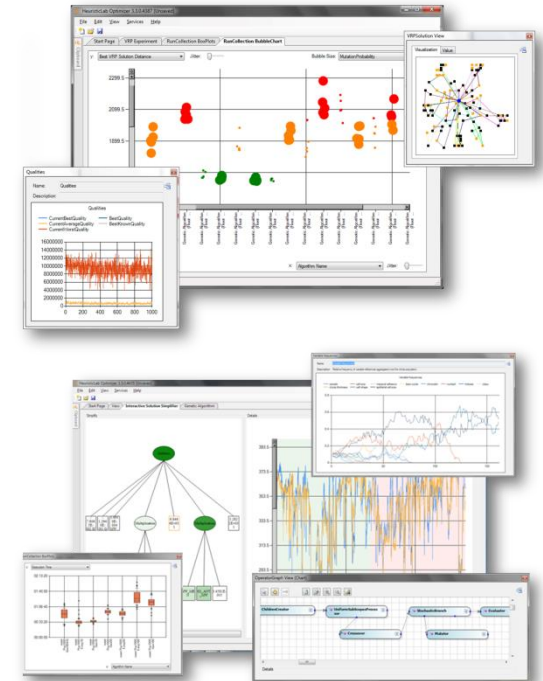
Objectives of the Tutorial



- Introduce general motivation and design principles of HeuristicLab
- Show where to get HeuristicLab
- Explain basic GUI usability concepts
- Demonstrate basic features
- Demonstrate editing and analysis of optimization experiments
- Demonstrate custom algorithms and graphical algorithm designer
- Demonstrate data-based modeling features
- Outline some additional features

Introduction

- Motivation and Goals
 - graphical user interface
 - paradigm independence
 - multiple algorithms and problems
 - large scale experiments and analyses
 - parallelization
 - extensibility, flexibility and reusability
 - visual and interactive algorithm development
 - multiple layers of abstraction
- Facts
 - development of HeuristicLab started in 2002
 - based on Microsoft .NET and C#
 - used in research and education
 - second place at the *Microsoft Innovation Award 2009*
 - open source (GNU General Public License)
 - version 3.3.0 released on May 18th, 2010
 - latest version 3.3.10 "Vancouver" released on July 10th, 2014



Where to get HeuristicLab?

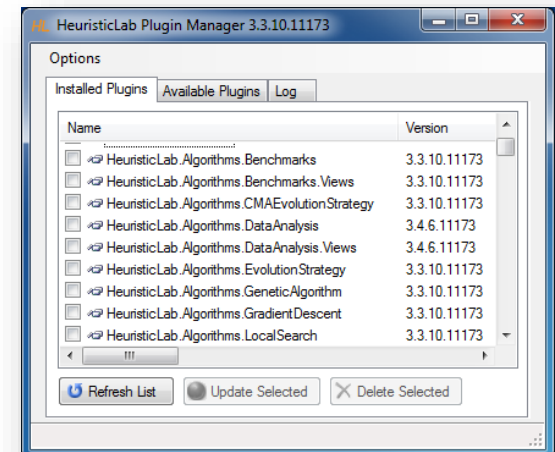
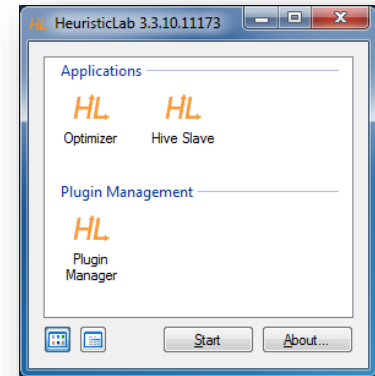


- Download binaries
 - deployed as ZIP archives
 - latest stable version 3.3.10 "Vancouver"
 - released on July 10th, 2014
 - daily trunk builds
 - <http://dev.heuristiclab.com/download>
- Check out sources
 - SVN repository
 - HeuristicLab 3.3.10 tag
 - <http://svn.heuristiclab.com/svn/core/tags/3.3.10>
 - Stable development version
 - <http://svn.heuristiclab.com/svn/core/stable>
- License
 - GNU General Public License (Version 3)
- System requirements
 - Microsoft .NET Framework 4.0 Full Version
 - enough RAM and CPU power ;-)

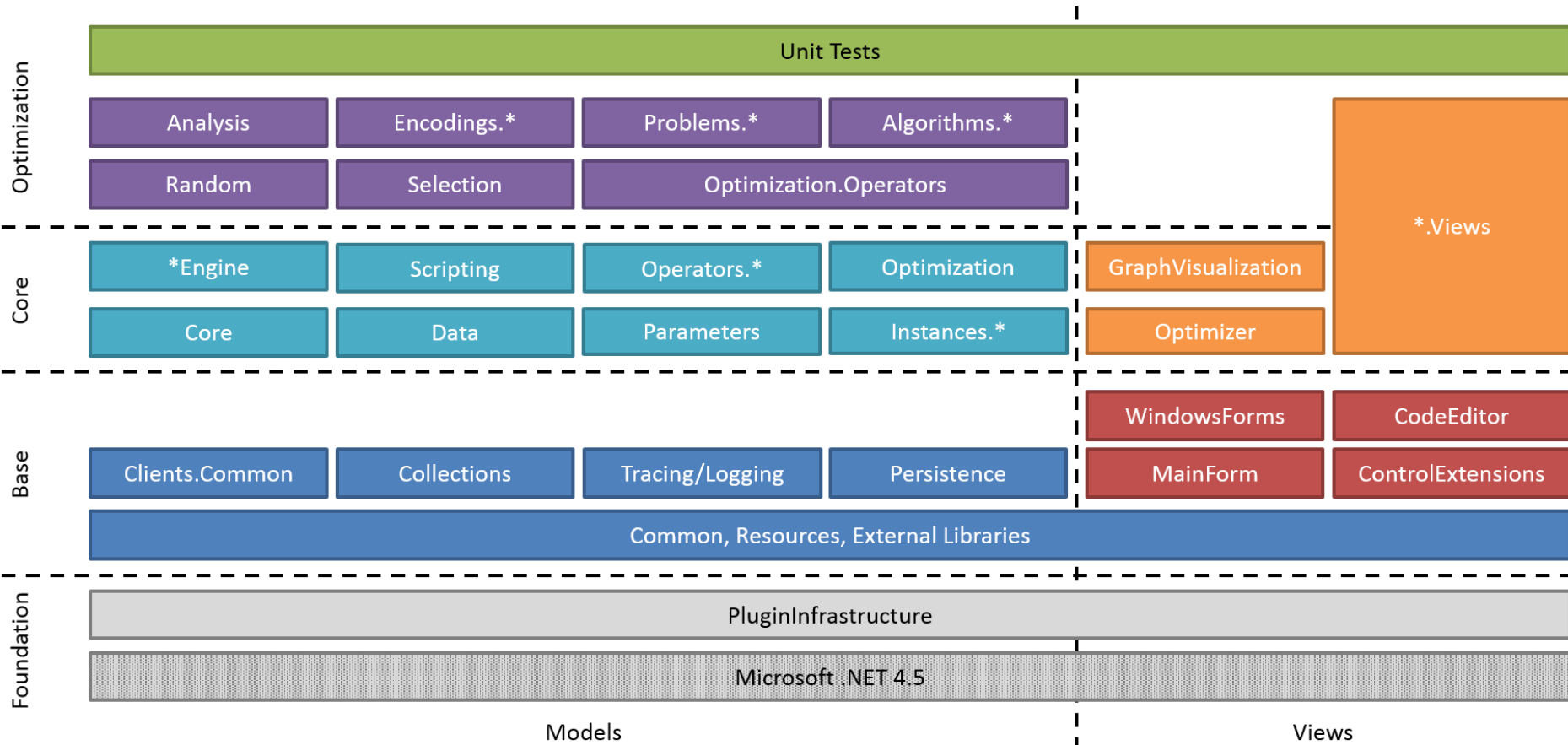
A screenshot of the HeuristicLab website homepage. The page features a navigation menu with links for Home, News, Download, Features, Documentation, Support, and Search. The main content area includes a welcome message, a list of features such as Graphical User Interface, Algorithm Prototyping, and Evolutionary Algorithms, and a download button for HeuristicLab 3.3.3. There are also sections for Research & Publications, License, and Contribute, along with a contact form and a 'Thank you!' message.

Plugin Infrastructure

- HeuristicLab consists of many assemblies
 - 142 plugins in HeuristicLab 3.3.10
 - plugins can be loaded or unloaded at runtime
 - plugins can be updated via internet
 - application plugins provide GUI frontends
- Extensibility
 - developing and deploying new plugins is easy
 - dependencies are explicitly defined, automatically checked and resolved
 - automatic discovery of interface implementations (service locator pattern)
- Plugin Manager
 - GUI to check, install, update or delete plugins



Plugin Architecture

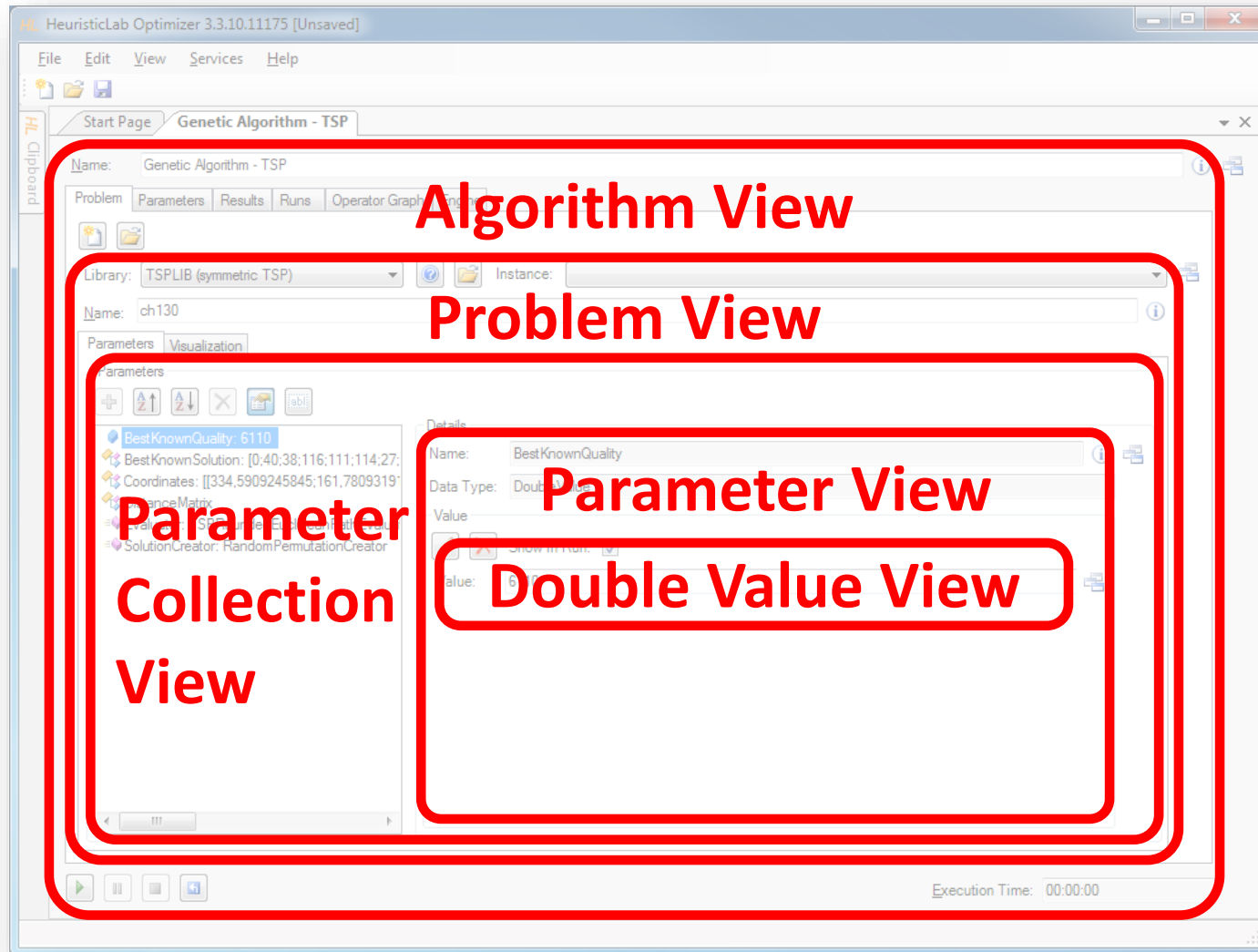


Graphical User Interface



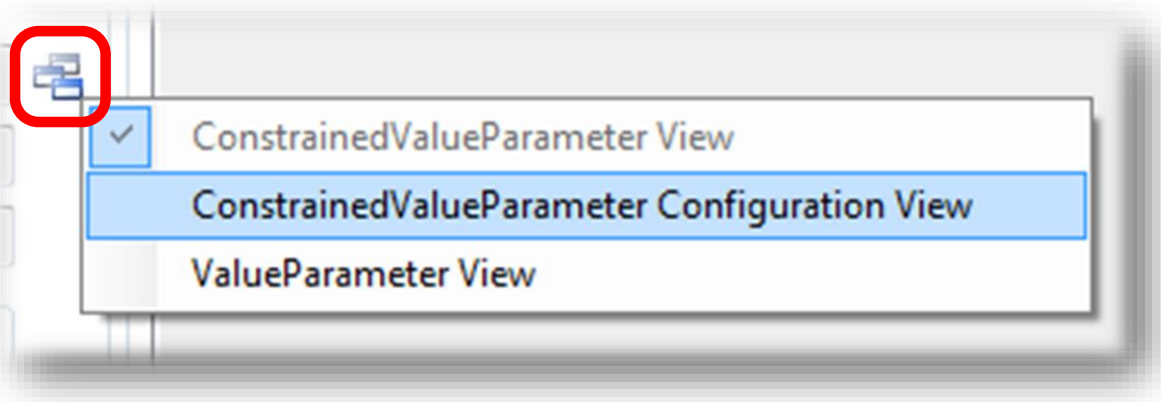
- HeuristicLab GUI is made up of views
 - views are visual representations of content objects
 - views are composed in the same way as their content
 - views and content objects are loosely coupled
 - multiple different views may exist for the same content
- Drag & Drop
 - views support drag & drop operations
 - content objects can be copied or moved (shift key)
 - enabled for collection items and content objects

Graphical User Interface



Graphical User Interface

- ViewHost
 - control which hosts views
 - right-click on windows icon to switch views
 - double-click on windows icon to open another view
 - drag & drop windows icon to copy contents



Available Algorithms

Population-based

- CMA-ES
- Evolution Strategy
- Genetic Algorithm
- Offspring Selection Genetic Algorithm
- Island Genetic Algorithm
- Island Offspring Selection Genetic Algorithm
- SASEGASA
- Relevant Alleles Preserving GA (RAPGA)
- Genetic Programming
- NSGA-II
- Scatter Search
- Particle Swarm Optimization

Trajectory-based

- Local Search
- Tabu Search
- Robust Taboo Search
- Variable Neighborhood Search
- Simulated Annealing

Data Analysis

- Linear Discriminant Analysis
- Linear Regression
- Multinomial Logit Classification
- k-Nearest Neighbor
- k-Means
- Neighbourhood Component Analysis
- Artificial Neural Networks
- Random Forests
- Support Vector Machines
- Gaussian Processes

Additional Algorithms

- User-defined Algorithm
- Performance Benchmarks
- Hungarian Algorithm
- Cross Validation
- LM-BFGS

Available Problems

Combinatorial Problems

- Traveling Salesman
- Vehicle Routing
- Knapsack
- Job Shop Scheduling
- Linear Assignment
- Quadratic Assignment
- OneMax

Genetic Programming Problems

- Symbolic Classification
- Symbolic Regression
- Symbolic Time-Series Prognosis
- Artificial Ant
- Lawn Mower

Additional Problems

- Single-Objective Test Function
- User-defined Problem
- External Evaluation Problem
(Anylogic, Scilab, MATLAB)
- Regression, Classification, Clustering
- Trading
- Grammatical Evolution

Agenda



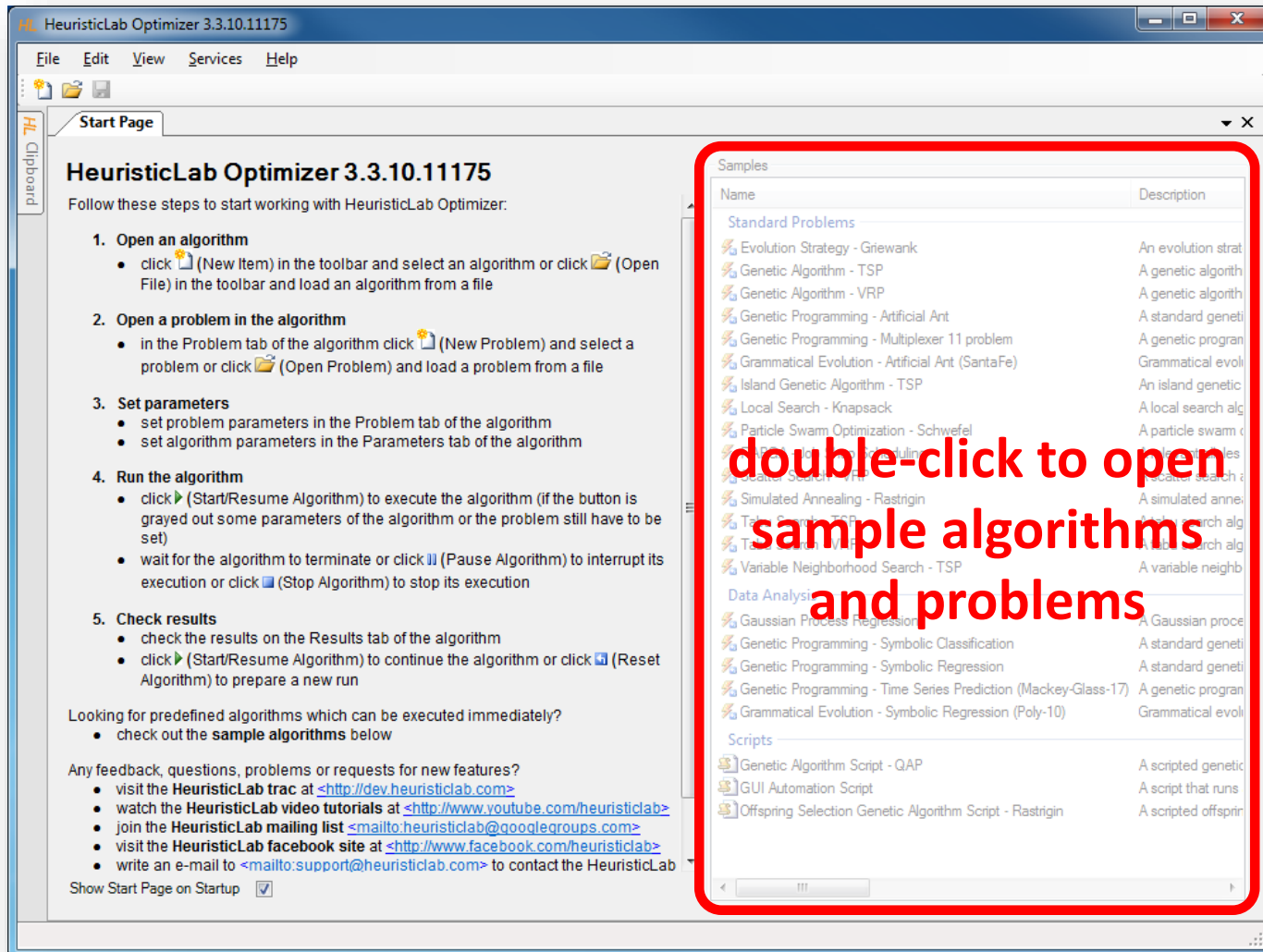
- Objectives of the Tutorial
- Introduction
- Where to get HeuristicLab?
- Plugin Infrastructure
- Graphical User Interface
- Available Algorithms & Problems
- **Demonstration Part I: Working with HeuristicLab**
- **Demonstration Part II: Data-based Modeling**
- Some Additional Features
- Planned Features
- Team
- Suggested Readings
- Bibliography
- Questions & Answers

Demonstration Part I: Working with HeuristicLab



- Create, Parameterize and Execute Algorithms
- Save and Load Items
- Create Batch Runs and Experiments
- Multi-core CPUs and Parallelization
- Analyze Runs
- Analyzers
- Building User-Defined Algorithms

HeuristicLab Optimizer



The screenshot shows the HeuristicLab Optimizer 3.3.10.11175 application window. The main area displays a 'Start Page' with instructions for getting started. A 'Samples' panel on the right is highlighted with a red border and contains a list of sample algorithms and problems. A red text overlay reads 'double-click to open sample algorithms and problems'.

HeuristicLab Optimizer 3.3.10.11175

Follow these steps to start working with HeuristicLab Optimizer:

- 1. Open an algorithm**
 - click (New Item) in the toolbar and select an algorithm or click (Open File) in the toolbar and load an algorithm from a file
- 2. Open a problem in the algorithm**
 - in the Problem tab of the algorithm click (New Problem) and select a problem or click (Open Problem) and load a problem from a file
- 3. Set parameters**
 - set problem parameters in the Problem tab of the algorithm
 - set algorithm parameters in the Parameters tab of the algorithm
- 4. Run the algorithm**
 - click (Start/Resume Algorithm) to execute the algorithm (if the button is grayed out some parameters of the algorithm or the problem still have to be set)
 - wait for the algorithm to terminate or click (Pause Algorithm) to interrupt its execution or click (Stop Algorithm) to stop its execution
- 5. Check results**
 - check the results on the Results tab of the algorithm
 - click (Start/Resume Algorithm) to continue the algorithm or click (Reset Algorithm) to prepare a new run

Looking for predefined algorithms which can be executed immediately?

- check out the **sample algorithms** below

Any feedback, questions, problems or requests for new features?

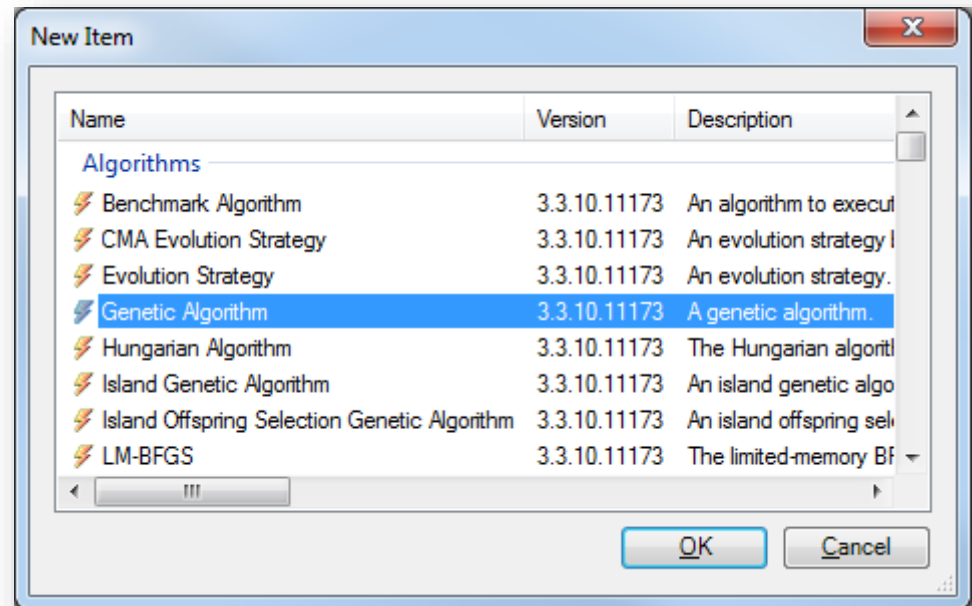
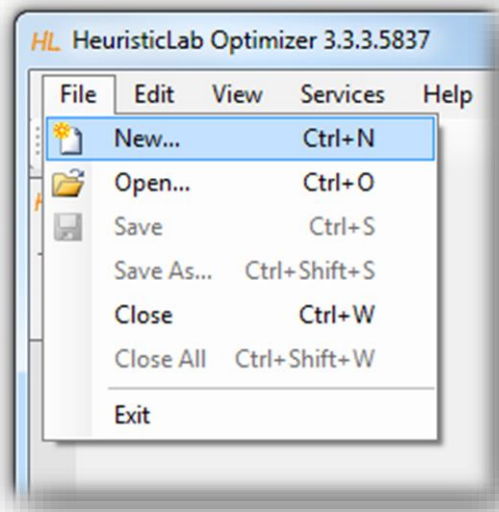
- visit the **HeuristicLab trac** at <http://dev.heuristiclab.com>
- watch the **HeuristicLab video tutorials** at <http://www.youtube.com/heuristiclab>
- join the **HeuristicLab mailing list** <mailto:heuristiclab@googlegroups.com>
- visit the **HeuristicLab facebook site** at <http://www.facebook.com/heuristiclab>
- write an e-mail to <mailto:support@heuristiclab.com> to contact the HeuristicLab

Show Start Page on Startup

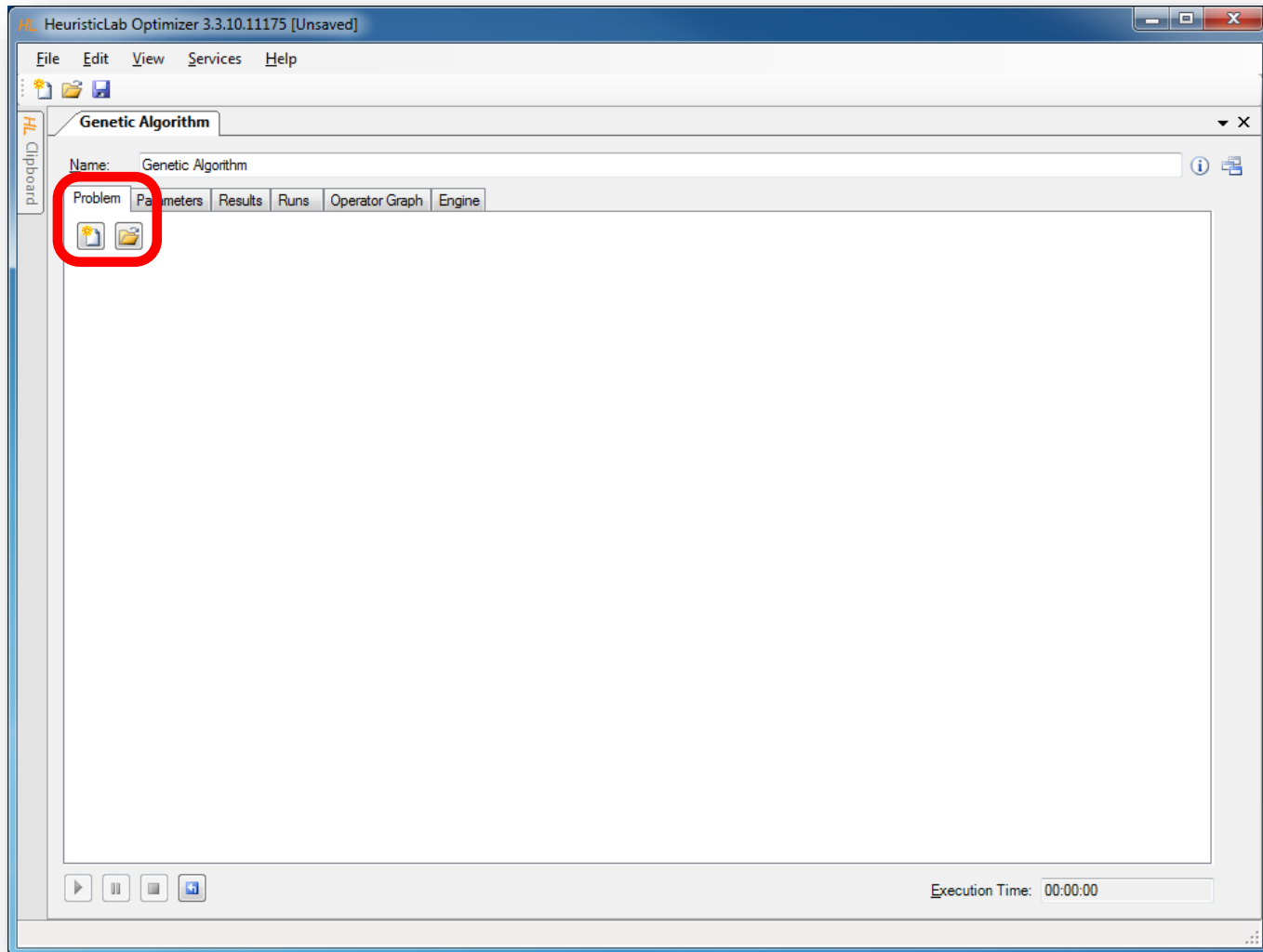
Name	Description
Standard Problems	
Evolution Strategy - Griewank	An evolution strat
Genetic Algorithm - TSP	A genetic algorith
Genetic Algorithm - VRP	A genetic algorith
Genetic Programming - Artificial Ant	A standard geneti
Genetic Programming - Multiplexer 11 problem	A genetic program
Grammatical Evolution - Artificial Ant (SantaFe)	Grammatical evoli
Island Genetic Algorithm - TSP	An island genetic
Local Search - Knapsack	A local search alg
Particle Swarm Optimization - Schwefel	A particle swarm c
Tabu Search - Traveling Salesman Problem	A tabu search alg
Tabu Search - TSP	A tabu search alg
Simulated Annealing - Rastrigin	A simulated anne
Tabu Search - Traveling Salesman Problem	A tabu search alg
Tabu Search - TSP	A tabu search alg
Variable Neighborhood Search - TSP	A variable neighb
Data Analysis	
Gaussian Process Regression	A Gaussian proce
Genetic Programming - Symbolic Classification	A standard geneti
Genetic Programming - Symbolic Regression	A standard geneti
Genetic Programming - Time Series Prediction (Mackey-Glass-17)	A genetic program
Grammatical Evolution - Symbolic Regression (Poly-10)	Grammatical evoli
Scripts	
Genetic Algorithm Script - QAP	A scripted geneti
GUI Automation Script	A script that runs
Offspring Selection Genetic Algorithm Script - Rastrigin	A scripted offsprir

double-click to open
sample algorithms
and problems

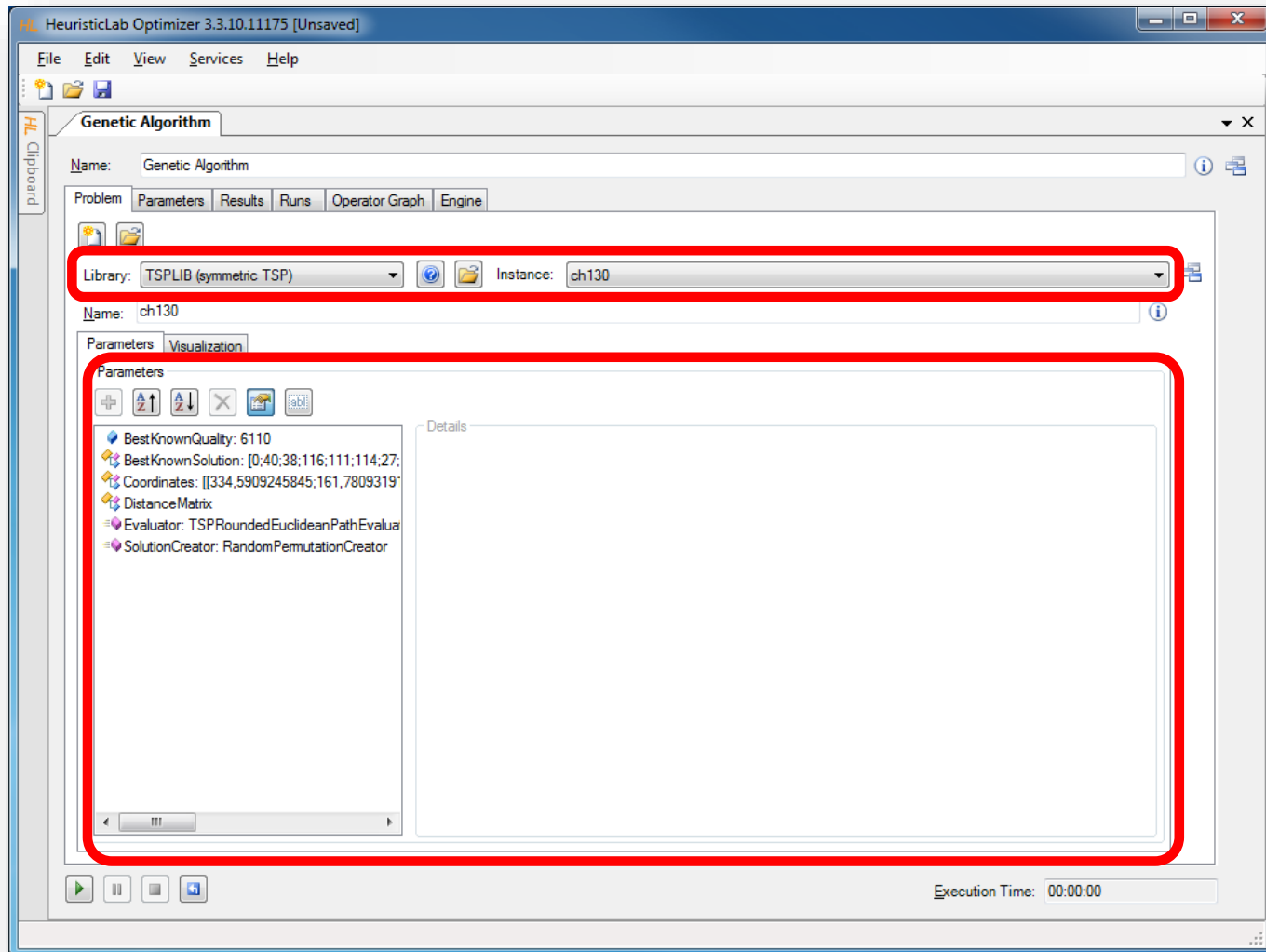
Create Algorithm



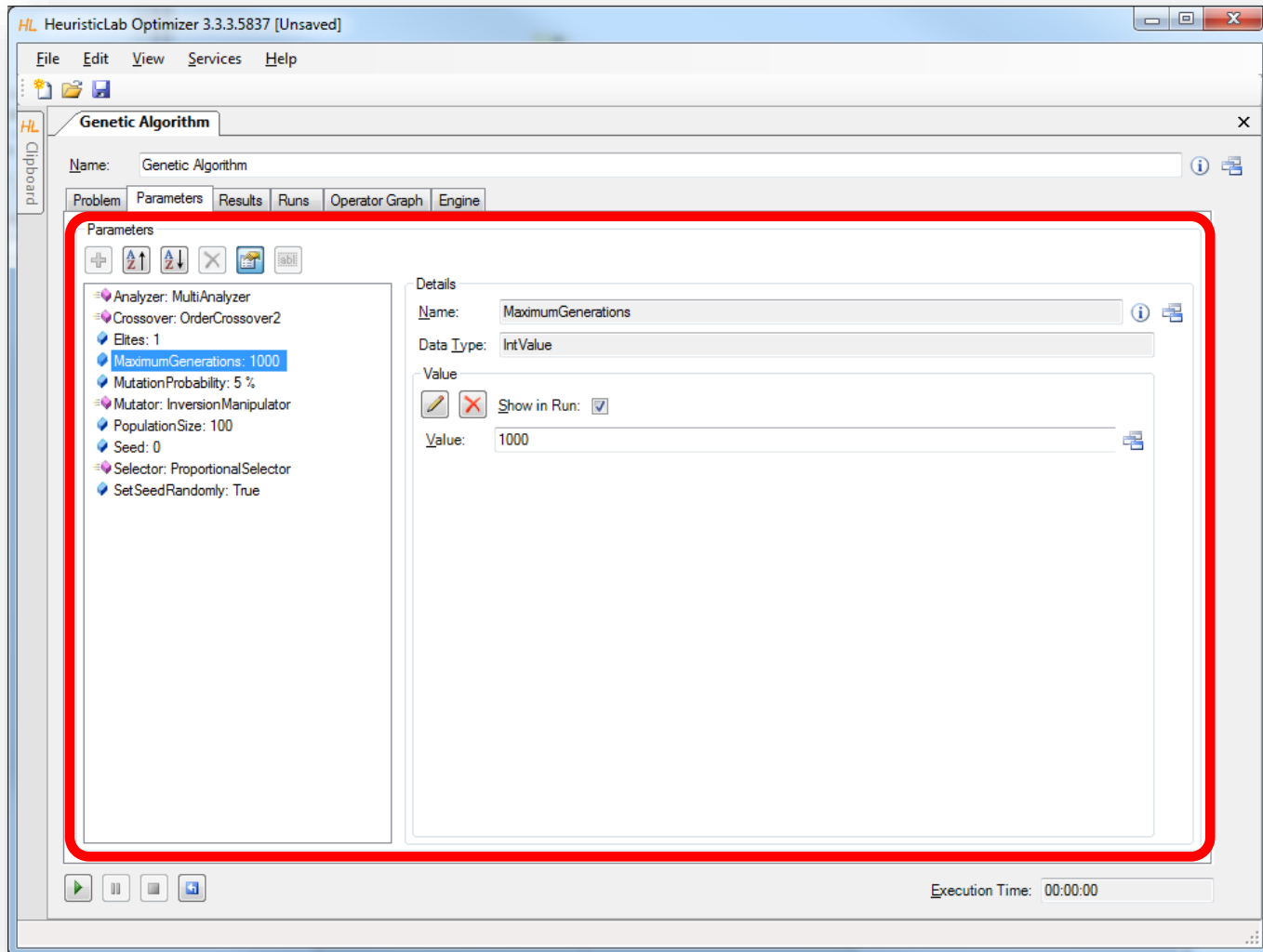
Create or Load Problem



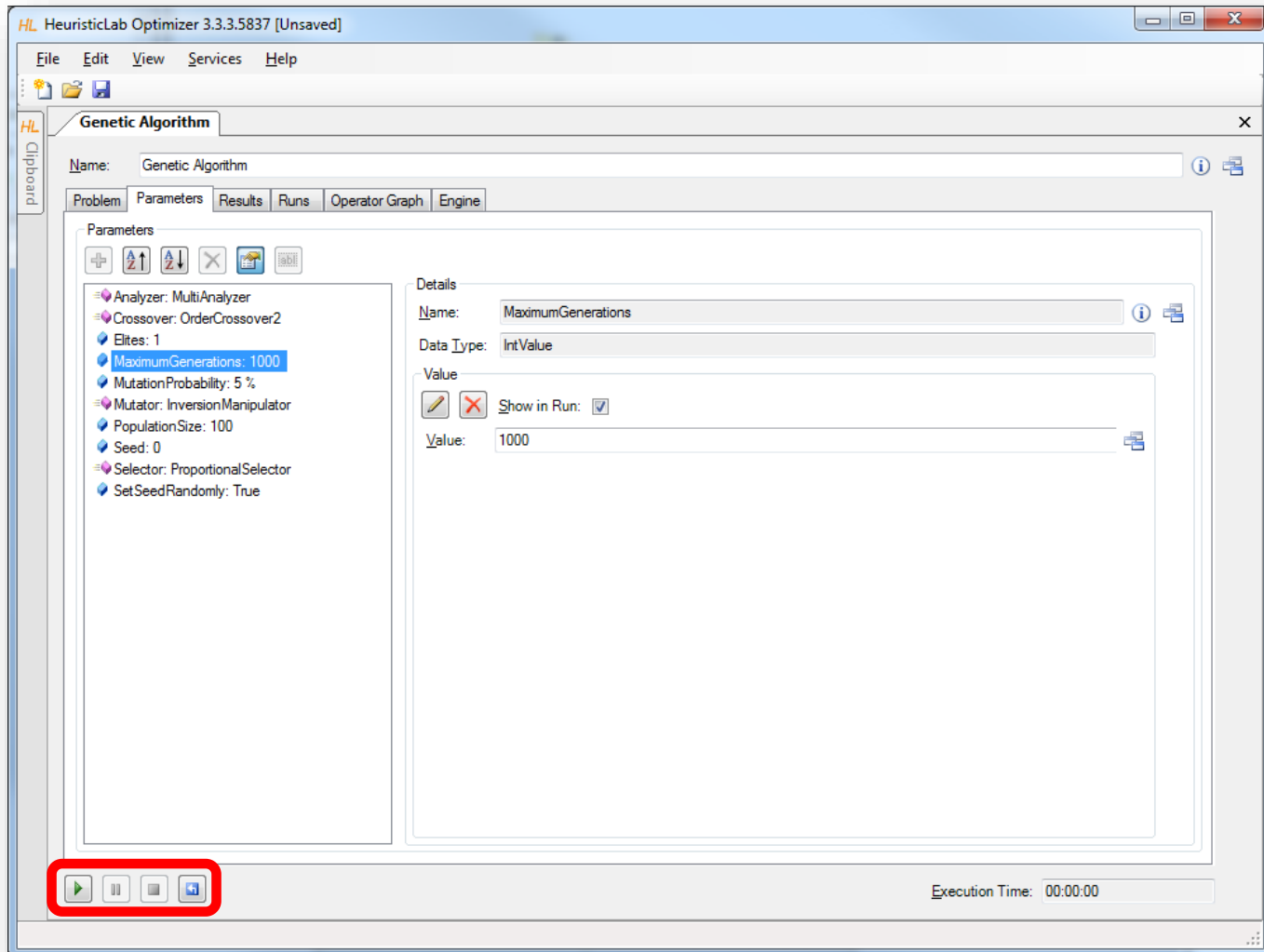
Import or Parameterize Problem Data



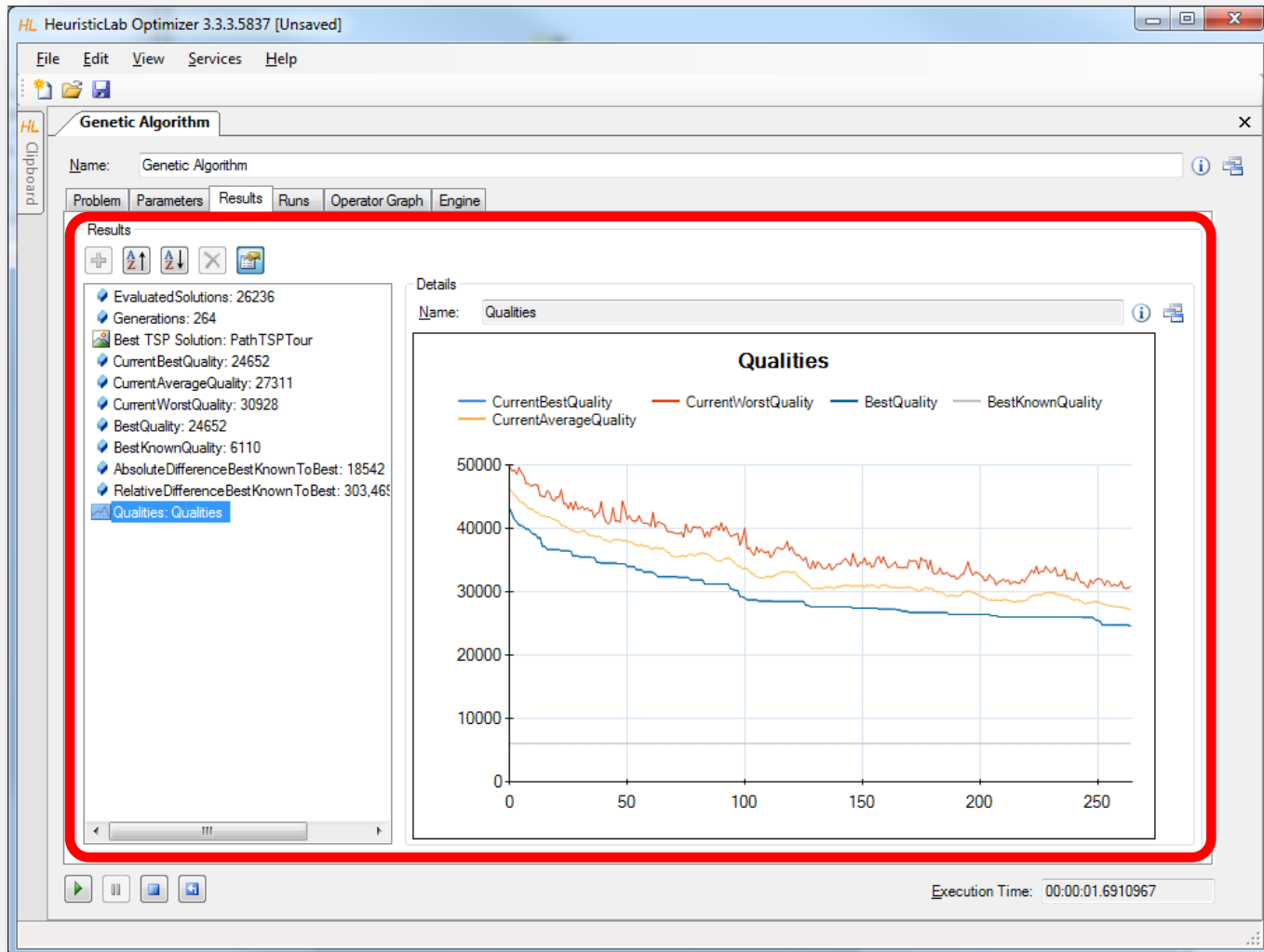
Parameterize Algorithm



Start, Pause, Resume, Stop and Reset

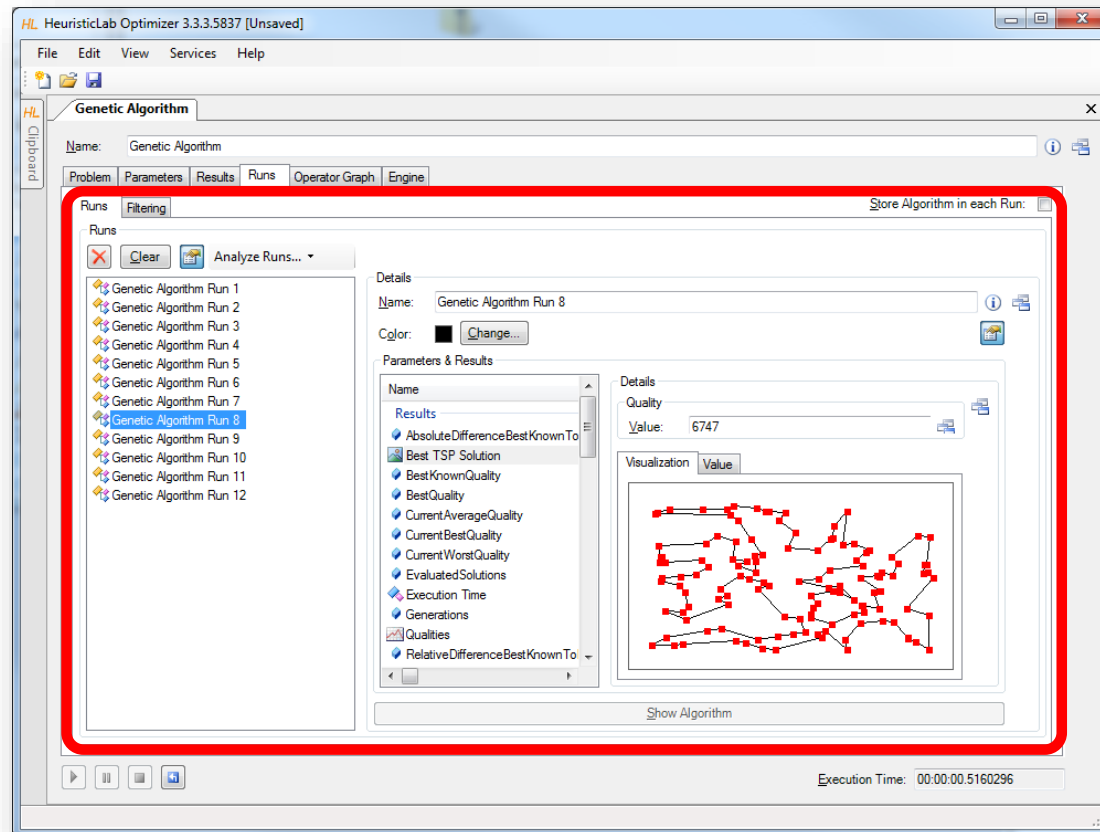


Inspect Results



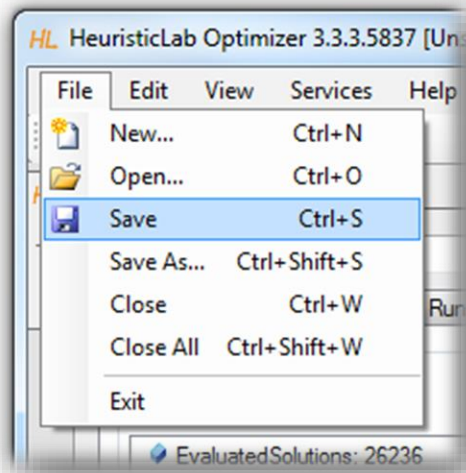
Compare Runs

- A run is created each time when the algorithm is stopped
 - runs contain all results and parameter settings
 - previous results are not forgotten and can be compared



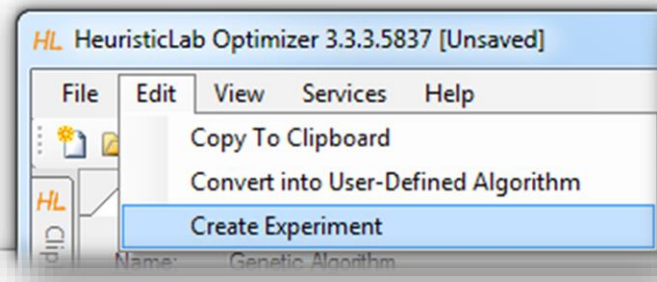
Save and Load

- Save to and load from disk
 - HeuristicLab items (i.e., algorithms, problems, experiments, ...) can be saved to and loaded from a file
 - algorithms can be paused, saved, loaded and resumed
 - data format is custom compressed XML
 - saving and loading files might take several minutes
 - saving and loading large experiments requires some memory

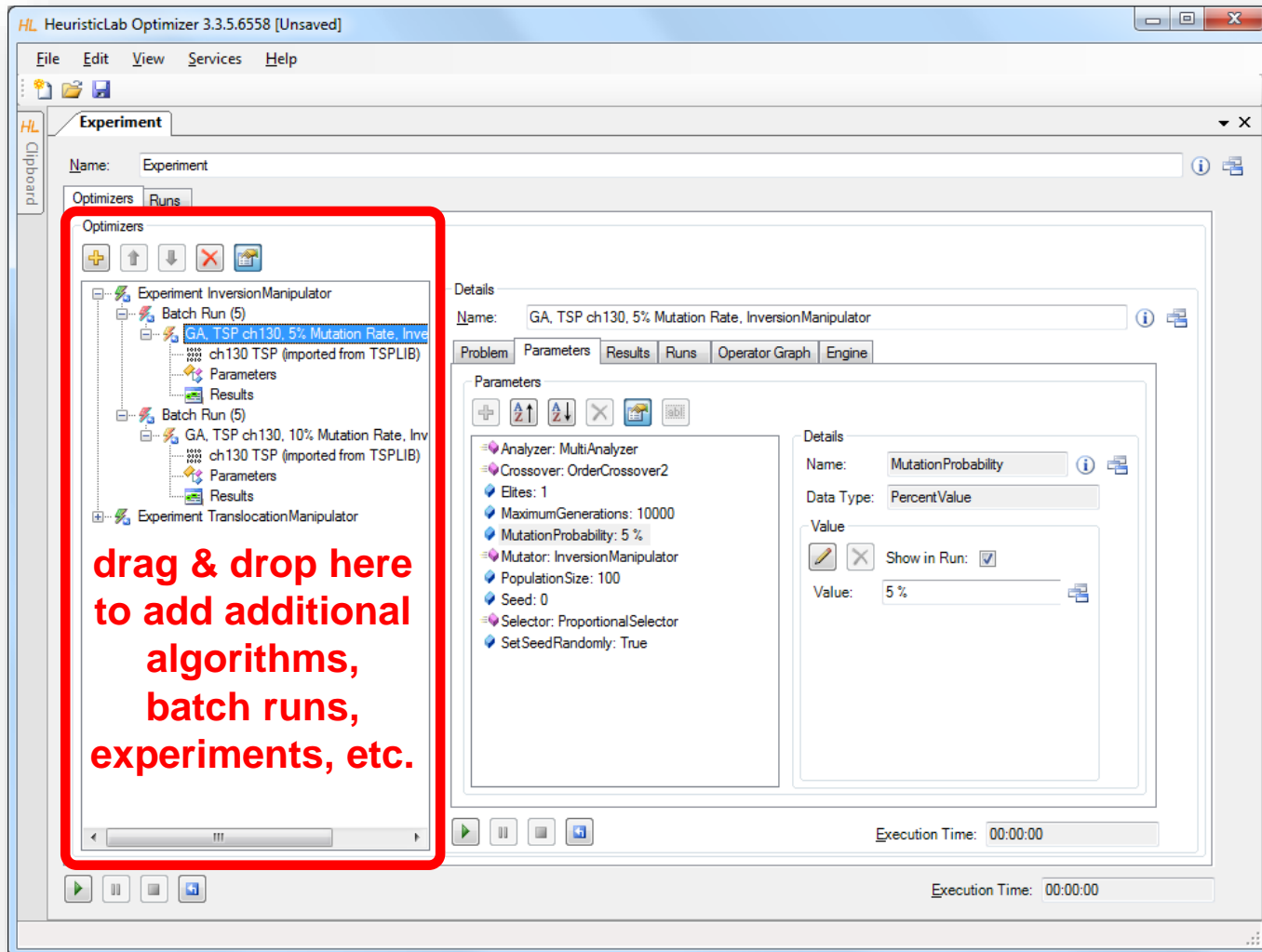


Create Batch Runs and Experiments

- Batch runs
 - execute the same optimizer (e.g. algorithm, batch run, experiment) several times
- Experiments
 - execute different optimizers
 - suitable for large scale algorithm comparison and analysis
- Experiments and batch runs can be nested
- Generated runs can be compared afterwards



Create Batch Runs and Experiments



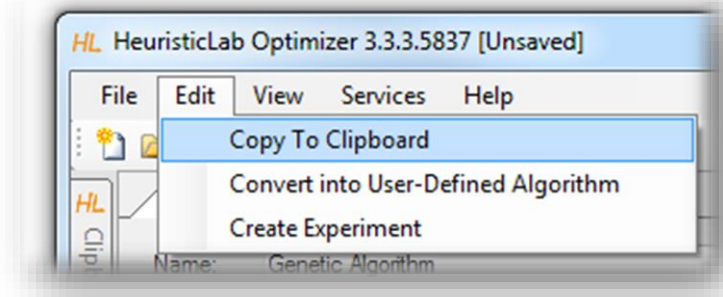
The screenshot shows the HeuristicLab Optimizer interface. On the left, a tree view under the 'Optimizers' tab shows a hierarchy: 'Experiment InversionManipulator' containing 'Batch Run (5)', which contains 'GA, TSP ch130, 5% Mutation Rate, Inve...', which contains 'ch130 TSP (imported from TSPLIB)', 'Parameters', and 'Results'. Below this, another 'Batch Run (5)' contains 'GA, TSP ch130, 10% Mutation Rate, Inv...', which contains 'ch130 TSP (imported from TSPLIB)', 'Parameters', and 'Results'. At the bottom of the tree is 'Experiment TranslocationManipulator'. A red box highlights the tree view with the text: **drag & drop here to add additional algorithms, batch runs, experiments, etc.**

The main area shows the 'Details' panel for the selected optimizer: 'GA, TSP ch130, 5% Mutation Rate, InversionManipulator'. The 'Parameters' tab is active, showing a list of parameters: Analyzer: MultiAnalyzer, Crossover: OrderCrossover2, Elites: 1, MaximumGenerations: 10000, MutationProbability: 5%, Mutator: InversionManipulator, PopulationSize: 100, Seed: 0, Selector: ProportionalSelector, and SetSeedRandomly: True. The 'Details' sub-panel for 'MutationProbability' shows: Name: MutationProbability, Data Type: PercentValue, Value: 5%, and Show in Run: checked.

At the bottom, the 'Execution Time' is displayed as 00:00:00.

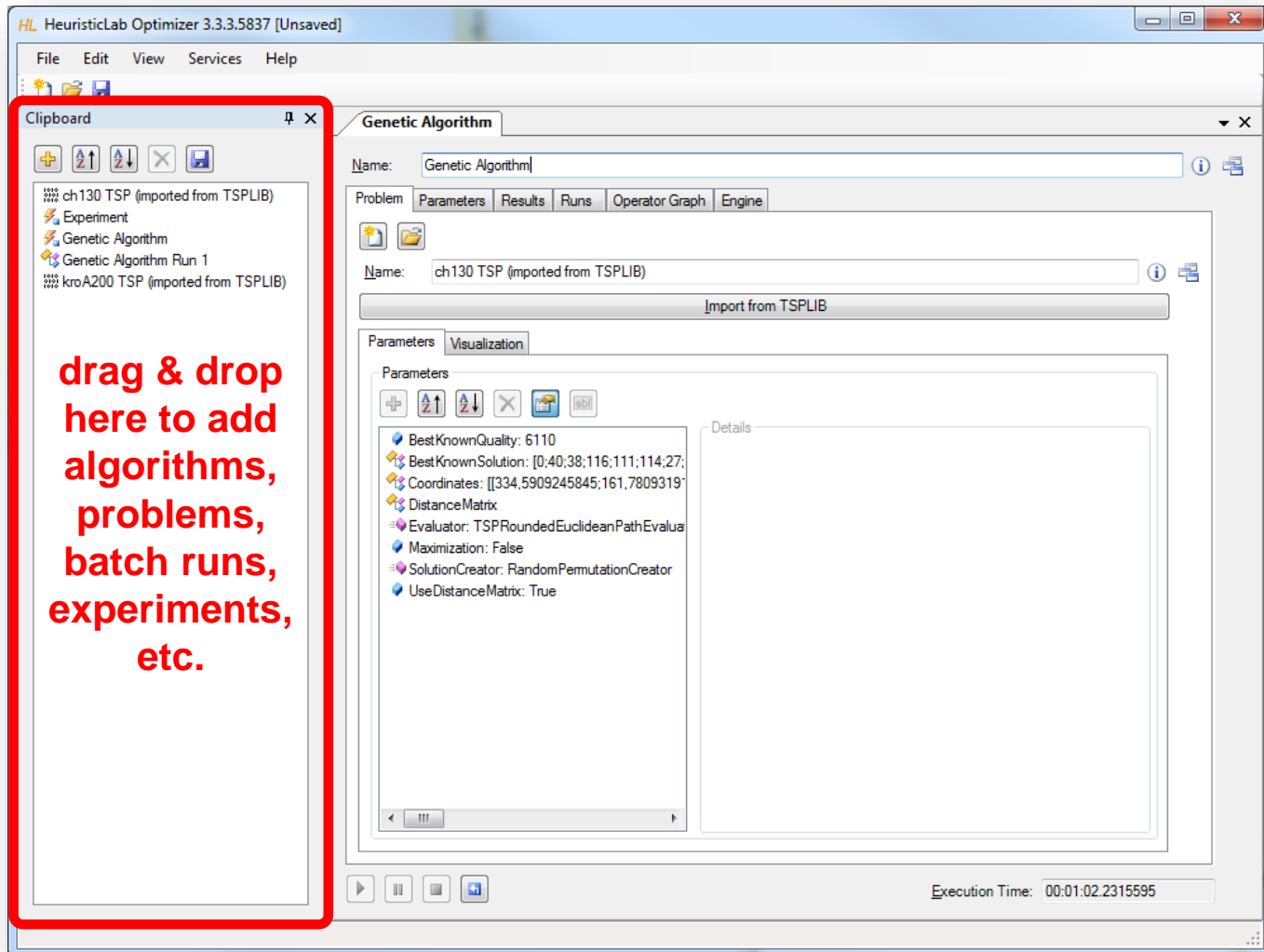
Clipboard

- Store items
 - click on the buttons to add or remove items
 - drag & drop items on the clipboard
 - use the menu to add a copy of a shown item to the clipboard

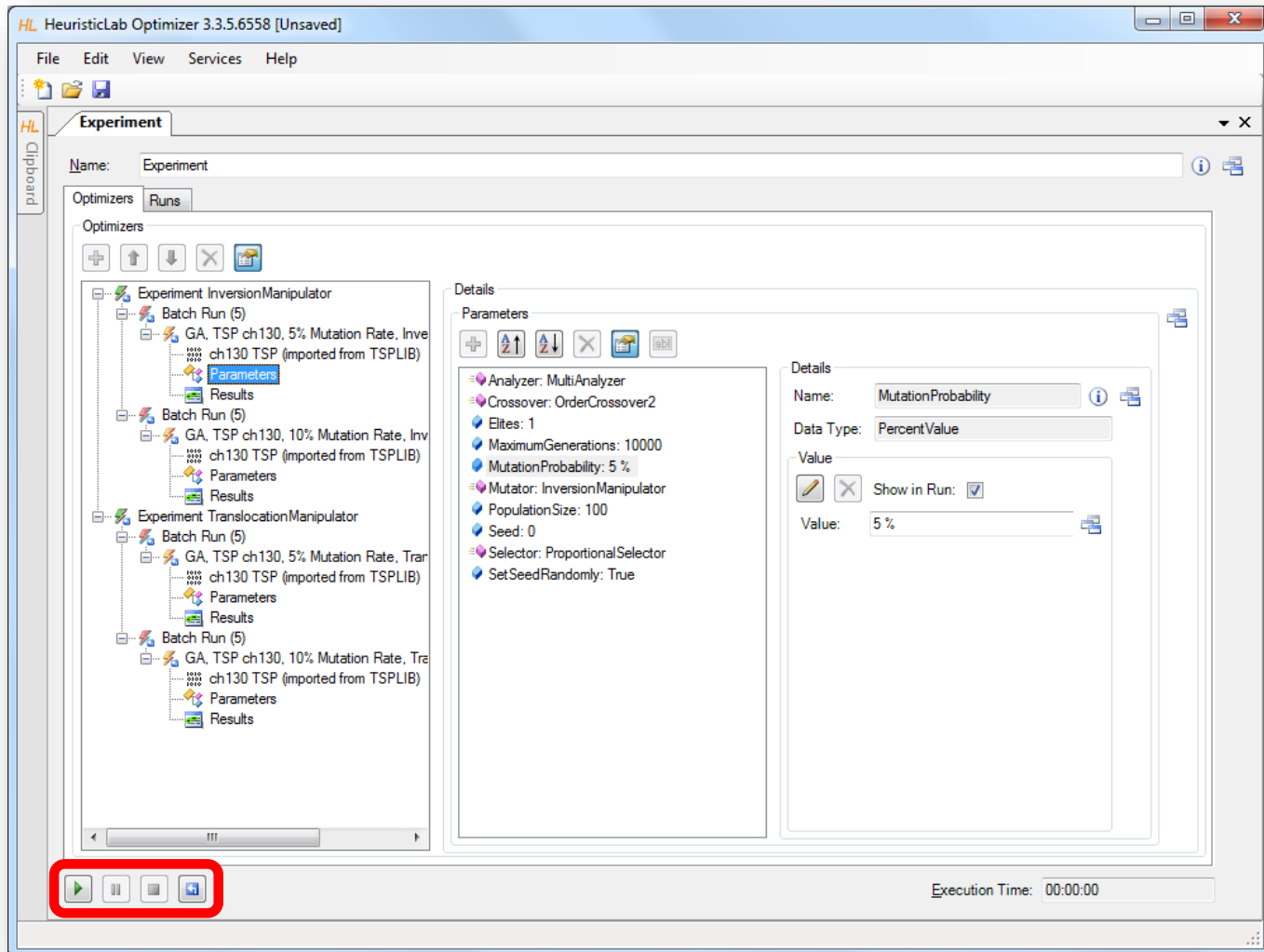


- Show items
 - double-click on an item in the clipboard to show its view
- Save and restore clipboard content
 - click on the save button to write the clipboard content to disk
 - clipboard is automatically restored when HeuristicLab is started the next time

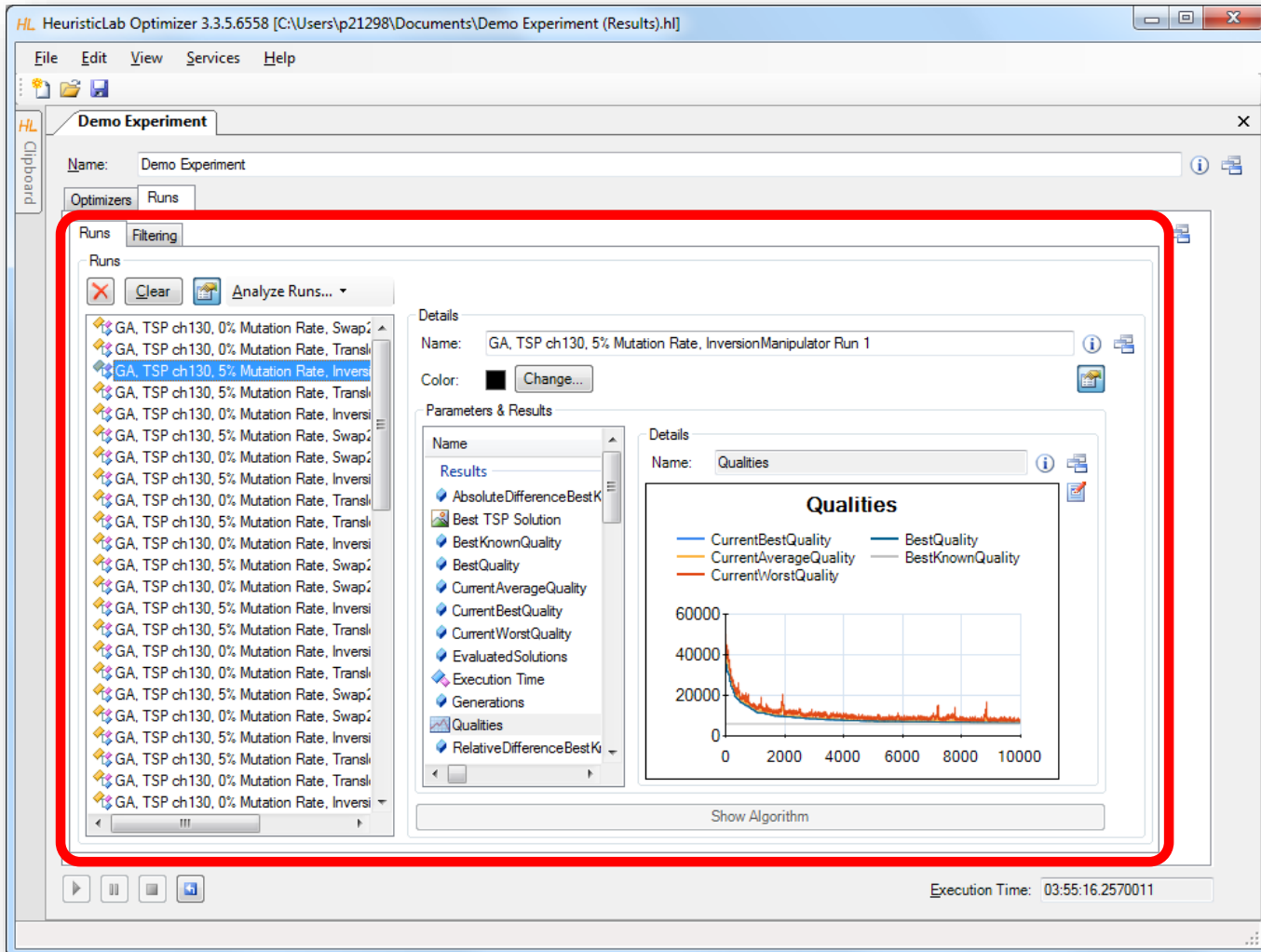
Clipboard



Start, Pause, Resume, Stop, Reset



Compare Runs



The screenshot displays the HeuristicLab Optimizer interface. The main window is titled "HL HeuristicLab Optimizer 3.3.5.6558 [C:\Users\p21298\Documents\Demo Experiment (Results).hl]". The interface includes a menu bar (File, Edit, View, Services, Help) and a toolbar. The "Demo Experiment" tab is active, showing the "Name: Demo Experiment" field. Below this, there are tabs for "Optimizers" and "Runs". The "Runs" tab is selected, and a red box highlights the "Runs" list and the "Details" panel. The "Runs" list contains multiple entries, each representing a different configuration of the Genetic Algorithm (GA) for the Traveling Salesman Problem (TSP) on a 130-city instance. The "Details" panel shows the selected run: "GA, TSP ch130, 5% Mutation Rate, InversionManipulator Run 1". The "Parameters & Results" section is expanded to show the "Qualities" results. A line graph titled "Qualities" plots the performance metrics over 10,000 generations. The y-axis represents quality, ranging from 0 to 60,000. The x-axis represents generations, ranging from 0 to 10,000. The graph shows four data series: CurrentBestQuality (blue), CurrentAverageQuality (orange), CurrentWorstQuality (red), and BestKnownQuality (grey). The CurrentBestQuality starts at approximately 60,000 and rapidly descends to about 10,000 within the first 2,000 generations, then continues to decrease slowly towards the BestKnownQuality. The CurrentAverageQuality and CurrentWorstQuality lines are clustered together, showing a similar downward trend.

HL HeuristicLab Optimizer 3.3.5.6558 [C:\Users\p21298\Documents\Demo Experiment (Results).hl]

File Edit View Services Help

Demo Experiment

Name: Demo Experiment

Optimizers Runs

Runs Filtering

Runs

Clear Analyze Runs...

GA, TSP ch130, 0% Mutation Rate, Swap; GA, TSP ch130, 0% Mutation Rate, Transl; GA, TSP ch130, 5% Mutation Rate, Invers; GA, TSP ch130, 5% Mutation Rate, Transl; GA, TSP ch130, 0% Mutation Rate, Invers; GA, TSP ch130, 5% Mutation Rate, Swap; GA, TSP ch130, 0% Mutation Rate, Swap; GA, TSP ch130, 5% Mutation Rate, Invers; GA, TSP ch130, 0% Mutation Rate, Transl; GA, TSP ch130, 5% Mutation Rate, Swap; GA, TSP ch130, 0% Mutation Rate, Swap; GA, TSP ch130, 5% Mutation Rate, Invers; GA, TSP ch130, 5% Mutation Rate, Transl; GA, TSP ch130, 0% Mutation Rate, Invers; GA, TSP ch130, 5% Mutation Rate, Transl; GA, TSP ch130, 0% Mutation Rate, Invers; GA, TSP ch130, 5% Mutation Rate, Swap; GA, TSP ch130, 0% Mutation Rate, Swap; GA, TSP ch130, 5% Mutation Rate, Invers; GA, TSP ch130, 5% Mutation Rate, Transl; GA, TSP ch130, 0% Mutation Rate, Transl; GA, TSP ch130, 0% Mutation Rate, Invers

Details

Name: GA, TSP ch130, 5% Mutation Rate, InversionManipulator Run 1

Color: Change...

Parameters & Results

Name

Results

- AbsoluteDifferenceBestK
- Best TSP Solution
- BestKnownQuality
- BestQuality
- CurrentAverageQuality
- CurrentBestQuality
- CurrentWorstQuality
- EvaluatedSolutions
- Execution Time
- Generations
- Qualities
- RelativeDifferenceBestK

Details

Name: Qualities

Qualities

CurrentBestQuality BestQuality
CurrentAverageQuality BestKnownQuality
CurrentWorstQuality

60000
40000
20000
0

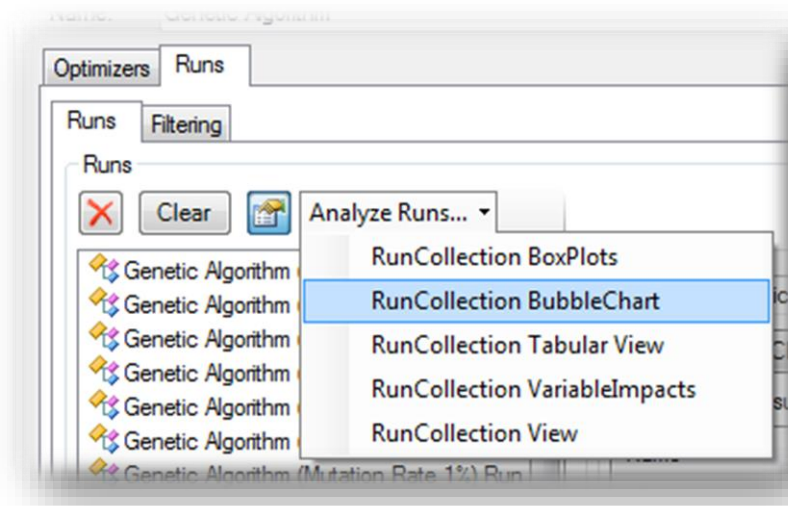
0 2000 4000 6000 8000 10000

Show Algorithm

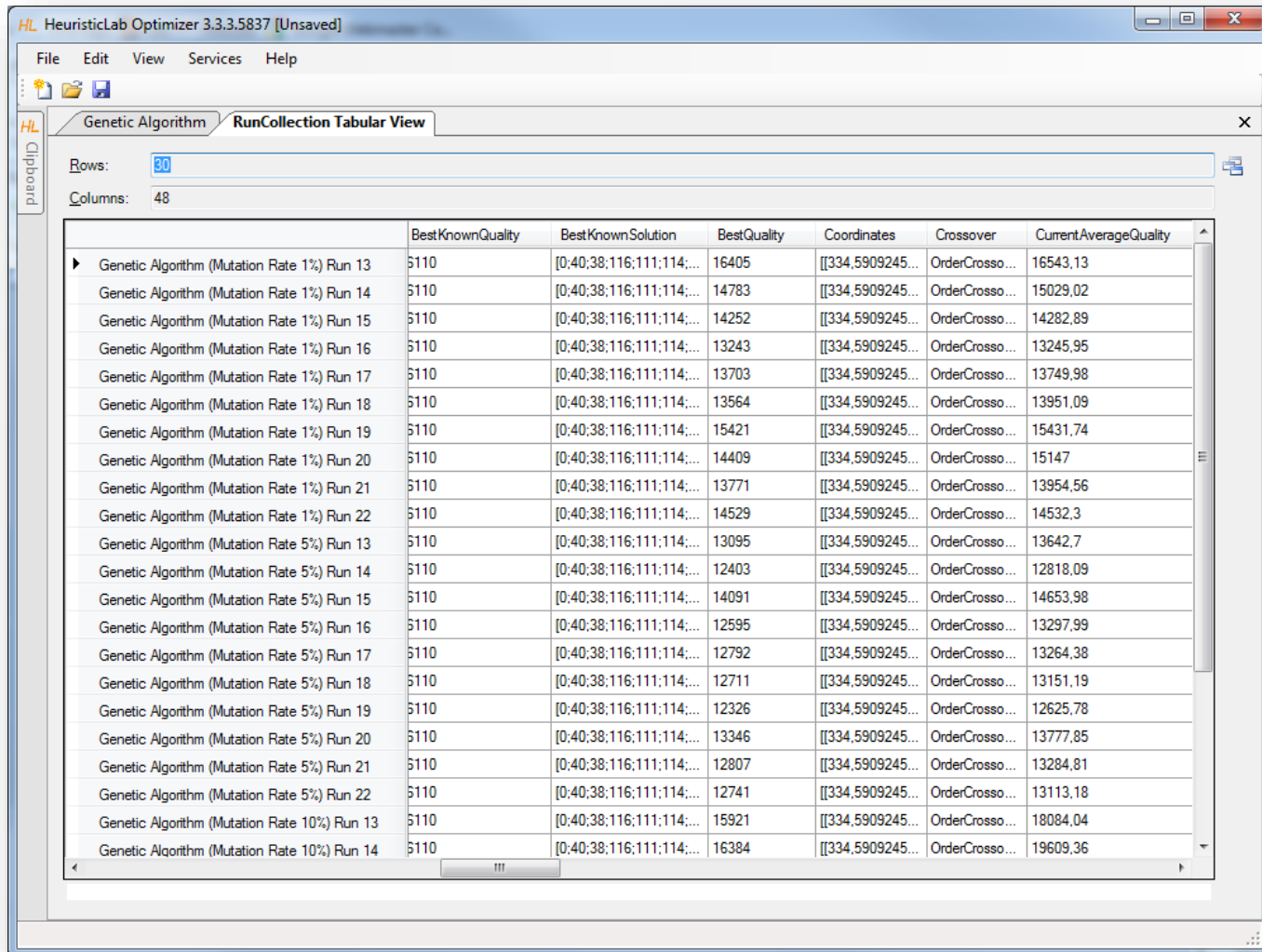
Execution Time: 03:55:16.2570011

Analyze Runs

- HeuristicLab provides interactive views to analyze and compare all runs of a run collection
 - textual analysis
 - RunCollection Tabular View
 - graphical analysis
 - RunCollection BubbleChart
 - RunCollection BoxPlots
- Filtering is automatically applied to all open run collection views



Runs – Tabular View

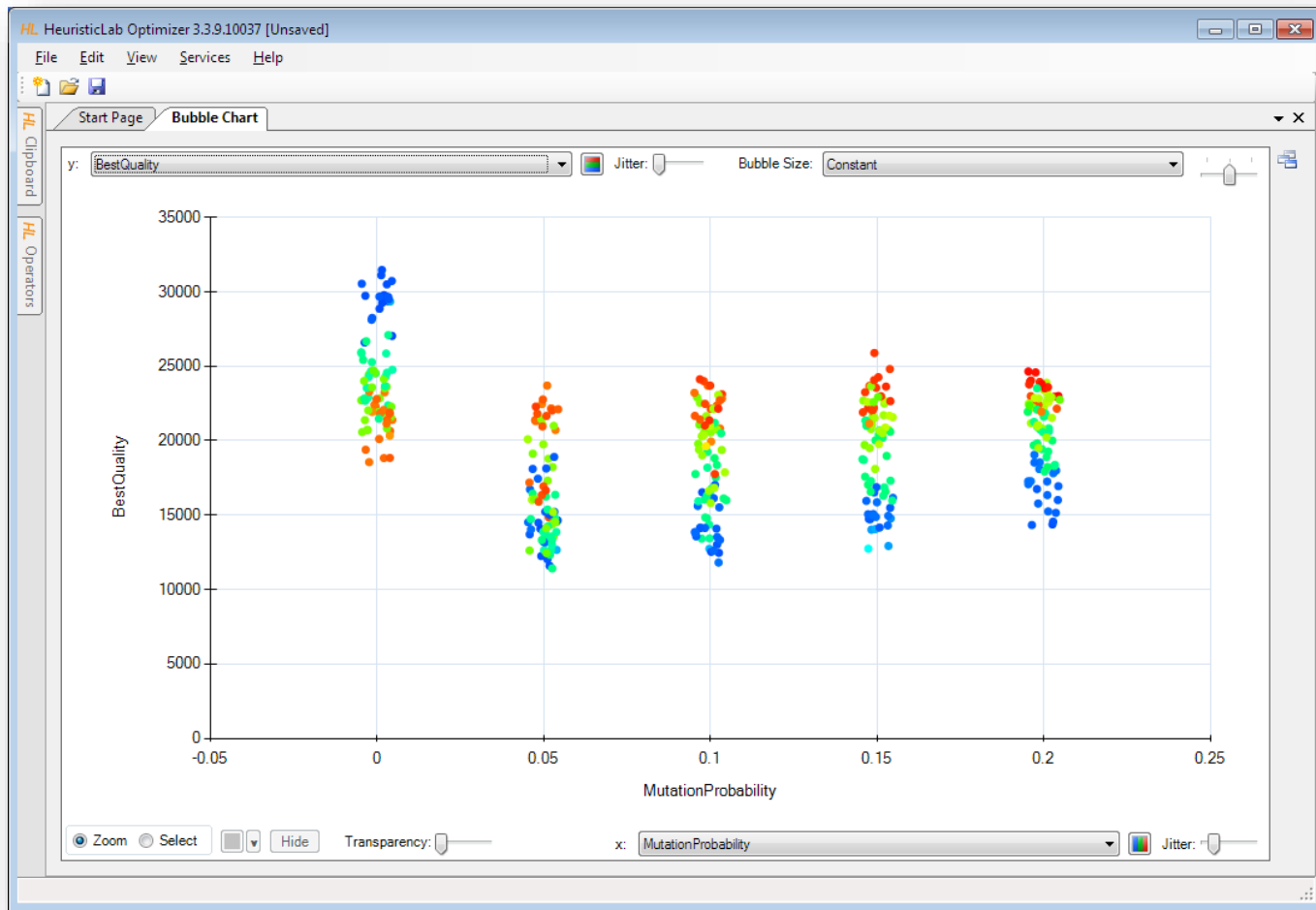


	BestKnownQuality	BestKnownSolution	BestQuality	Coordinates	Crossover	CurrentAverageQuality
▶ Genetic Algorithm (Mutation Rate 1%) Run 13	5110	[0;40;38;116;111;114;...	16405	[[334,5909245...	OrderCrosso...	16543,13
Genetic Algorithm (Mutation Rate 1%) Run 14	5110	[0;40;38;116;111;114;...	14783	[[334,5909245...	OrderCrosso...	15029,02
Genetic Algorithm (Mutation Rate 1%) Run 15	5110	[0;40;38;116;111;114;...	14252	[[334,5909245...	OrderCrosso...	14282,89
Genetic Algorithm (Mutation Rate 1%) Run 16	5110	[0;40;38;116;111;114;...	13243	[[334,5909245...	OrderCrosso...	13245,95
Genetic Algorithm (Mutation Rate 1%) Run 17	5110	[0;40;38;116;111;114;...	13703	[[334,5909245...	OrderCrosso...	13749,98
Genetic Algorithm (Mutation Rate 1%) Run 18	5110	[0;40;38;116;111;114;...	13564	[[334,5909245...	OrderCrosso...	13951,09
Genetic Algorithm (Mutation Rate 1%) Run 19	5110	[0;40;38;116;111;114;...	15421	[[334,5909245...	OrderCrosso...	15431,74
Genetic Algorithm (Mutation Rate 1%) Run 20	5110	[0;40;38;116;111;114;...	14409	[[334,5909245...	OrderCrosso...	15147
Genetic Algorithm (Mutation Rate 1%) Run 21	5110	[0;40;38;116;111;114;...	13771	[[334,5909245...	OrderCrosso...	13954,56
Genetic Algorithm (Mutation Rate 1%) Run 22	5110	[0;40;38;116;111;114;...	14529	[[334,5909245...	OrderCrosso...	14532,3
Genetic Algorithm (Mutation Rate 5%) Run 13	5110	[0;40;38;116;111;114;...	13095	[[334,5909245...	OrderCrosso...	13642,7
Genetic Algorithm (Mutation Rate 5%) Run 14	5110	[0;40;38;116;111;114;...	12403	[[334,5909245...	OrderCrosso...	12818,09
Genetic Algorithm (Mutation Rate 5%) Run 15	5110	[0;40;38;116;111;114;...	14091	[[334,5909245...	OrderCrosso...	14653,98
Genetic Algorithm (Mutation Rate 5%) Run 16	5110	[0;40;38;116;111;114;...	12595	[[334,5909245...	OrderCrosso...	13297,99
Genetic Algorithm (Mutation Rate 5%) Run 17	5110	[0;40;38;116;111;114;...	12792	[[334,5909245...	OrderCrosso...	13264,38
Genetic Algorithm (Mutation Rate 5%) Run 18	5110	[0;40;38;116;111;114;...	12711	[[334,5909245...	OrderCrosso...	13151,19
Genetic Algorithm (Mutation Rate 5%) Run 19	5110	[0;40;38;116;111;114;...	12326	[[334,5909245...	OrderCrosso...	12625,78
Genetic Algorithm (Mutation Rate 5%) Run 20	5110	[0;40;38;116;111;114;...	13346	[[334,5909245...	OrderCrosso...	13777,85
Genetic Algorithm (Mutation Rate 5%) Run 21	5110	[0;40;38;116;111;114;...	12807	[[334,5909245...	OrderCrosso...	13284,81
Genetic Algorithm (Mutation Rate 5%) Run 22	5110	[0;40;38;116;111;114;...	12741	[[334,5909245...	OrderCrosso...	13113,18
Genetic Algorithm (Mutation Rate 10%) Run 13	5110	[0;40;38;116;111;114;...	15921	[[334,5909245...	OrderCrosso...	18084,04
Genetic Algorithm (Mutation Rate 10%) Run 14	5110	[0;40;38;116;111;114;...	16384	[[334,5909245...	OrderCrosso...	19609,36

Runs – Tabular View

- Sort columns
 - click on column header to sort column
 - Ctrl-click on column header to sort multiple columns
- Show or hide columns
 - right-click on table to open dialog to show or hide columns
- Compute statistical values
 - select multiple numerical values to see count, sum, minimum, maximum, average and standard deviation
- Select, copy and paste into other applications

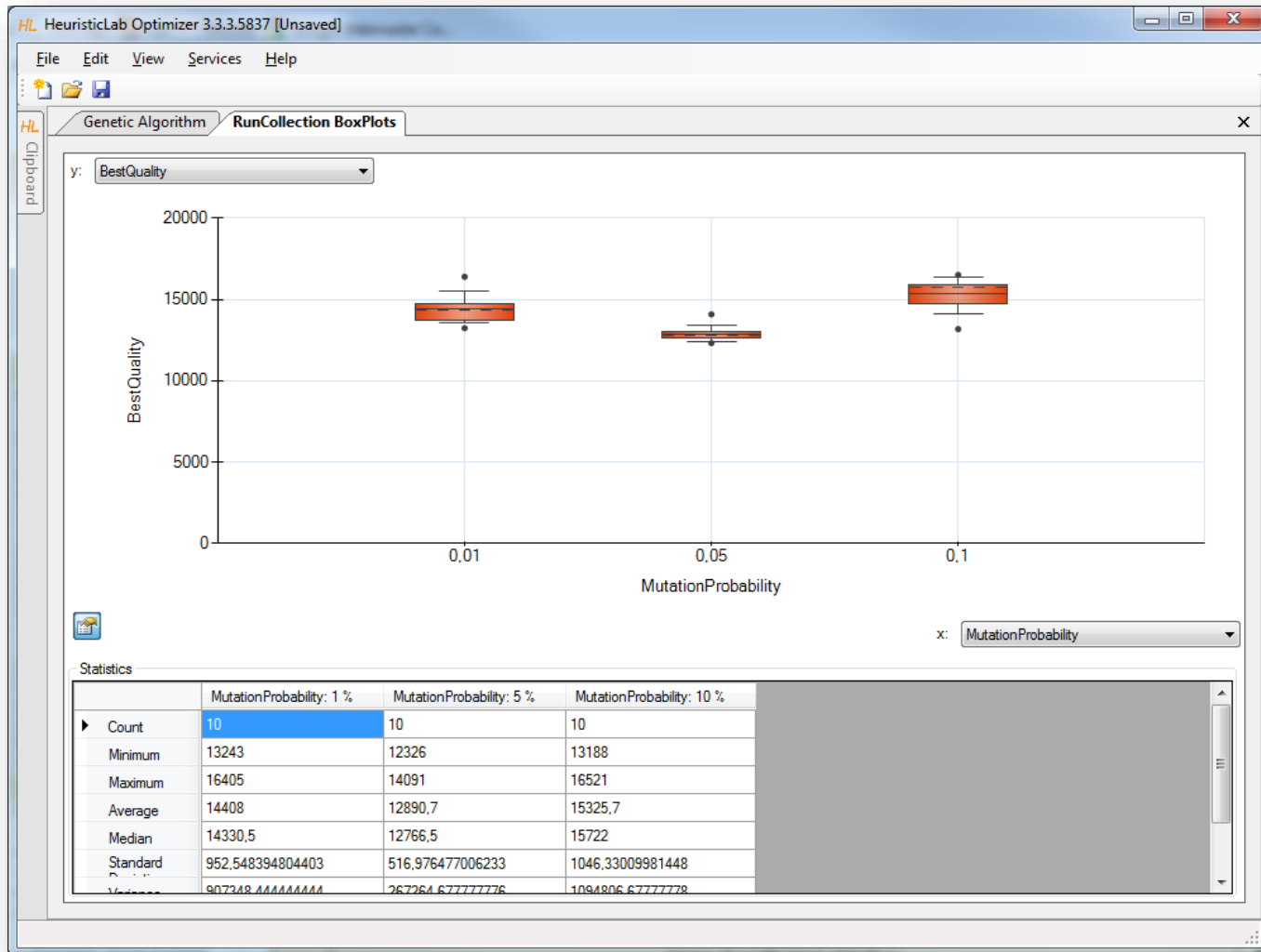
Runs – BubbleChart



Runs – BubbleChart

- Choose values to plot
 - choose which values to show on the x-axis, the y-axis and as bubble size
 - possible values are all parameter settings and results
- Add jitter
 - add jitter to separate overlapping bubbles
- Zoom in and out
 - click on Zoom and click and drag in the chart area to zoom in
 - double click on the chart area background or on the circle buttons beside the scroll bars to zoom out
- Color bubbles
 - click on Select, choose a color and click and drag in the chart area to select and color bubbles
 - apply coloring automatically by clicking on the axis coloring buttons
- Show runs
 - double click on a bubble to open its run
- Export image
 - right-click to open context menu to copy or save image
 - save image as pixel (BMP, JPG, PNG, GIF, TIF) or vector graphics (EMF)
- Show box plots
 - right-click to open context menu to show box plots view

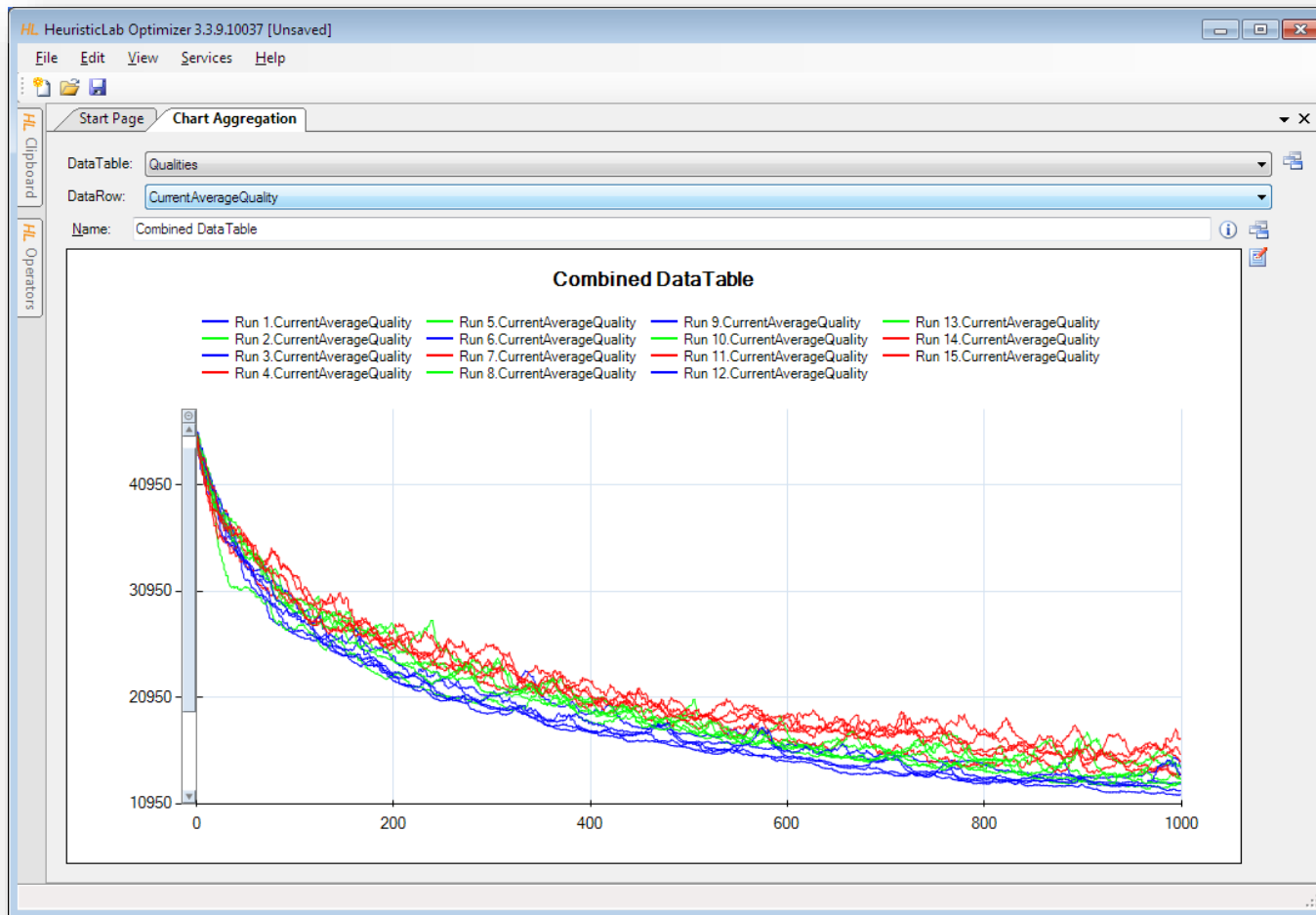
Runs – BoxPlots



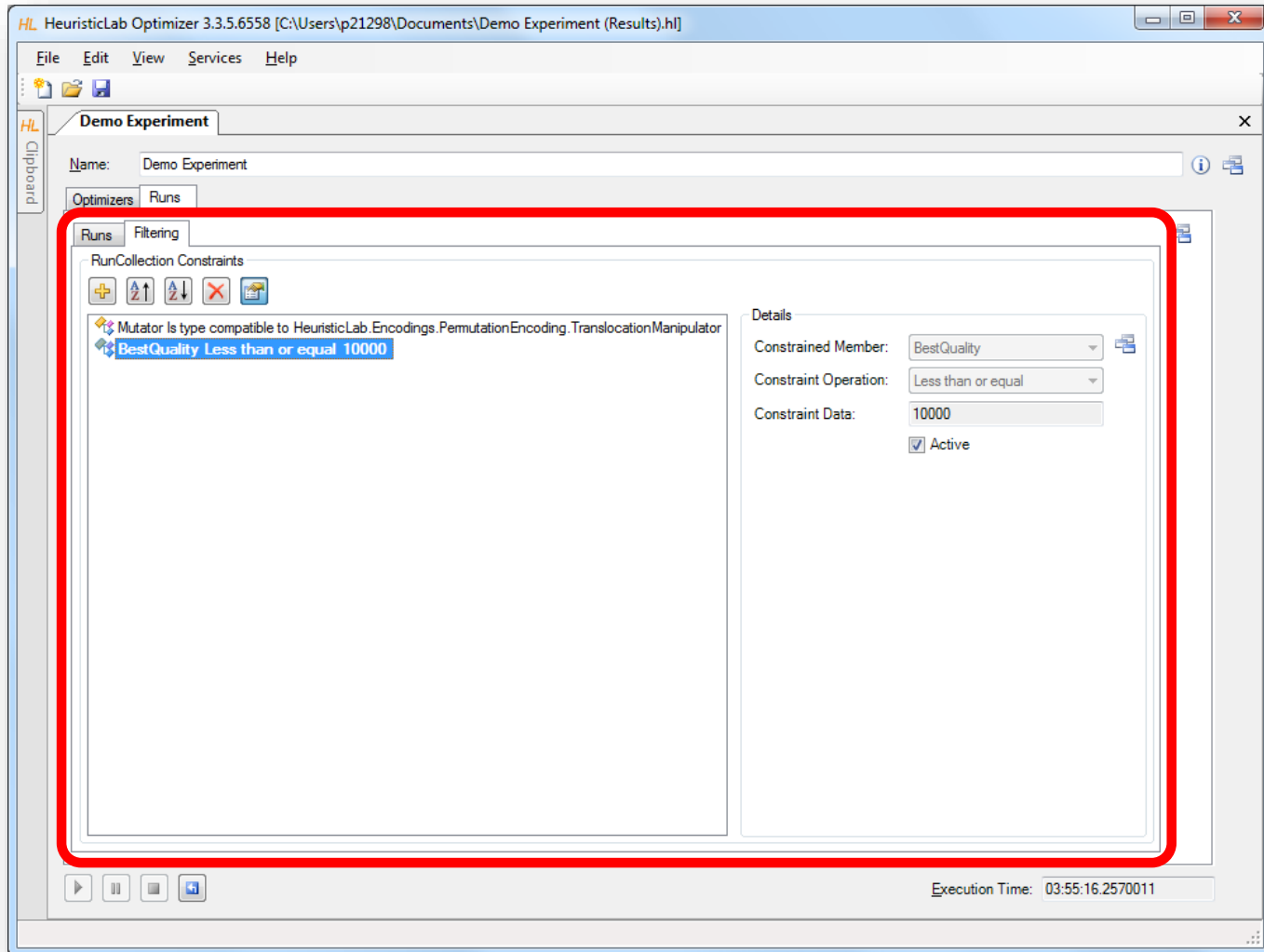
Runs – BoxPlots

- Choose values to plot
 - choose which values to show on the x-axis and y-axis
 - possible values are all parameter settings and results
- Zoom in and out
 - click on Zoom and click and drag in the chart area to zoom in
 - double click on the chart area background or on the circle buttons beside the scroll bars to zoom out
- Show or hide statistical values
 - click on the lower left button to show or hide statistical values
- Export image
 - right-click to open context menu to copy or save image
 - save image as pixel (BMP, JPG, PNG, GIF, TIF) or vector graphics (EMF)

Runs – Multi-Line Chart



Filter Runs

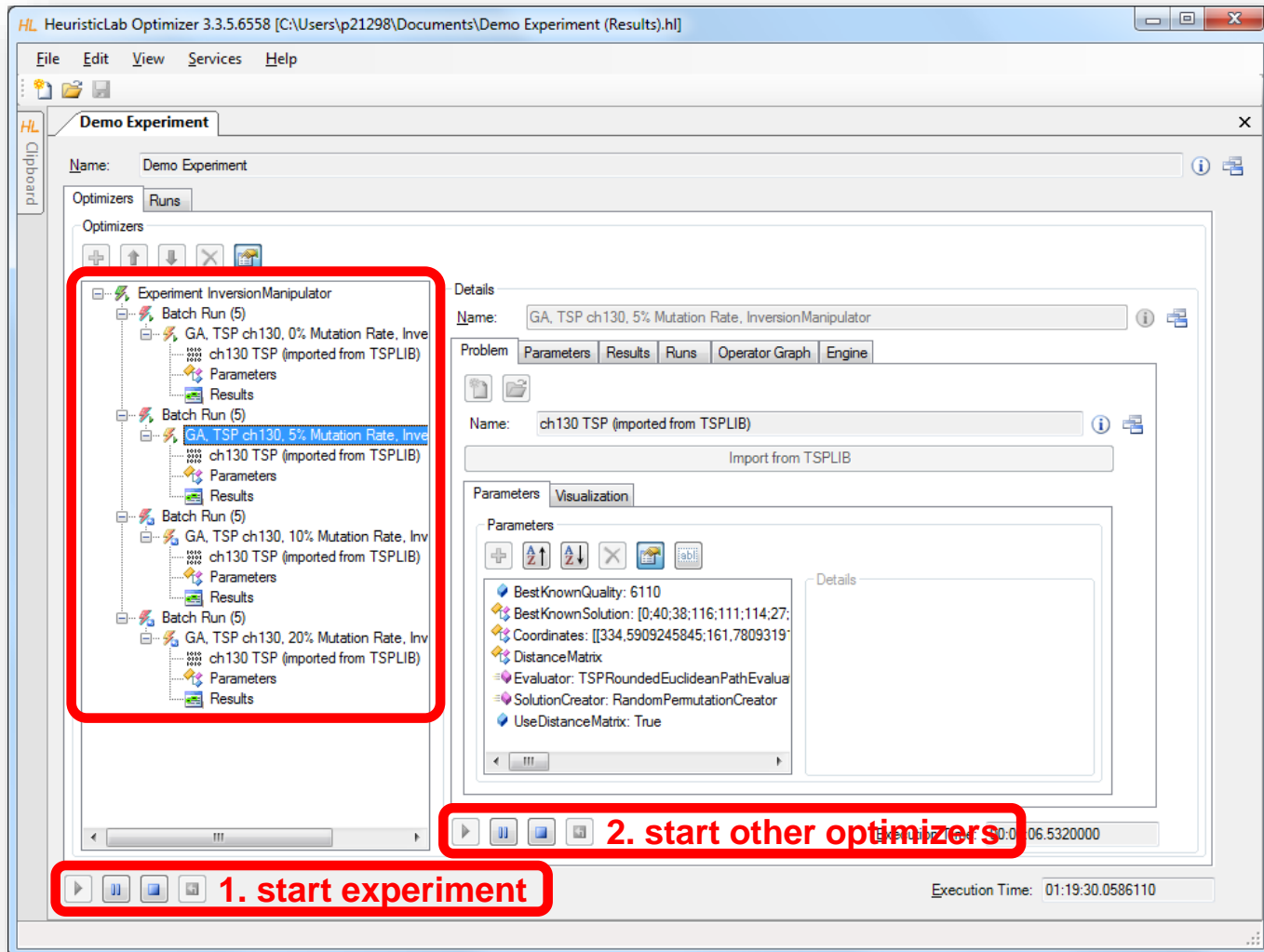


Multi-core CPUs and Parallelization



- Parallel execution of optimizers in experiments
 - optimizers in an experiment are executed sequentially from top to bottom per default
 - experiments support parallel execution of their optimizers
 - select a not yet executed optimizer and start it manually to utilize another core
 - execution of one of the next optimizers is started automatically after an optimizer is finished
- Parallel execution of algorithms
 - HeuristicLab provides special operators for parallelization
 - engines decide how to execute parallel operations
 - sequential engine executes everything sequentially
 - parallel engine executes parallel operations on multiple cores
 - Hive engine (under development) executes parallel operations on multiple computers
 - all implemented algorithms support parallel solution evaluation

Parallel Execution of Experiments



The screenshot shows the HeuristicLab Optimizer interface. The main window is titled "Demo Experiment" and contains a tree view of the experiment structure. The tree is organized as follows:

- Experiment InversionManipulator
 - Batch Run (5)
 - GA, TSP ch130, 0% Mutation Rate, Inve
 - ch130 TSP (imported from TSPLIB)
 - Parameters
 - Results
 - Batch Run (5)
 - GA, TSP ch130, 5% Mutation Rate, Inve
 - ch130 TSP (imported from TSPLIB)
 - Parameters
 - Results
 - Batch Run (5)
 - GA, TSP ch130, 10% Mutation Rate, Inv
 - ch130 TSP (imported from TSPLIB)
 - Parameters
 - Results
 - Batch Run (5)
 - GA, TSP ch130, 20% Mutation Rate, Inv
 - ch130 TSP (imported from TSPLIB)
 - Parameters
 - Results

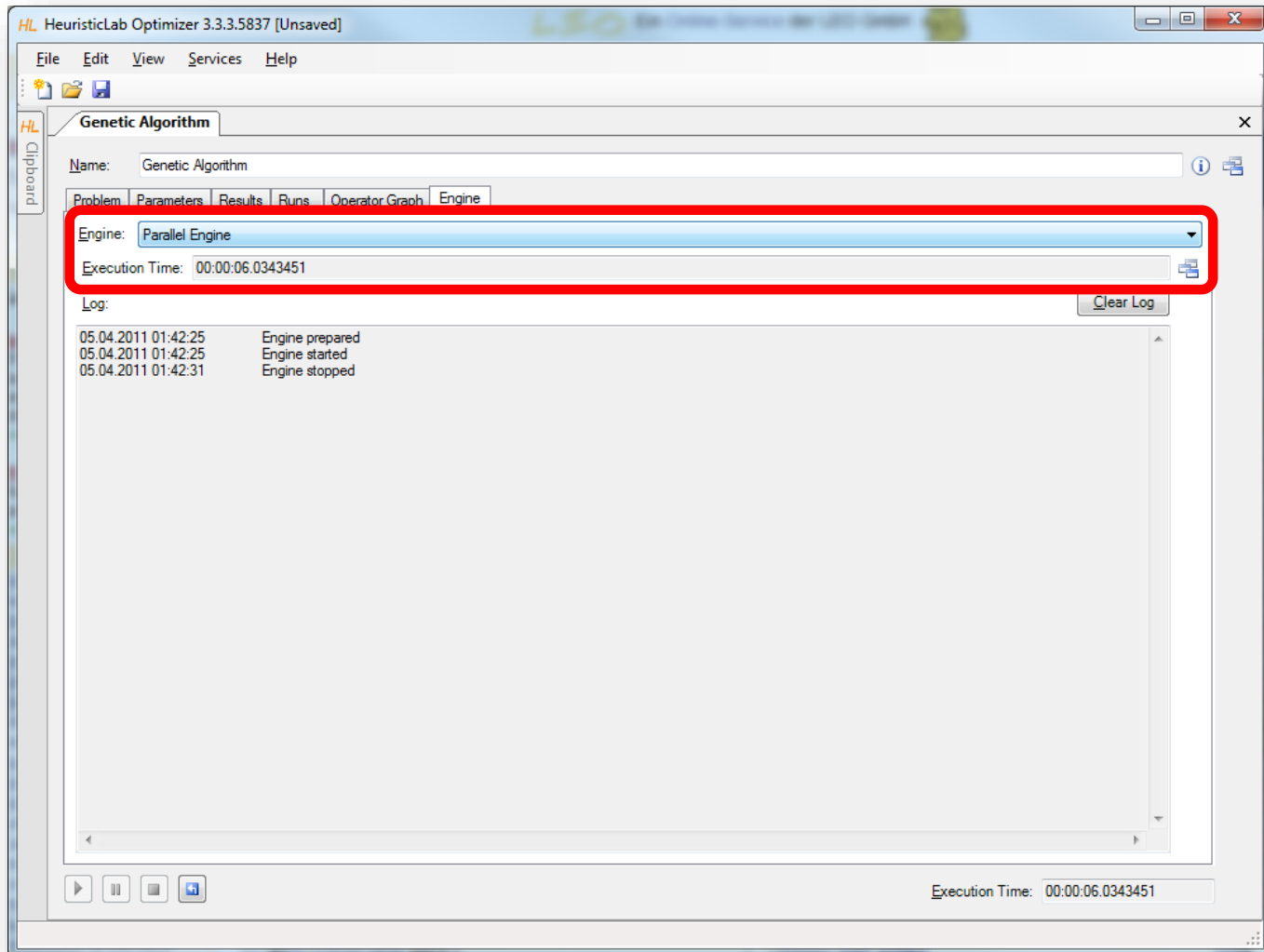
The "Details" panel on the right shows the configuration for the selected experiment:

- Name: GA, TSP ch130, 5% Mutation Rate, InversionManipulator
- Problem: Parameters Results Runs Operator Graph Engine
- Name: ch130 TSP (imported from TSPLIB)
- Parameters Visualization
- Parameters
 - BestKnownQuality: 6110
 - BestKnownSolution: [0;40;38;116;111;114;27;
 - Coordinates: [[334.5909245845;161.7809319;
 - DistanceMatrix
 - Evaluator: TSPRoundedEuclideanPathEvalua
 - SolutionCreator: RandomPemutationCreator
 - UseDistanceMatrix: True

At the bottom of the interface, there are two red boxes with white text:

- A red box containing the text "1. start experiment" is positioned over the play button icon in the bottom toolbar.
- A red box containing the text "2. start other optimizers" is positioned over the play button icon in the bottom toolbar, specifically over the second play button icon.

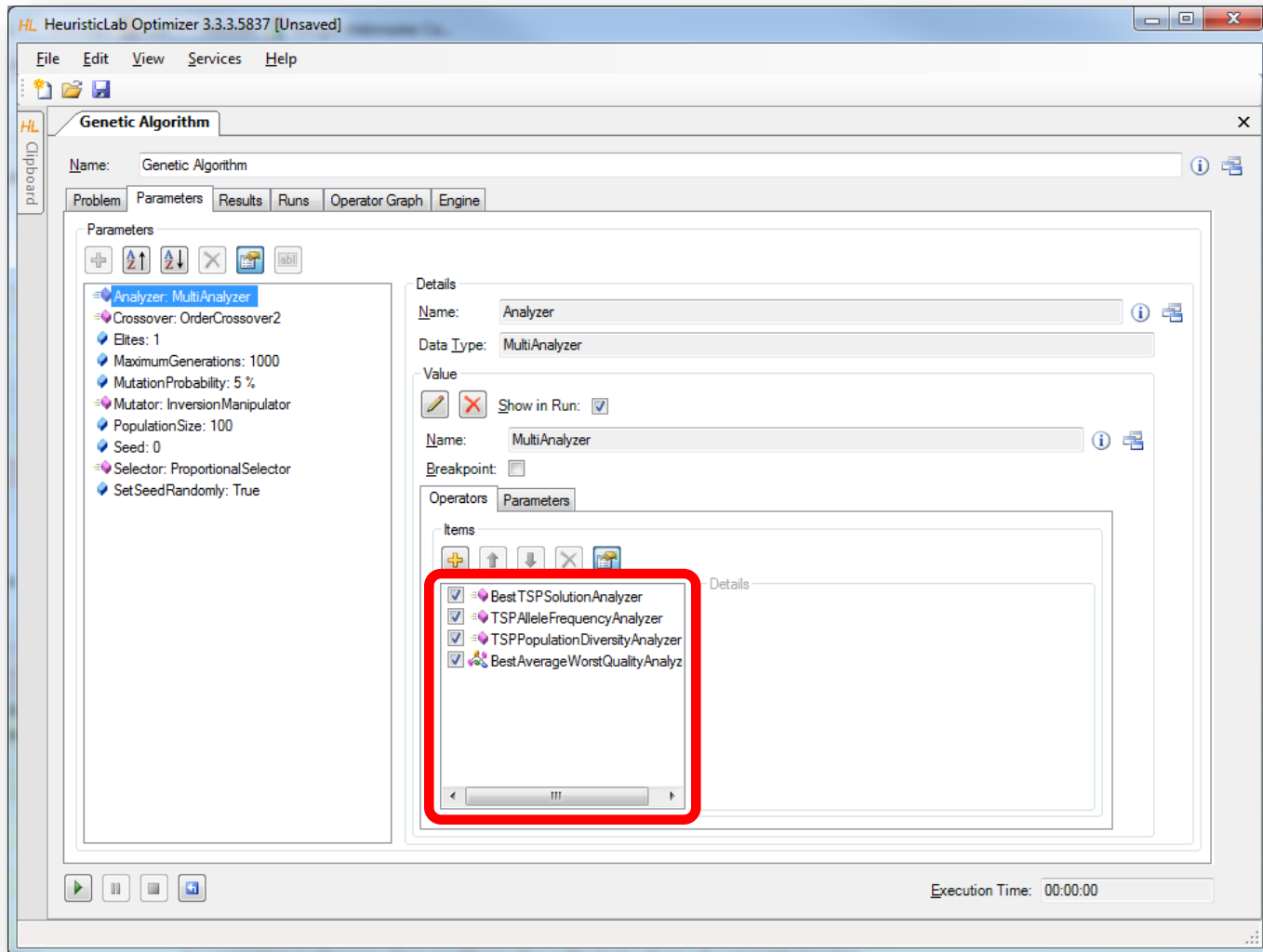
Parallel Execution of Algorithms



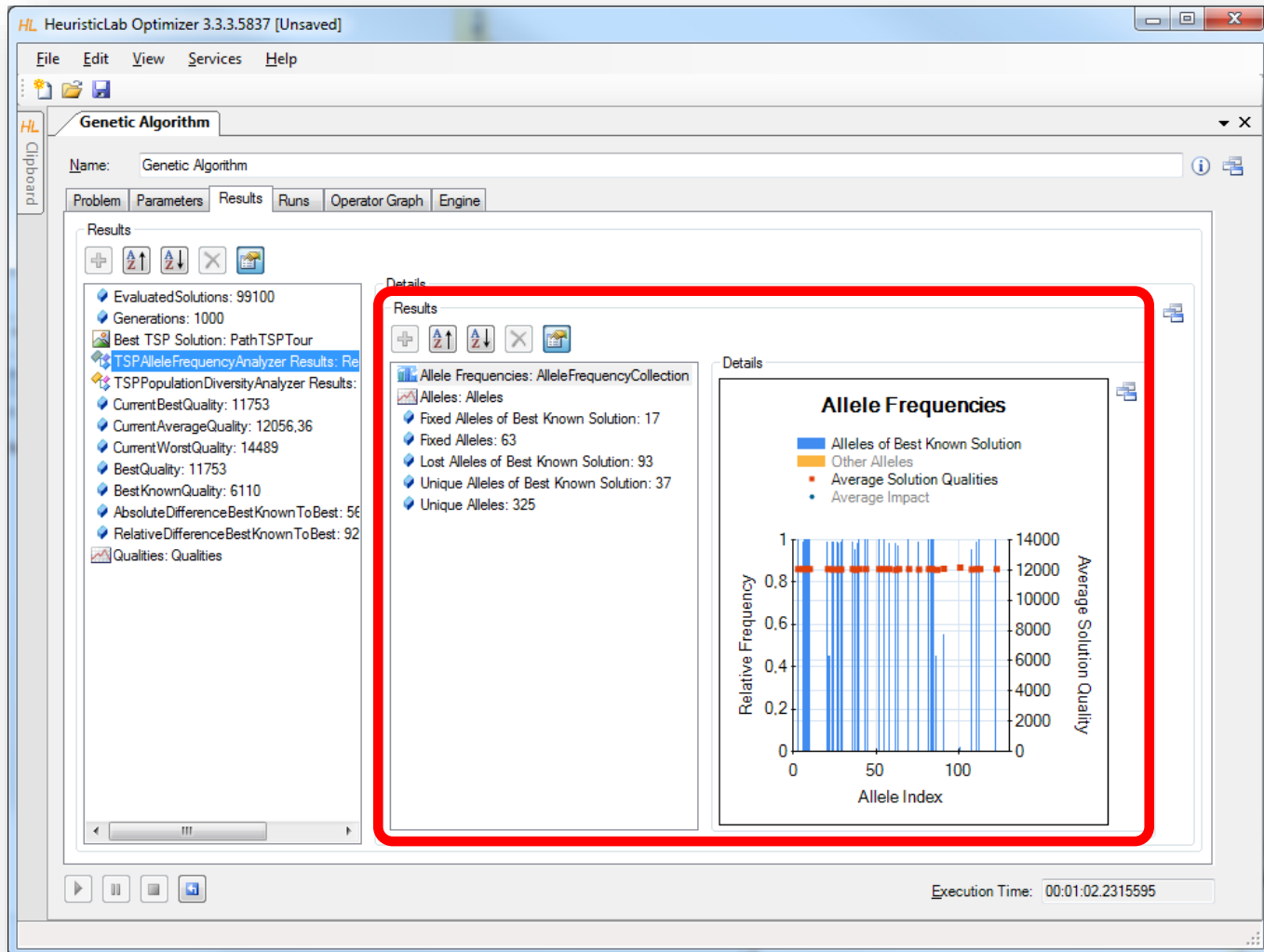
Analyzers

- Special operators for analysis purposes
 - are executed after each iteration
 - serve as general purpose extension points of algorithms
 - can be selected and parameterized in the algorithm
 - perform algorithm-specific and/or problem-specific tasks
 - some analyzers are quite costly regarding runtime and memory
 - implementing and adding custom analyzers is easy
- Examples
 - TSPAlleleFrequencyAnalyzer
 - TSPPopulationDiversityAnalyzer
 - SuccessfulOffspringAnalyzer
 - SymbolicDataAnalysisVariableFrequencyAnalyzer
 - SymbolicRegressionSingleObjectiveTrainingBestSolutionAnalyzer
 - ...

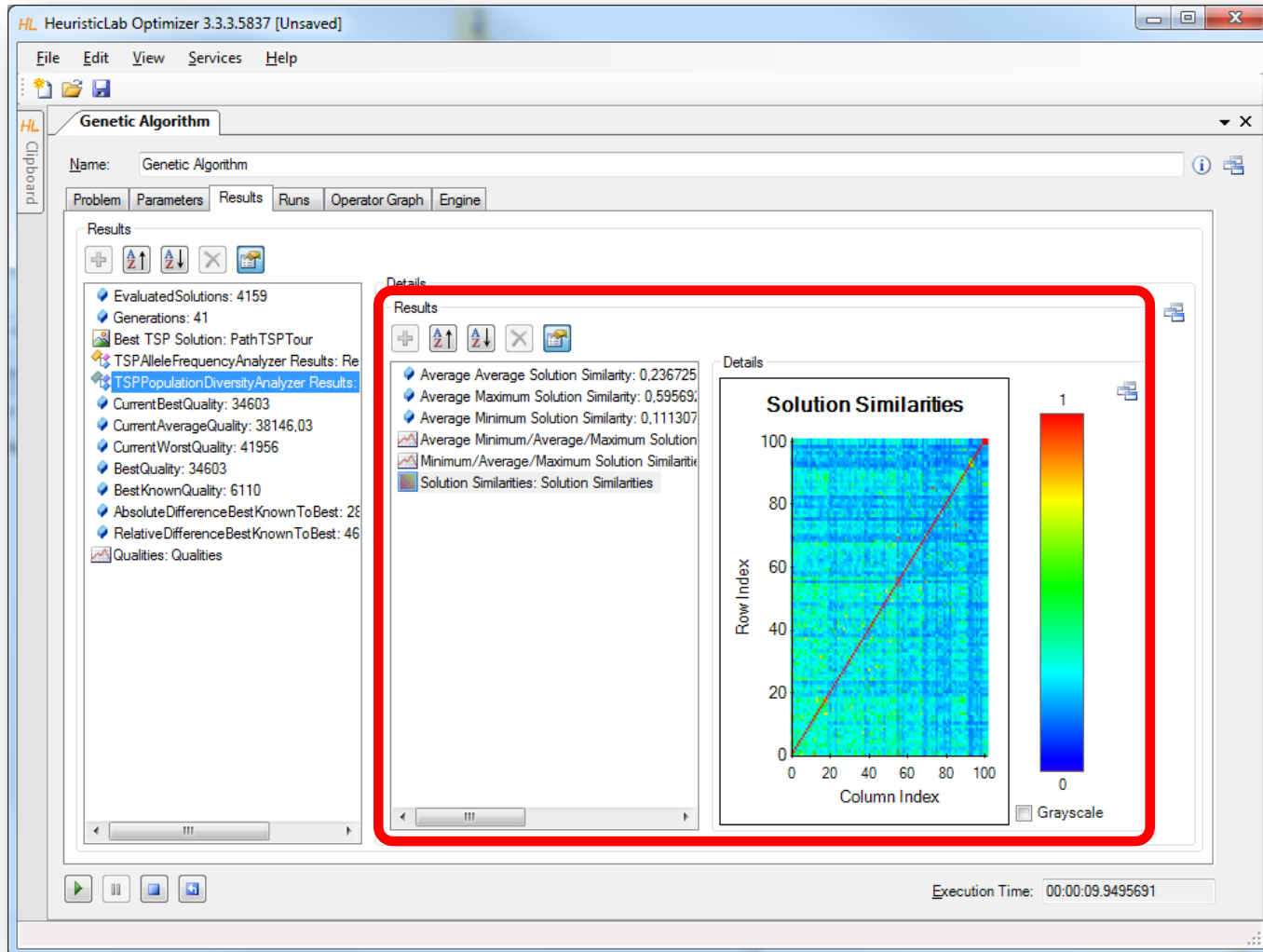
Analyzers



TSPAlleleFrequencyAnalyzer

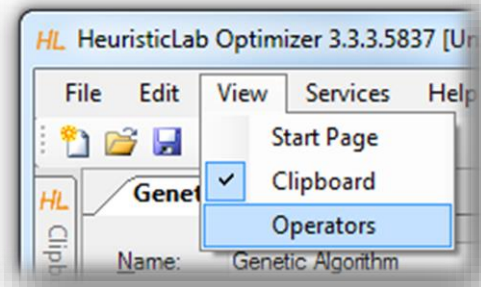
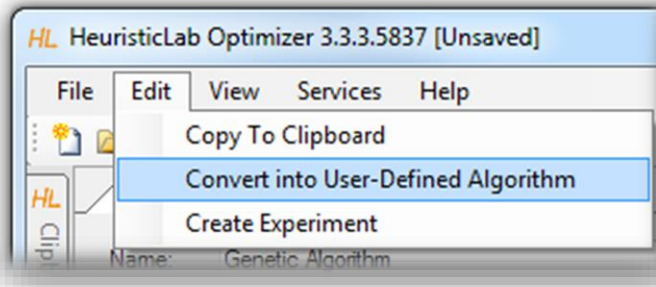


TSP Population Diversity Analyzer



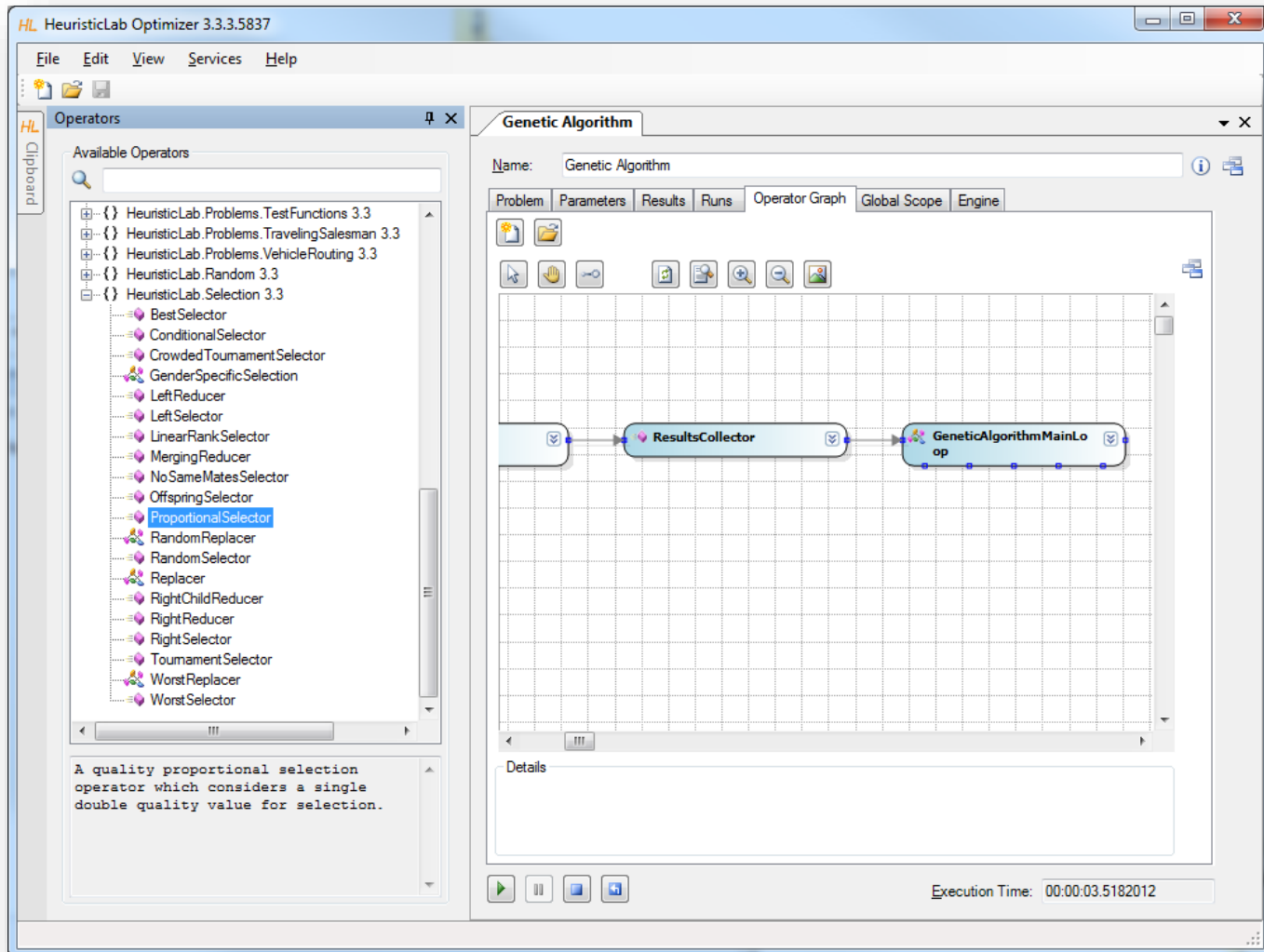
Building User-Defined Algorithms

- Operator graphs
 - algorithms are represented as operator graphs
 - operator graphs of user-defined algorithms can be changed
 - algorithms can be defined in the graphical algorithm designer
 - use the menu to convert a standard algorithm into a user-defined algorithm



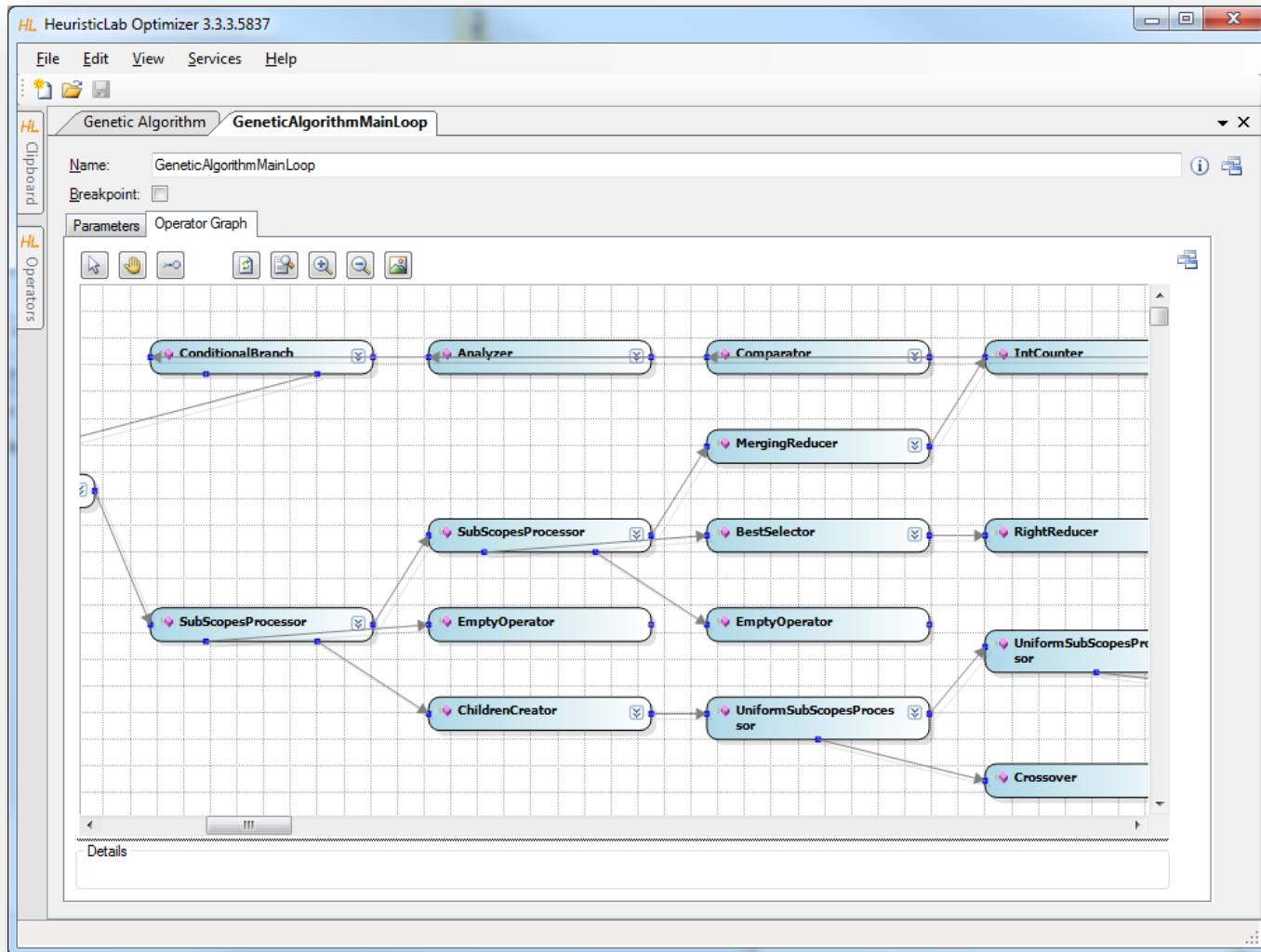
- Operators sidebar
 - drag & drop operators into an operator graph
- Programmable operators
 - add programmable operators in order to implement custom logic in an algorithm
 - no additional development environment needed
- Debug algorithms
 - use the debug engine to obtain detailed information during algorithm execution

Building User-Defined Algorithms

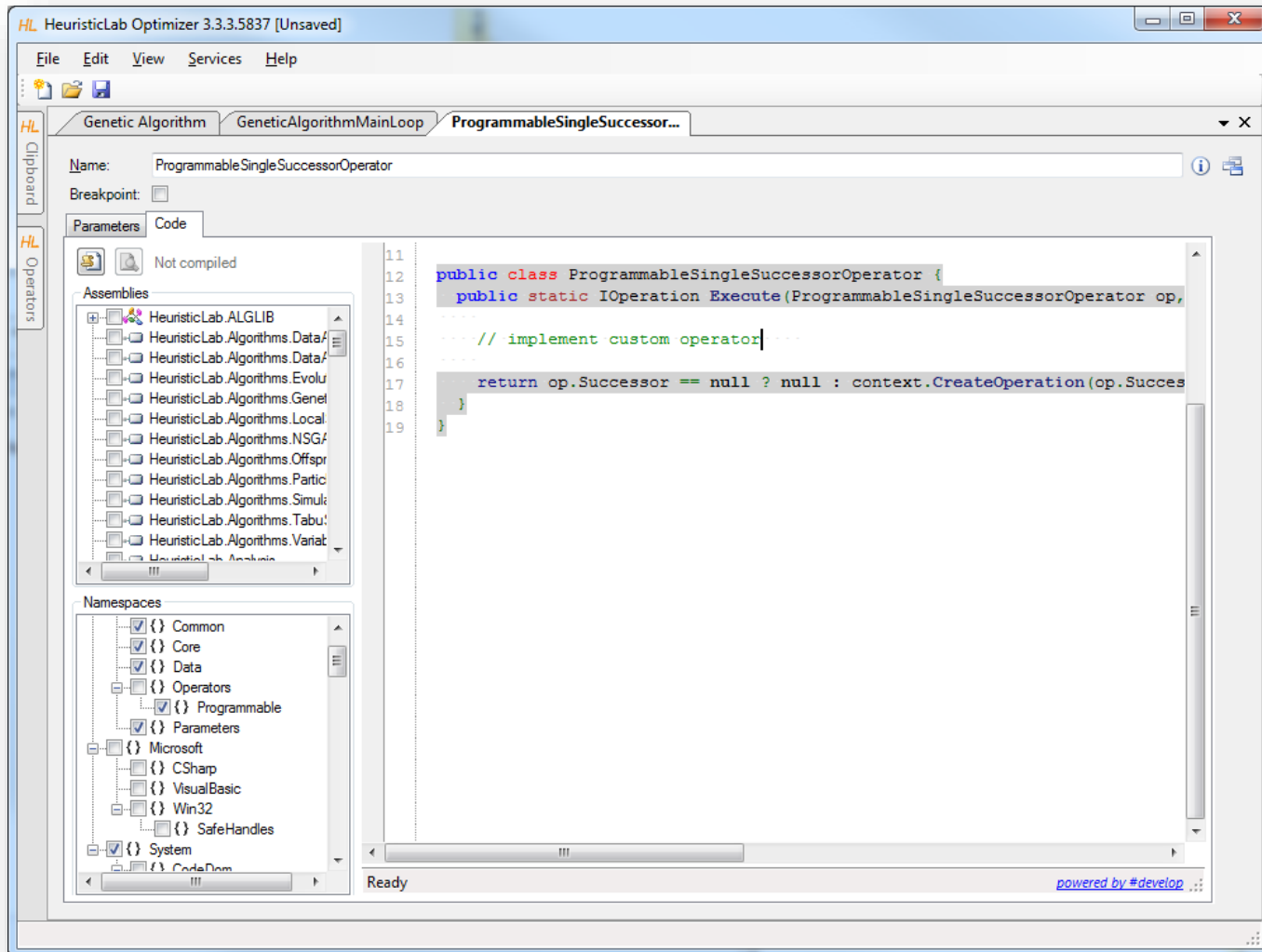


The screenshot displays the HeuristicLab Optimizer 3.3.3.5837 interface. The main window is titled "Genetic Algorithm" and shows a configuration panel with tabs for "Problem", "Parameters", "Results", "Runs", "Operator Graph", "Global Scope", and "Engine". The "Operator Graph" tab is active, showing a flow diagram with two operators: "ResultsCollector" and "GeneticAlgorithmMainLoop". The "Available Operators" list on the left includes various selection and reduction operators, with "ProportionalSelector" highlighted. A description for "ProportionalSelector" is visible at the bottom left: "A quality proportional selection operator which considers a single double quality value for selection." The "Execution Time" at the bottom right is 00:00:03.5182012.

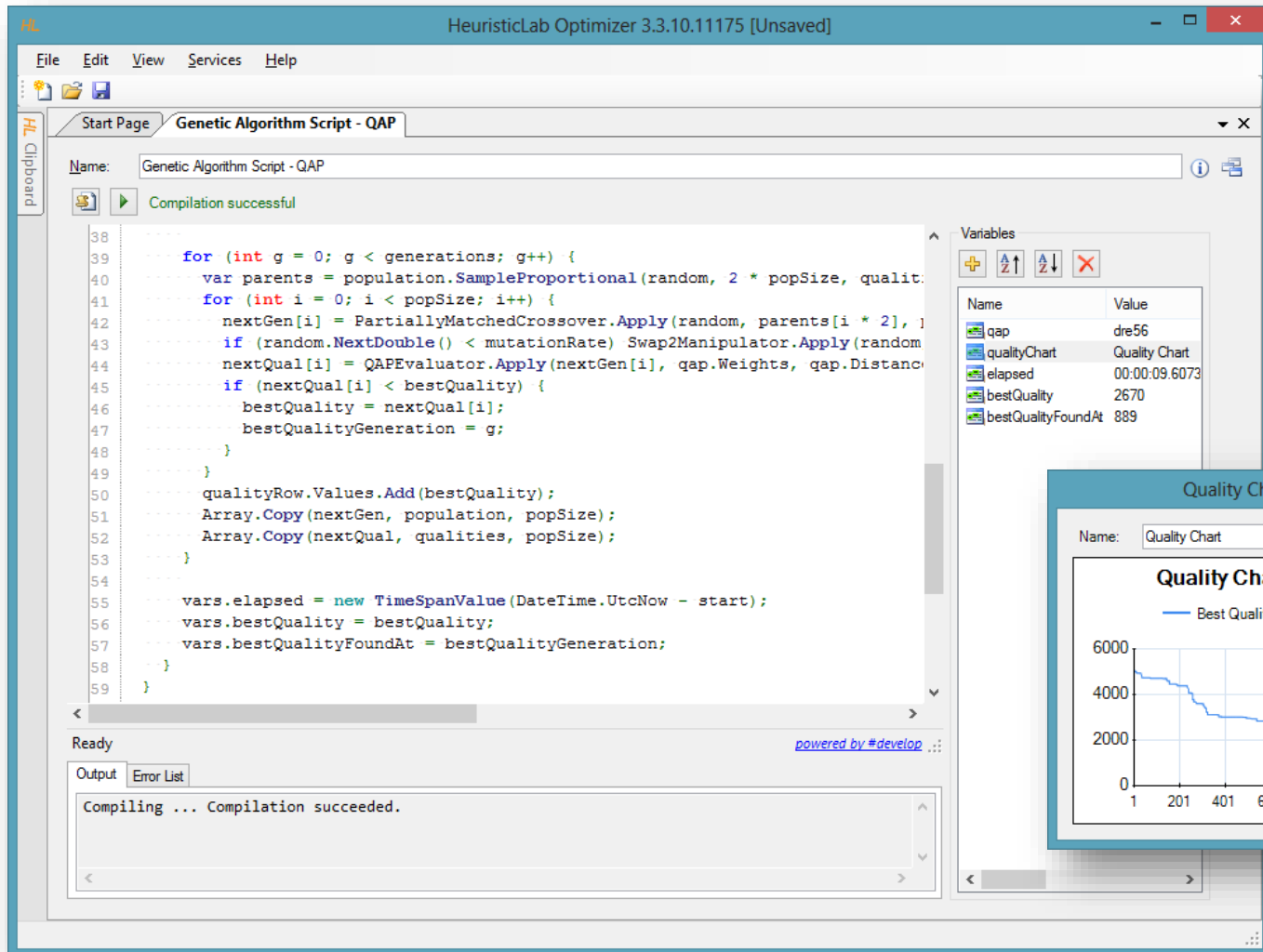
Building User-Defined Algorithms



Programmable Operators



Scripts



HeuristicLab Optimizer 3.3.10.11175 [Unsaved]

File Edit View Services Help

Start Page Genetic Algorithm Script - QAP

Name: Genetic Algorithm Script - QAP

Compilation successful

```
38
39
40
41
42
43
44
45
46
47
48
49
50
51
52
53
54
55
56
57
58
59
}
}
```

Variables

Name	Value
gap	dre56
qualityChart	Quality Chart
elapsed	00:00:09.6073
bestQuality	2670
bestQualityFoundAt	889

Ready *powered by #develop*

Output Error List

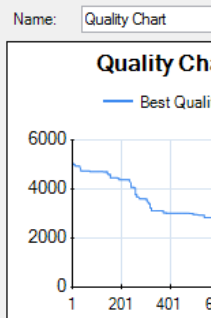
Compiling ... Compilation succeeded.

Quality Chart

Name: Quality Chart

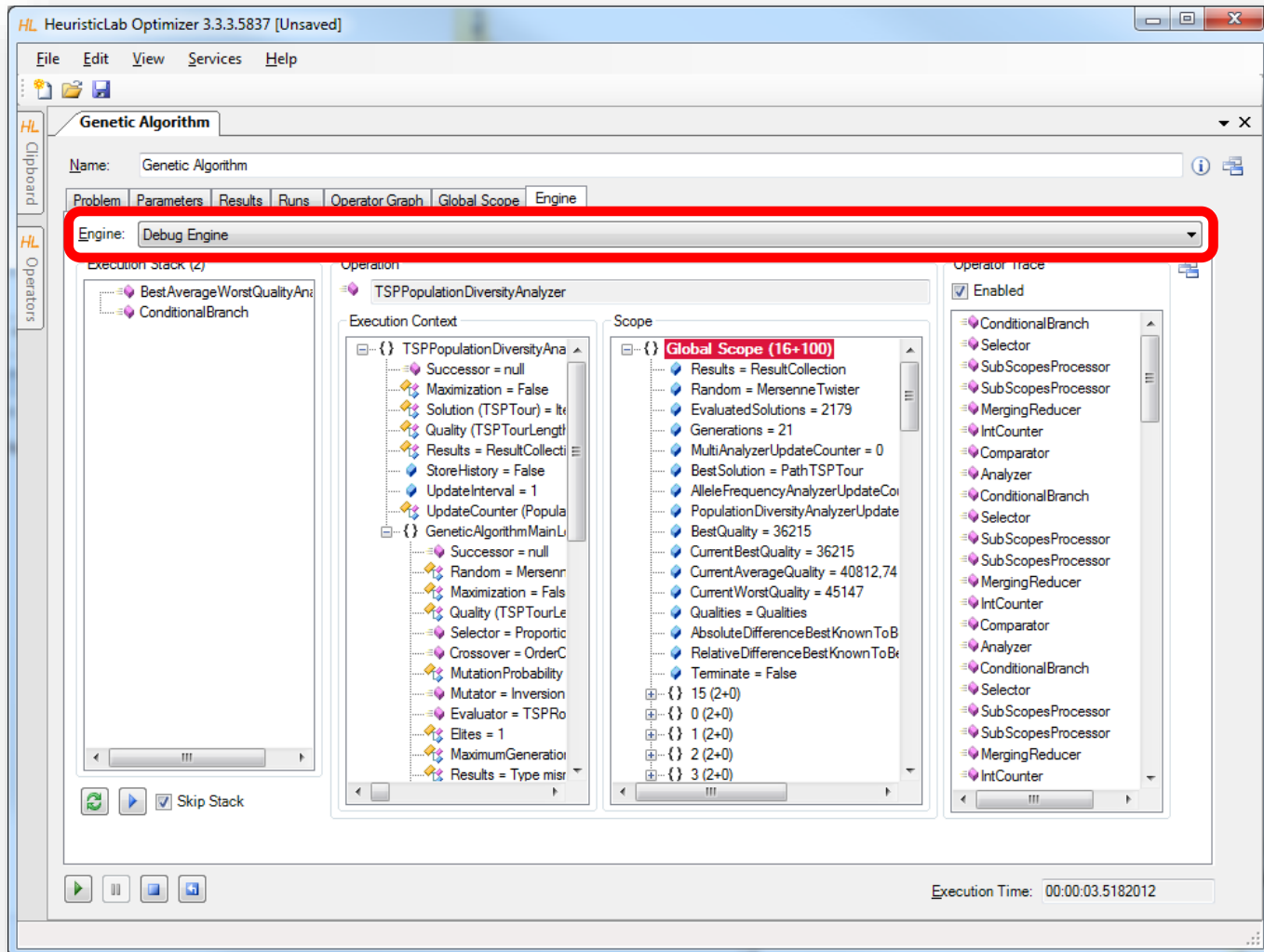
Quality Chart

Best Quality



Generations	Best Quality
1	5000
201	4500
401	3000
601	2800
801	2500

Debugging Algorithms



Agenda



- Objectives of the Tutorial
- Introduction
- Where to get HeuristicLab?
- Plugin Infrastructure
- Graphical User Interface
- Available Algorithms & Problems
- **Demonstration Part I: Working with HeuristicLab**
- **Demonstration Part II: Data-based Modeling**
- Some Additional Features
- Planned Features
- Team
- Suggested Readings
- Bibliography
- Questions & Answers

Demonstration Part II: Data-based Modeling



- Introduction
- Regression with HeuristicLab
- Model simplification and export
- Variable relevance analysis
- Classification with HeuristicLab

Introduction to Data-based Modeling



- Dataset: Matrix $(x_{i,j})_{i=1..N, j=1..K}$
 - N observations of K input variables
 - $x_{i,j}$ = i-th observation of j-th variable
 - Additionally: Vector of labels $(y_1 \dots y_N)^T$
- Goal: learn association of input variable values to labels

Data Analysis in HeuristicLab



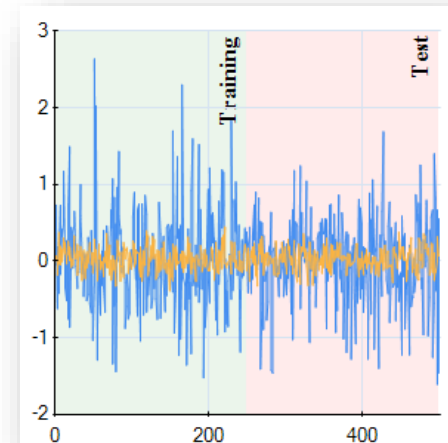
- Symbolic regression and classification using genetic programming
- External Libraries:
 - Linear Regression, Logistic Regression,
 - k-Nearest Neighbours, k-Means,
 - Random Forest, Support Vector Machines, Neural Networks, Gaussian Processes

Case Study: Regression

- Poly-10 benchmark problem dataset
 - 10 input variables $x_1 \dots x_{10}$
 - $y = x_1x_2 + x_3x_4 + x_5x_6 + x_1x_7x_9 + x_3x_6x_{10}$
 - non-linear modeling approach necessary
 - frequently used in GP literature
 - available as benchmark problem instance in HeuristicLab

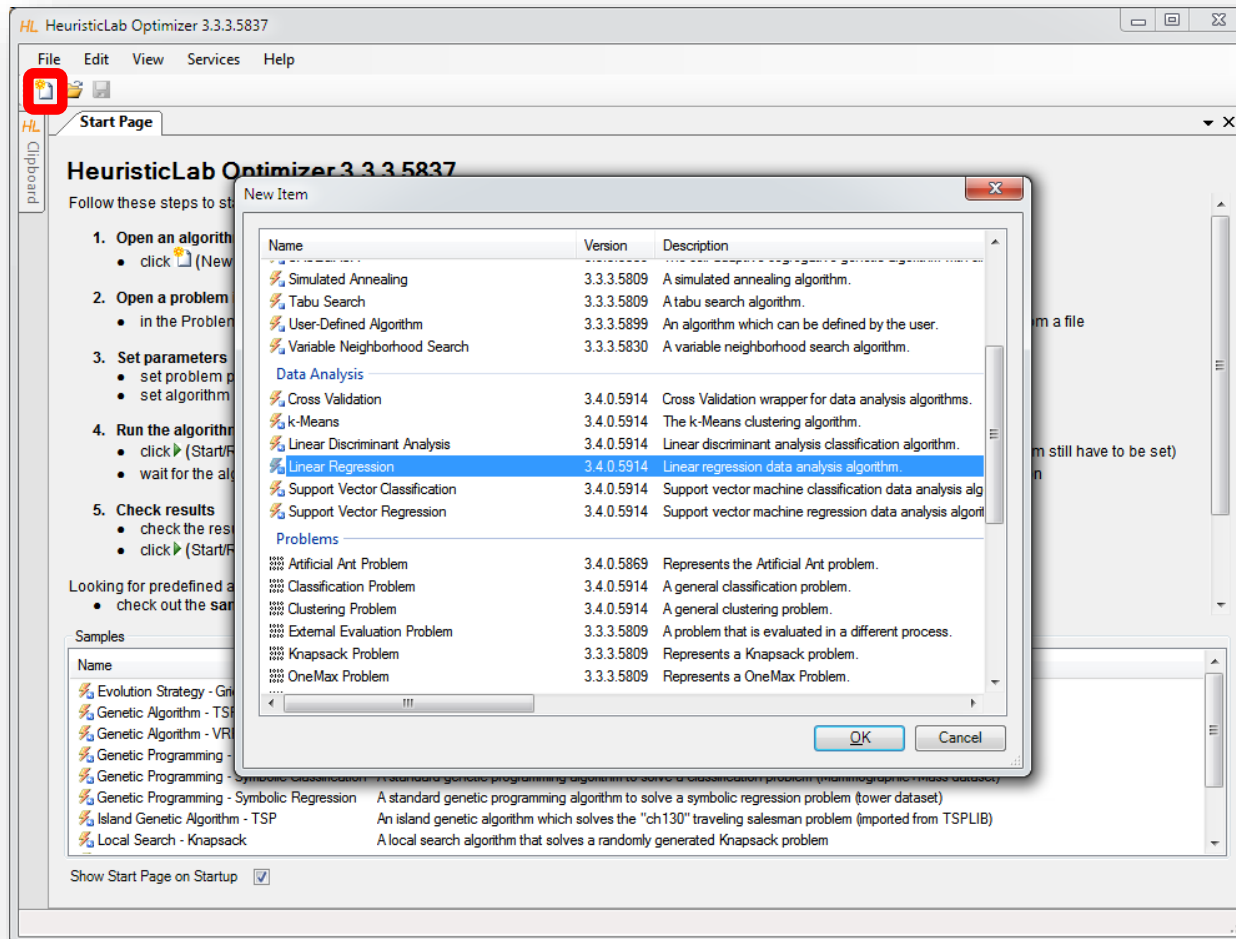
Demonstration

- problem configuration
 - data import
 - target and input variables
 - data partitions (training and test)
- algorithm configuration
- analysis of results
 - accuracy metrics
 - visualization of model output

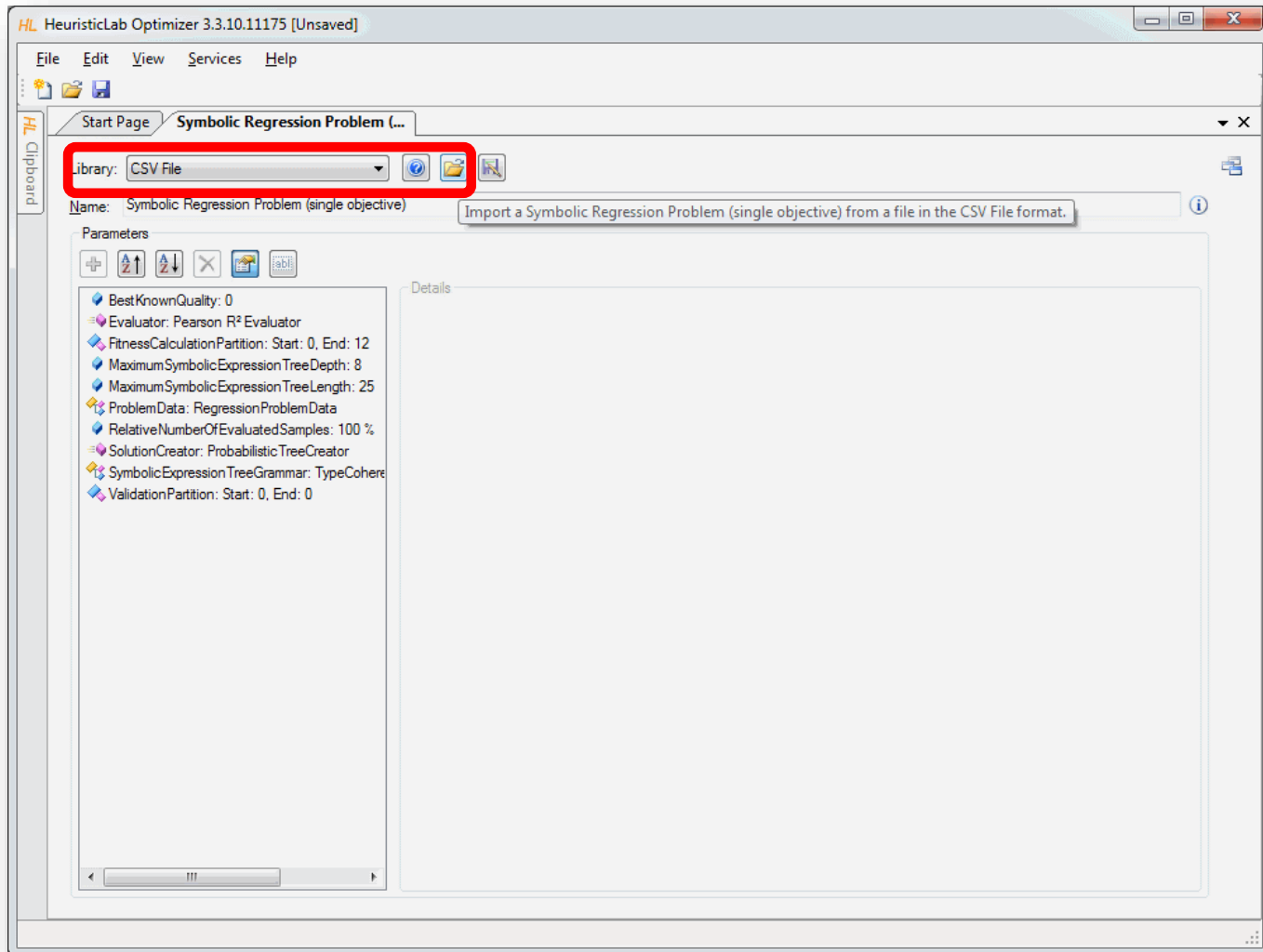


Linear Regression

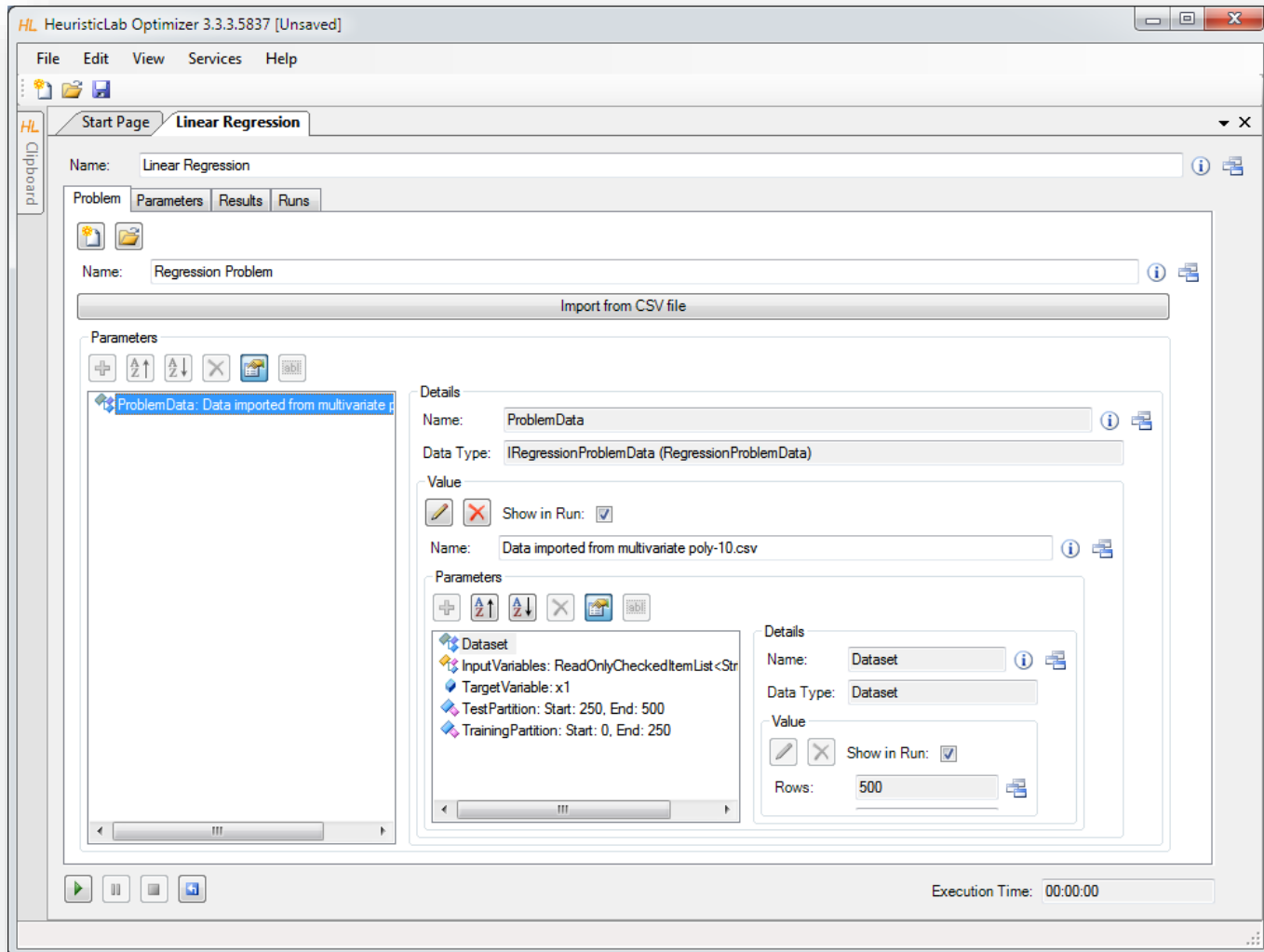
- Create new algorithm



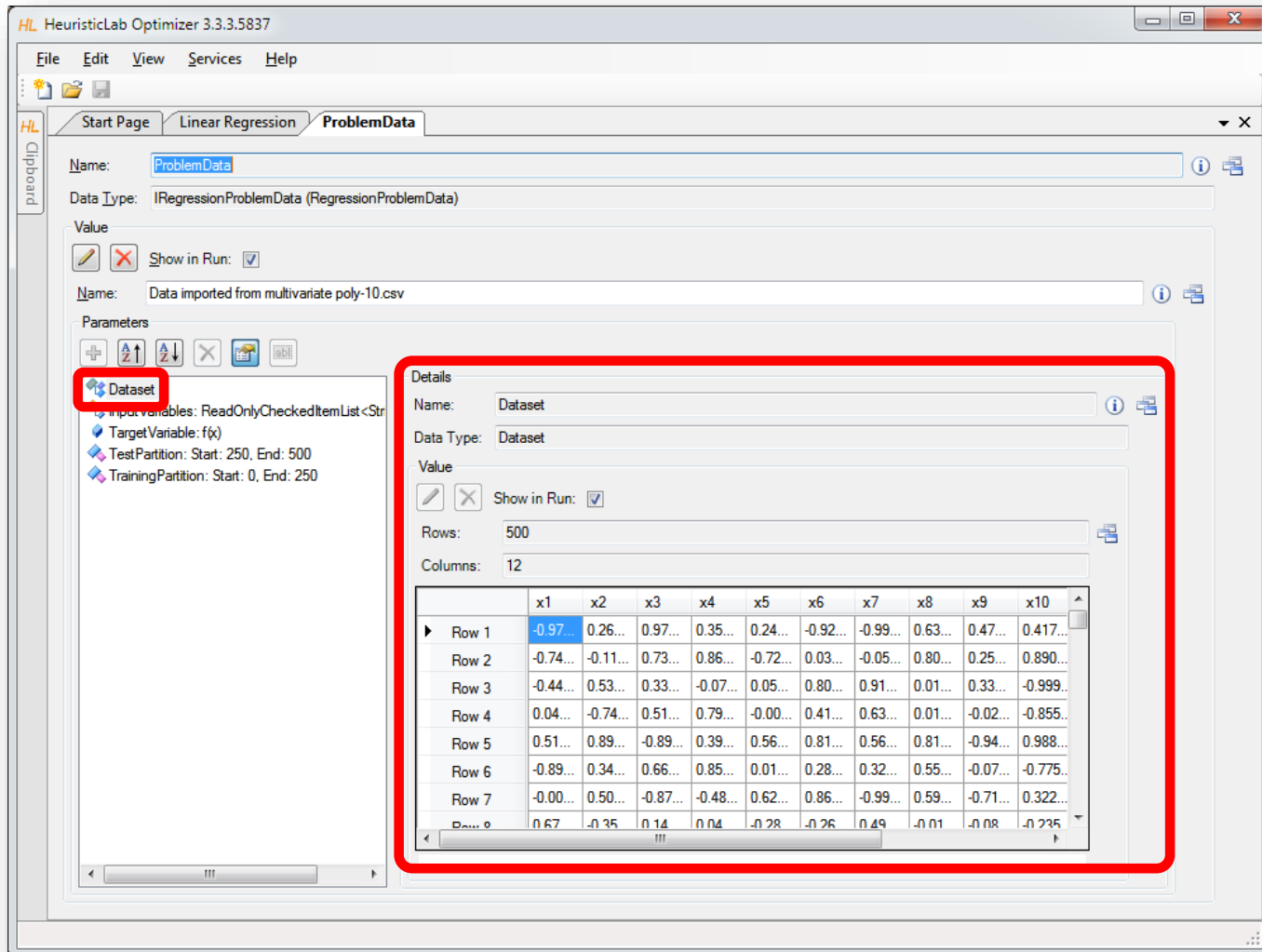
Import Data from CSV-File



Inspect and Configure Dataset



Inspect Imported Data



HL HeuristicLab Optimizer 3.3.3.5837

File Edit View Services Help

Start Page Linear Regression ProblemData

Name: ProblemData

Data Type: IRegressionProblemData (RegressionProblemData)

Value

Show in Run:

Name: Data imported from multivariate poly-10.csv

Parameters

Dataset

Input variables: ReadOnlyCheckedItemList<Str>

Target Variable: f(x)

TestPartition: Start: 250, End: 500

TrainingPartition: Start: 0, End: 250

Details

Name: Dataset

Data Type: Dataset

Value

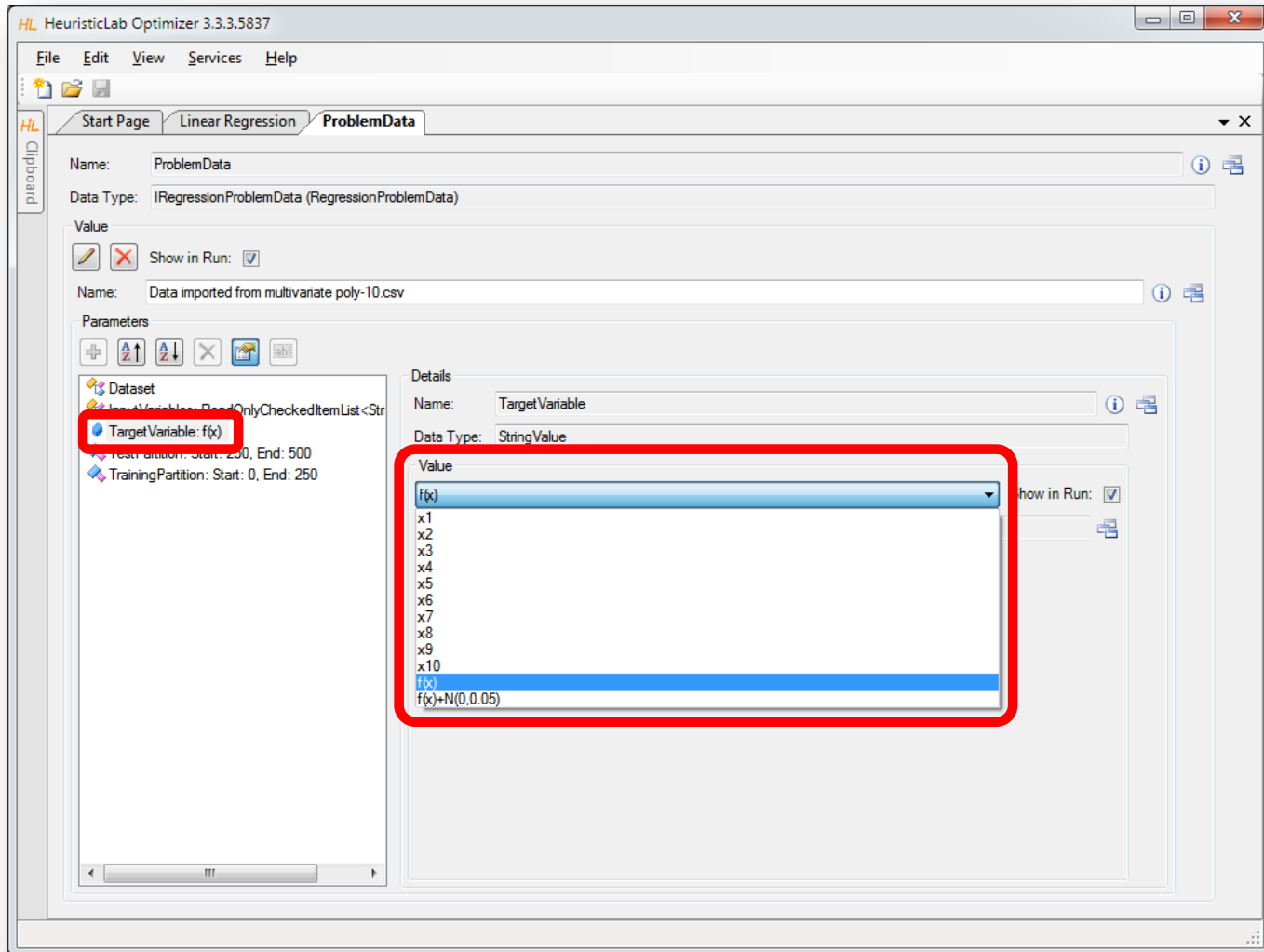
Show in Run:

Rows: 500

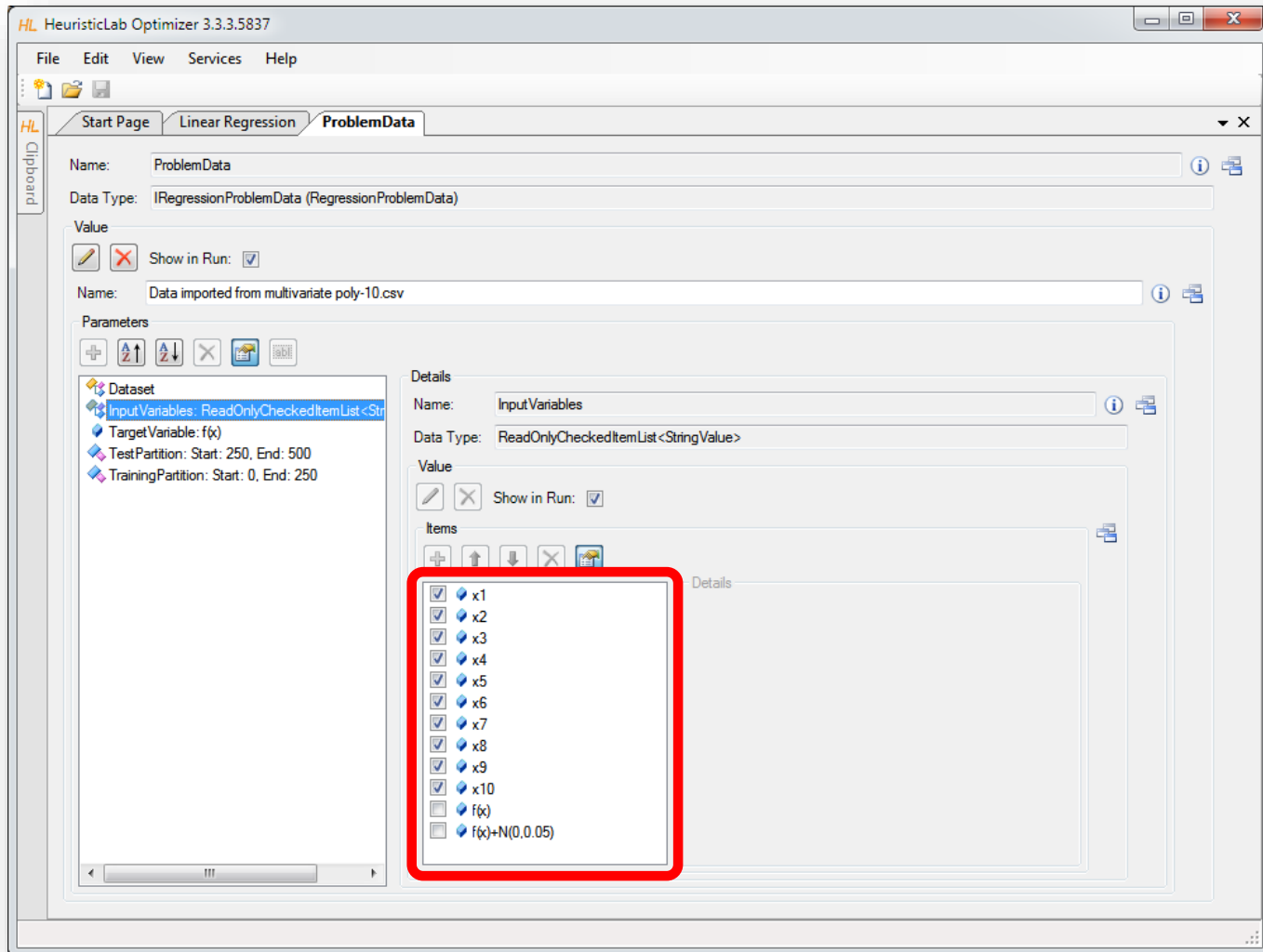
Columns: 12

	x1	x2	x3	x4	x5	x6	x7	x8	x9	x10
Row 1	-0.97...	0.26...	0.97...	0.35...	0.24...	-0.92...	-0.99...	0.63...	0.47...	0.417...
Row 2	-0.74...	-0.11...	0.73...	0.86...	-0.72...	0.03...	-0.05...	0.80...	0.25...	0.890...
Row 3	-0.44...	0.53...	0.33...	-0.07...	0.05...	0.80...	0.91...	0.01...	0.33...	-0.999...
Row 4	0.04...	-0.74...	0.51...	0.79...	-0.00...	0.41...	0.63...	0.01...	-0.02...	-0.855...
Row 5	0.51...	0.89...	-0.89...	0.39...	0.56...	0.81...	0.56...	0.81...	-0.94...	0.988...
Row 6	-0.89...	0.34...	0.66...	0.85...	0.01...	0.28...	0.32...	0.55...	-0.07...	-0.775...
Row 7	-0.00...	0.50...	-0.87...	-0.48...	0.62...	0.86...	-0.99...	0.59...	-0.71...	0.322...
Row 8	0.67...	-0.35...	0.14...	0.04...	-0.28...	-0.26...	0.49...	-0.01...	-0.08...	-0.235...

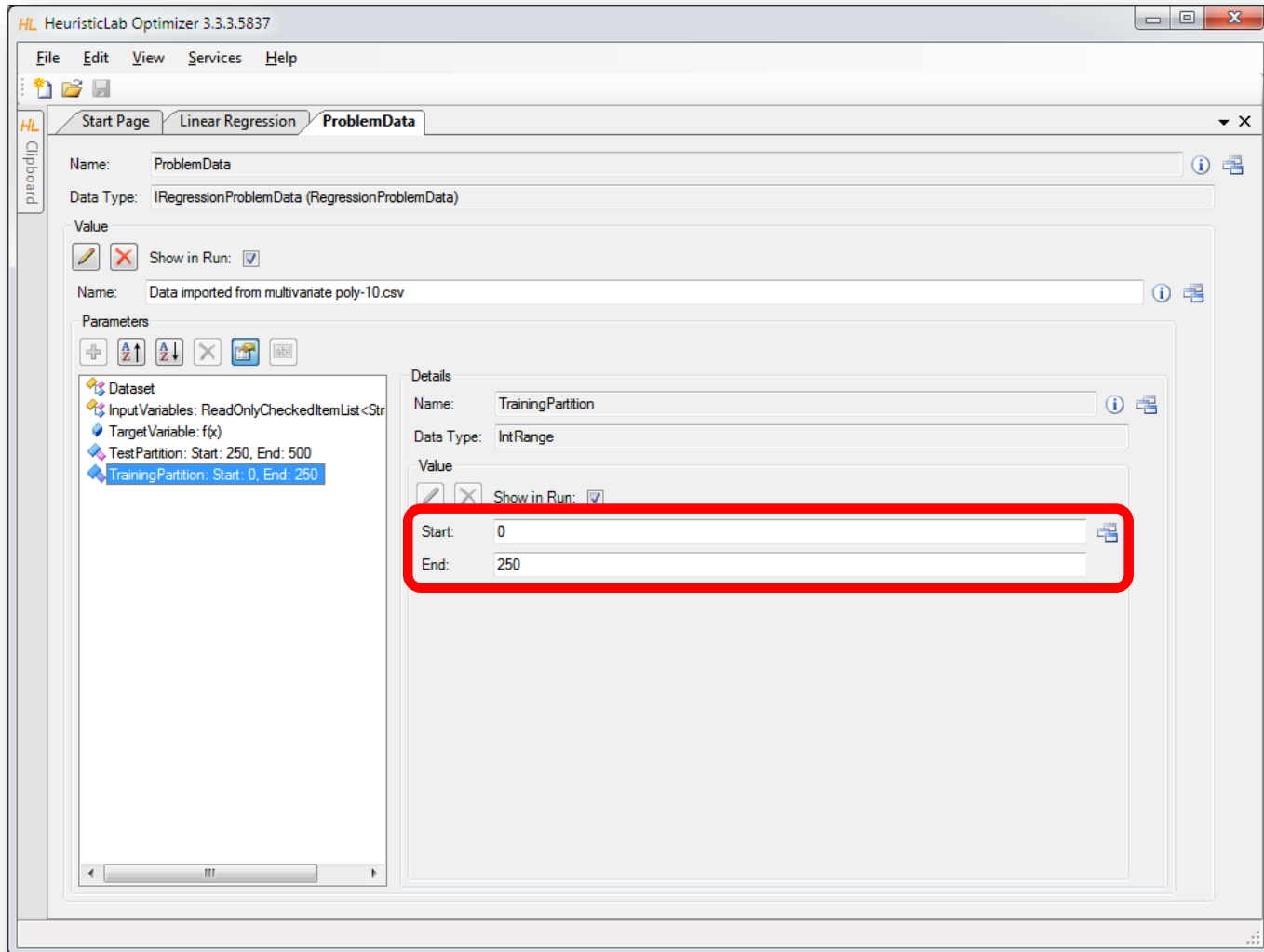
Set Target Variable



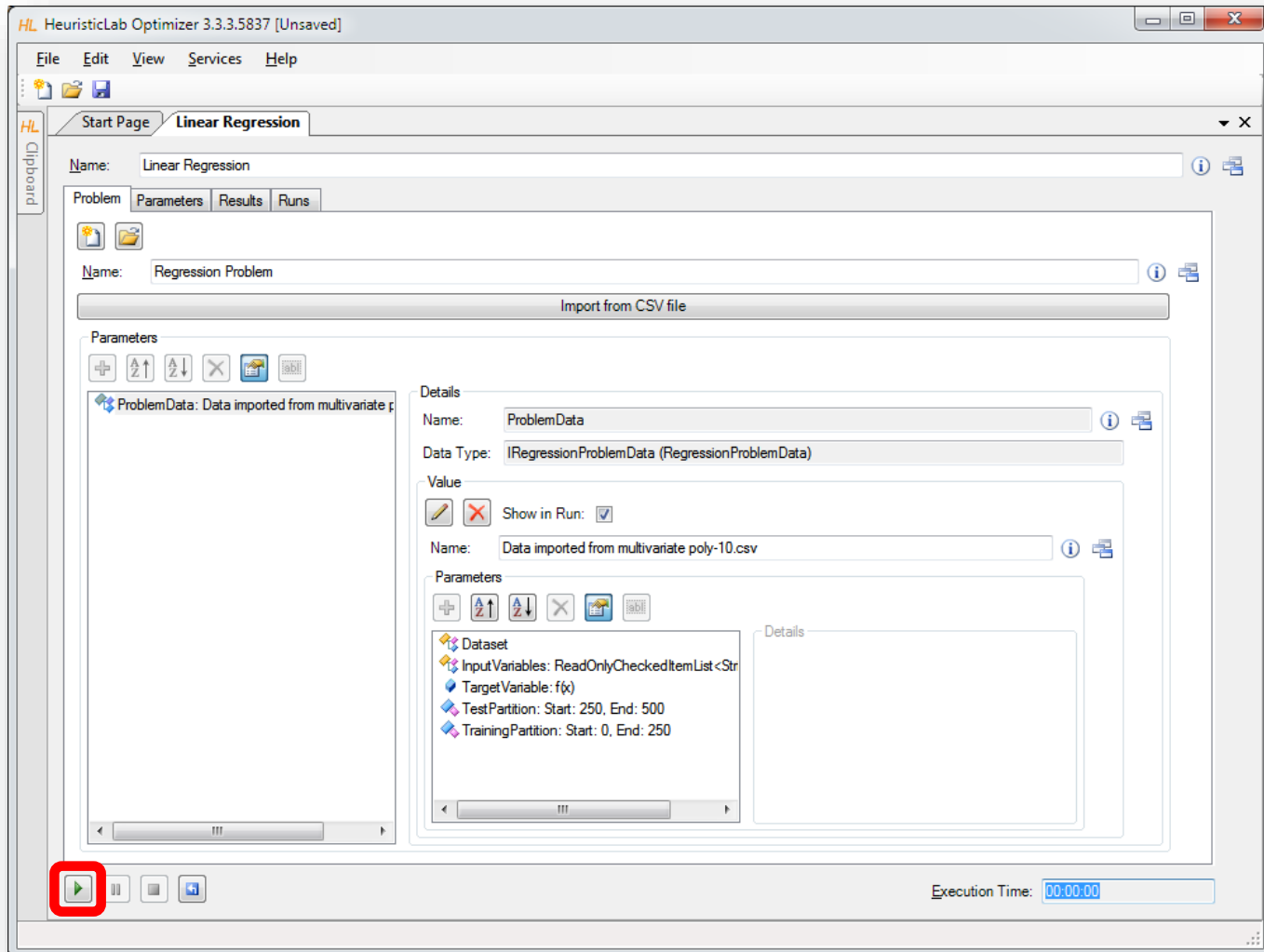
Select Input Variables



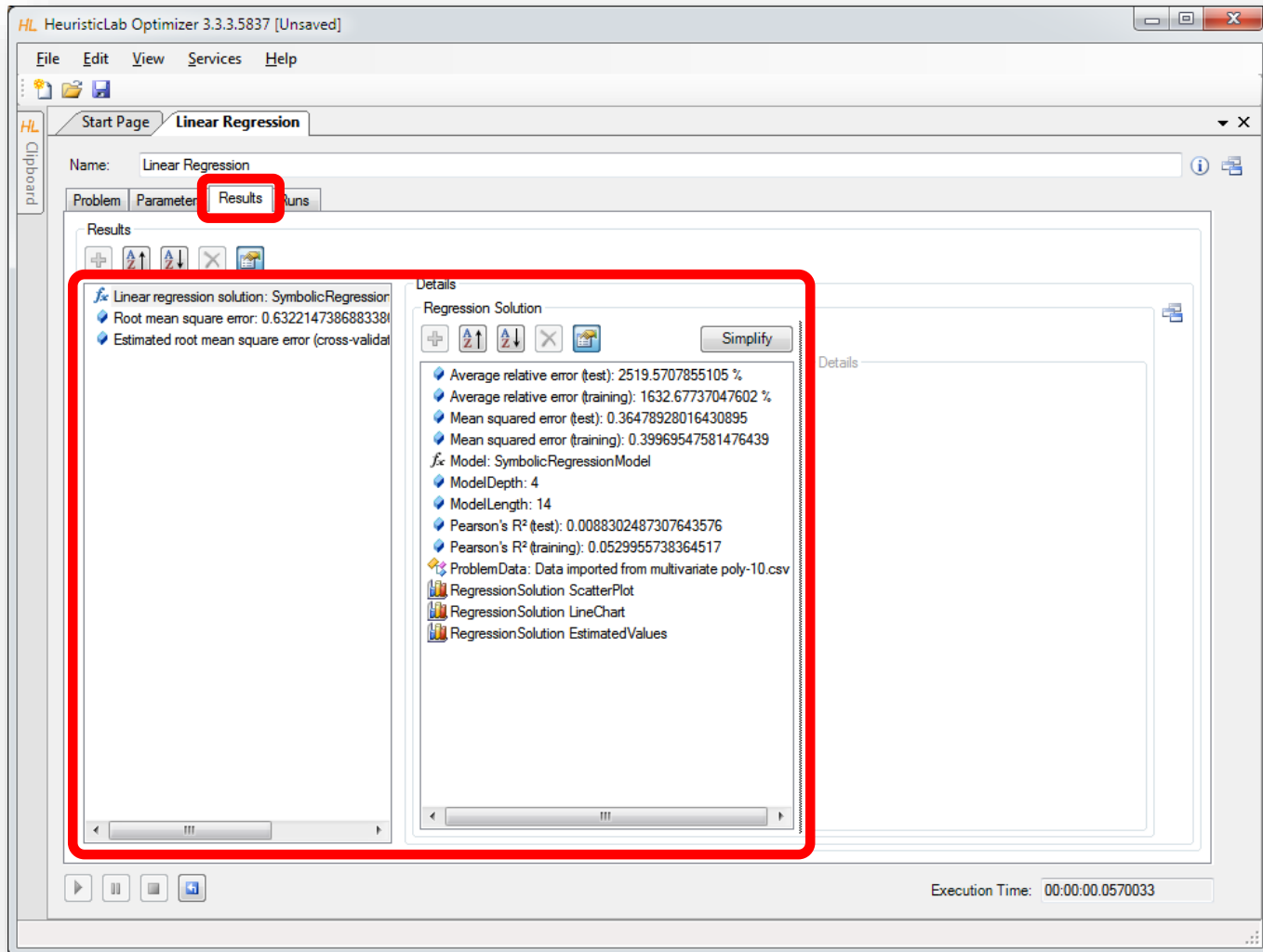
Configure Training and Test Partitions



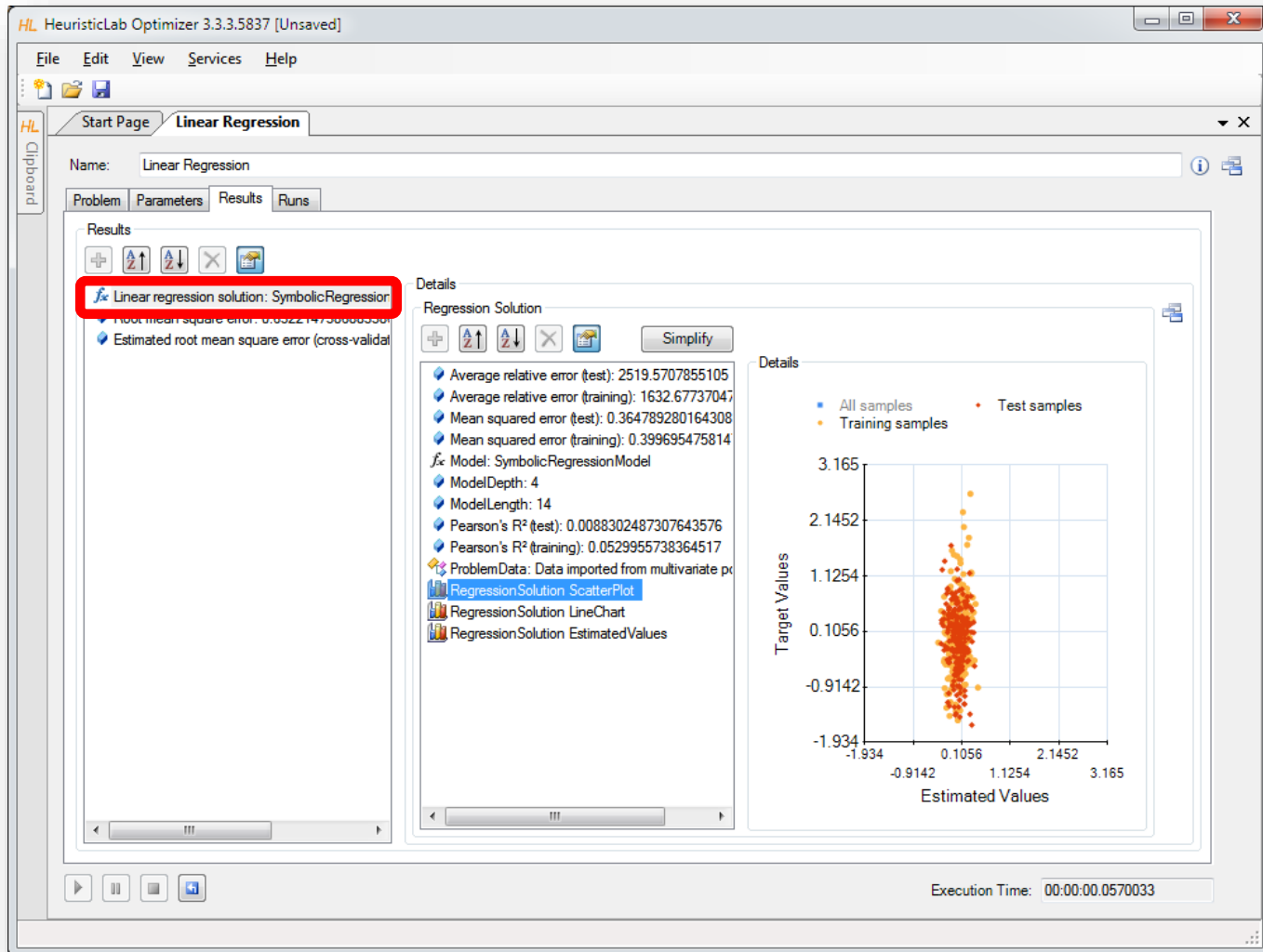
Run Linear Regression



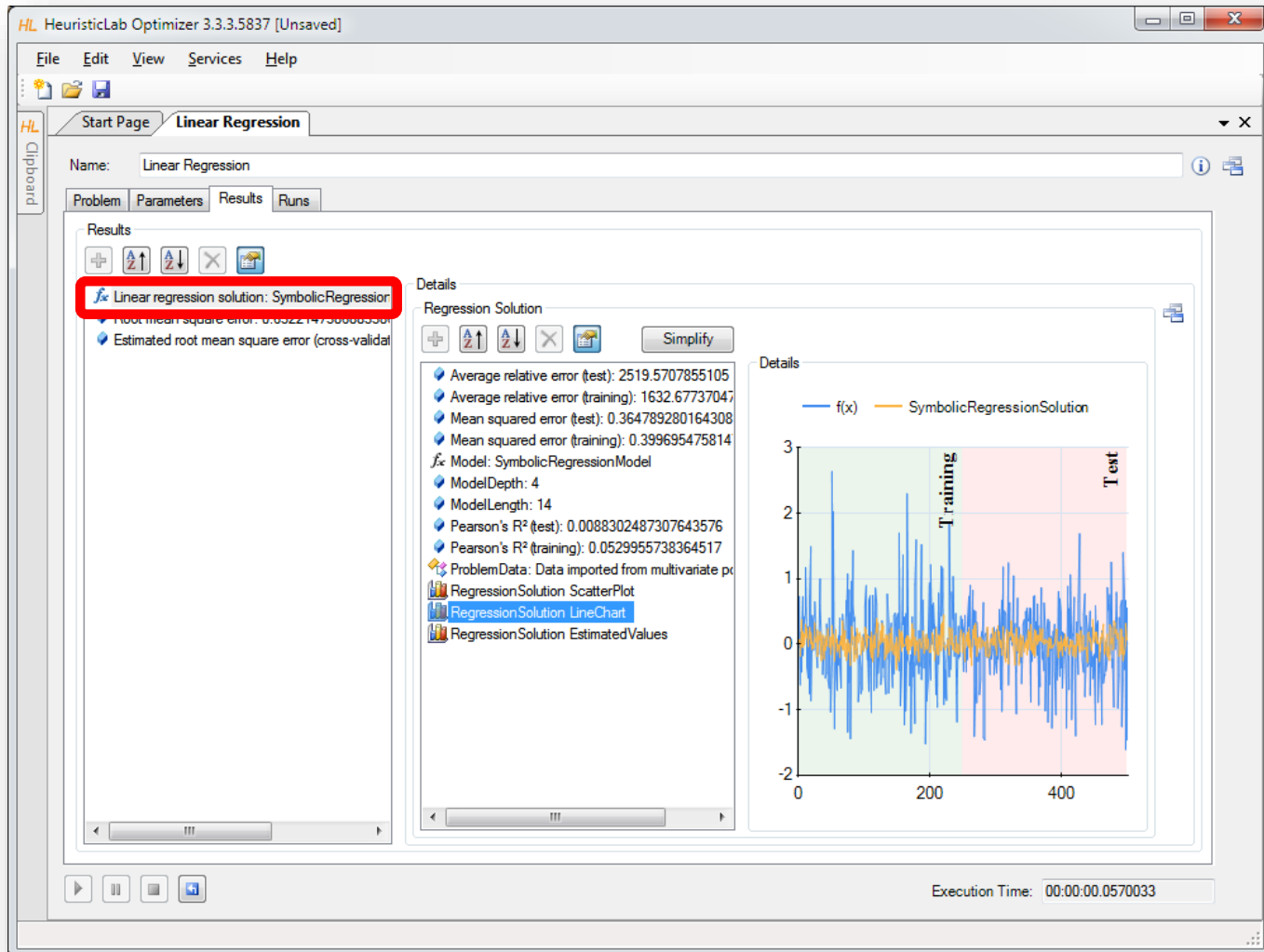
Inspect Results



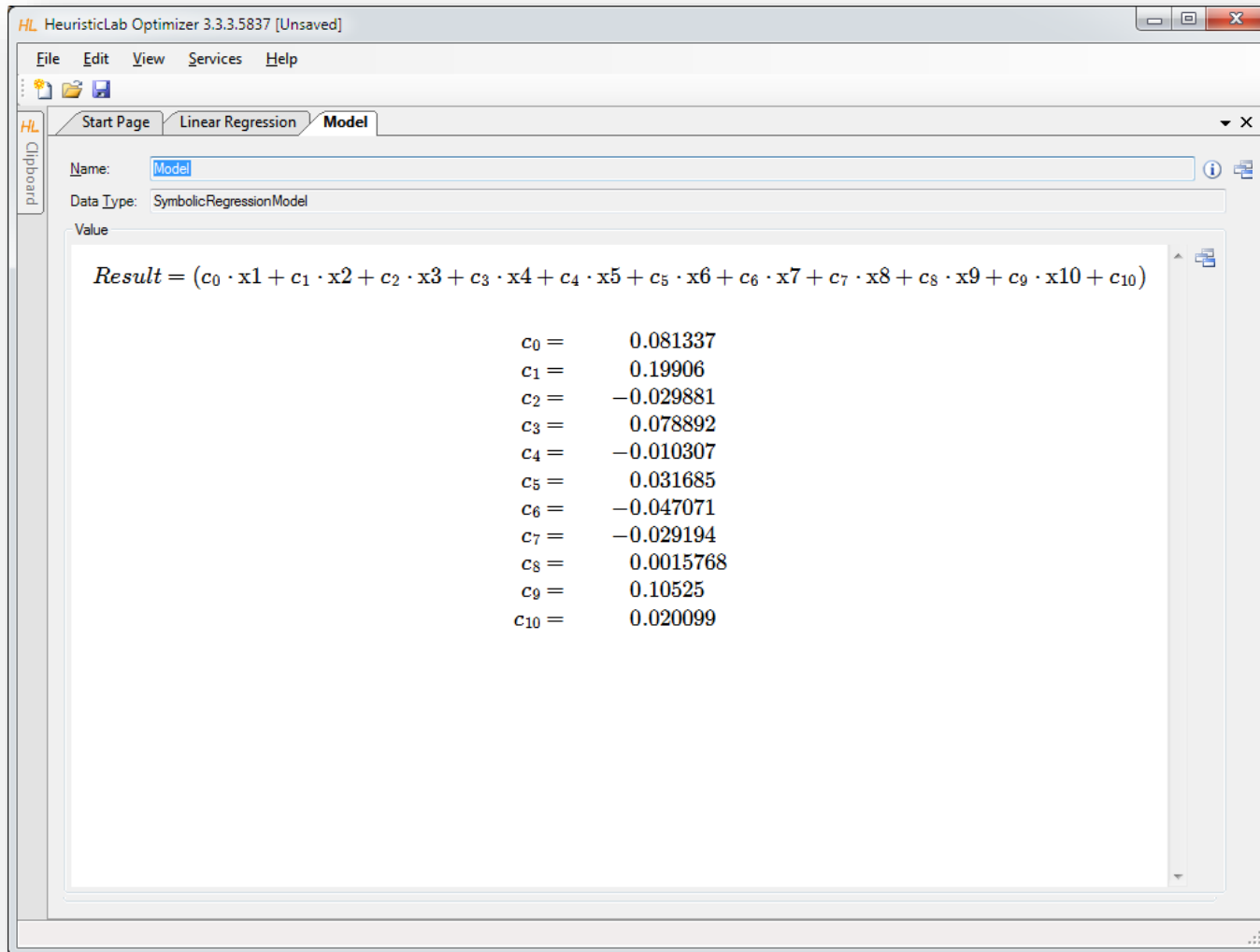
Inspect Scatterplot of Predicted and Target Values



Inspect Linechart



Inspect the Model



HL HeuristicLab Optimizer 3.3.3.5837 [Unsaved]

File Edit View Services Help

HL Start Page Linear Regression **Model**

Name: Model

Data Type: SymbolicRegressionModel

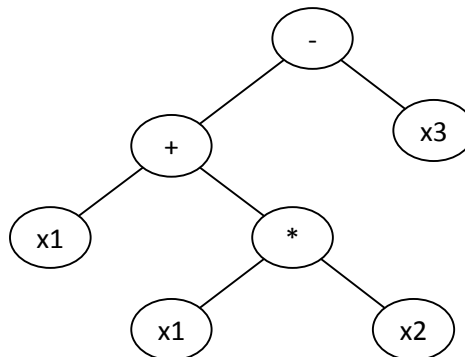
Value

$$\text{Result} = (c_0 \cdot x_1 + c_1 \cdot x_2 + c_2 \cdot x_3 + c_3 \cdot x_4 + c_4 \cdot x_5 + c_5 \cdot x_6 + c_6 \cdot x_7 + c_7 \cdot x_8 + c_8 \cdot x_9 + c_9 \cdot x_{10} + c_{10})$$

c_0	=	0.081337
c_1	=	0.19906
c_2	=	-0.029881
c_3	=	0.078892
c_4	=	-0.010307
c_5	=	0.031685
c_6	=	-0.047071
c_7	=	-0.029194
c_8	=	0.0015768
c_9	=	0.10525
c_{10}	=	0.020099

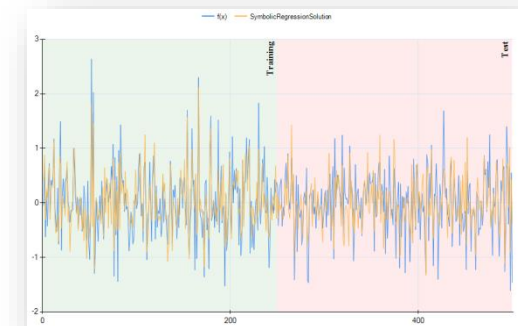
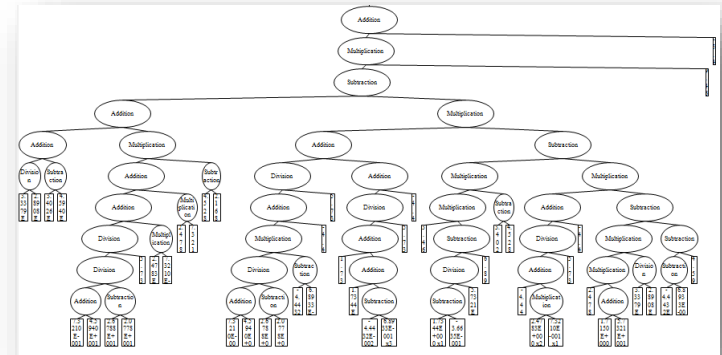
Symbolic Regression with HeuristicLab

- Linear regression produced an inaccurate model.
- Next: produce a nonlinear symbolic regression model using genetic programming
- Genetic programming
 - evolve variable-length models
 - model representation: symbolic expression tree
 - structure and model parameters are evolved side-by-side
 - white-box models

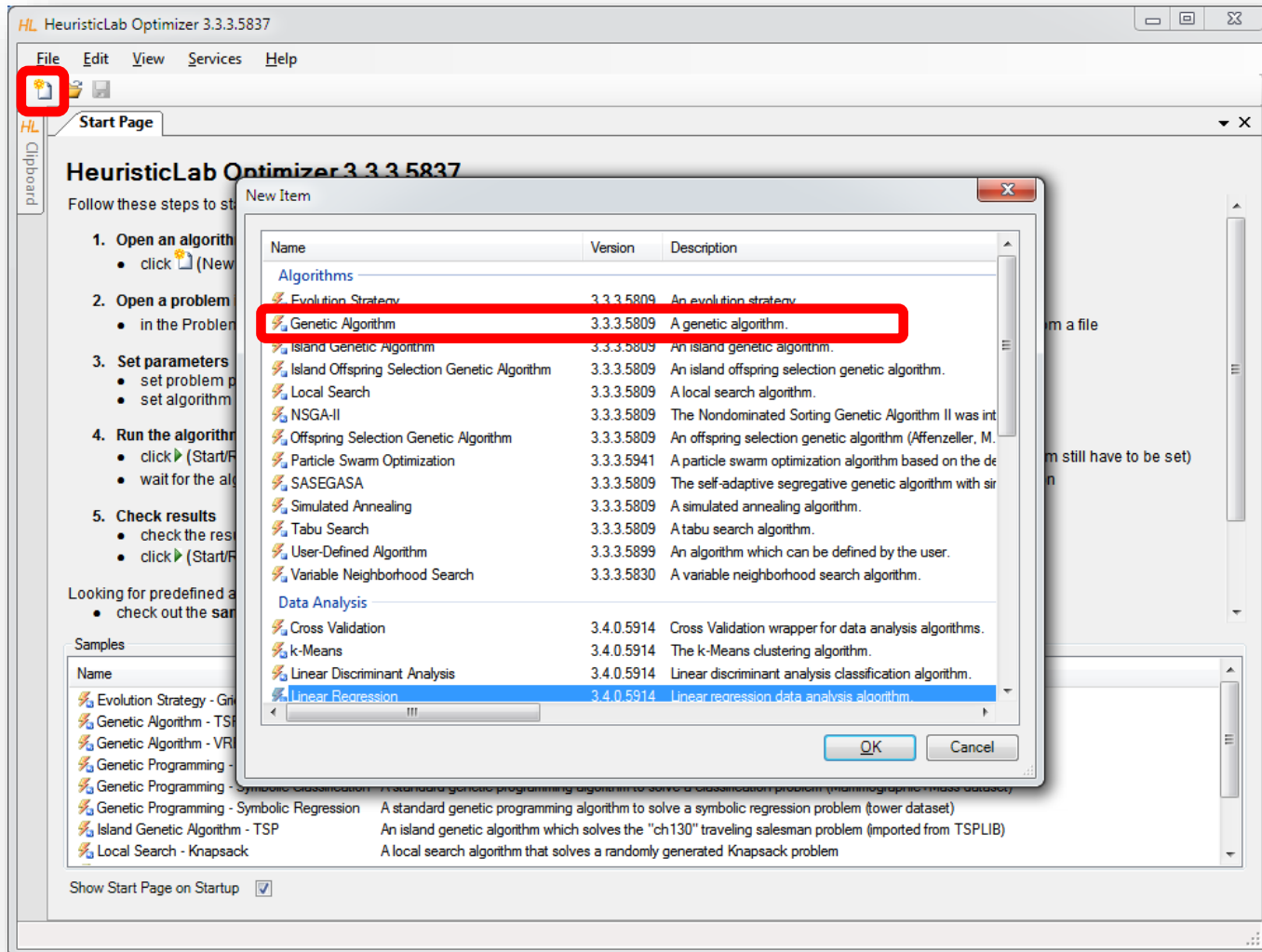


Symbolic Regression with HeuristicLab

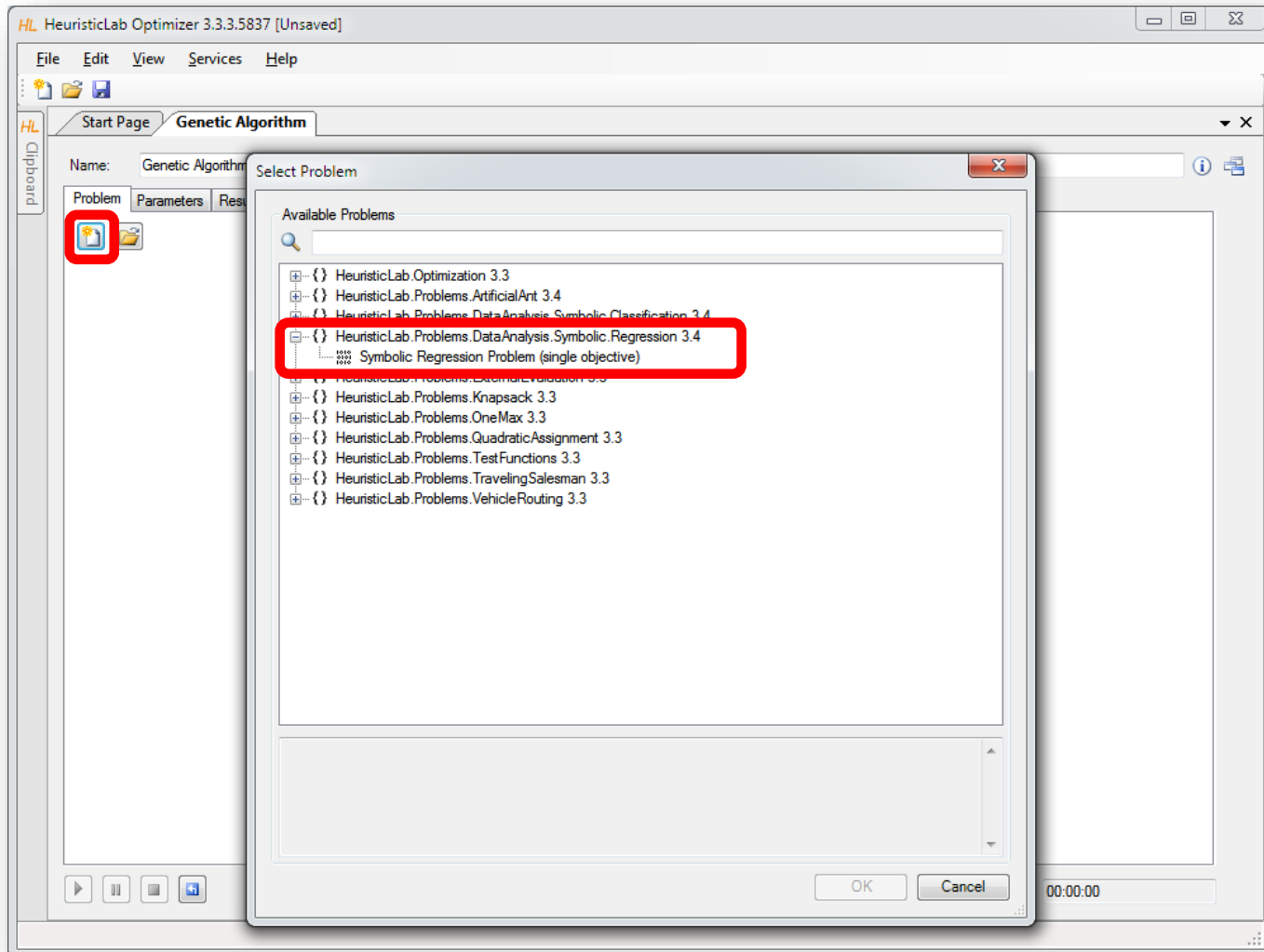
- Demonstration
 - problem configuration
 - function set and terminal set
 - model size constraints
 - evaluation
- Algorithm configuration
 - selection
 - mutation
- Analysis of results
 - model accuracy
 - model structure and parameters



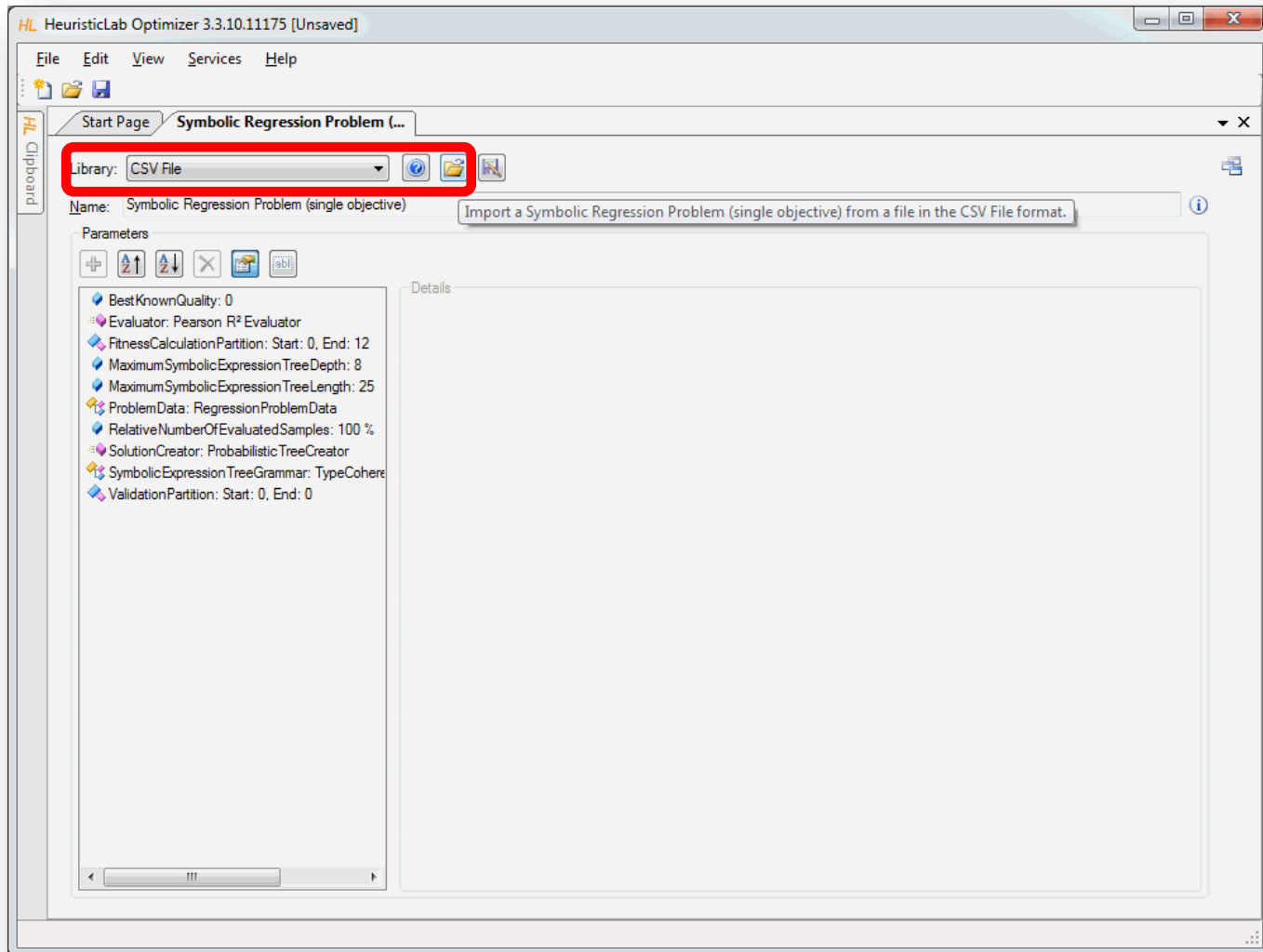
Create New Genetic Algorithm



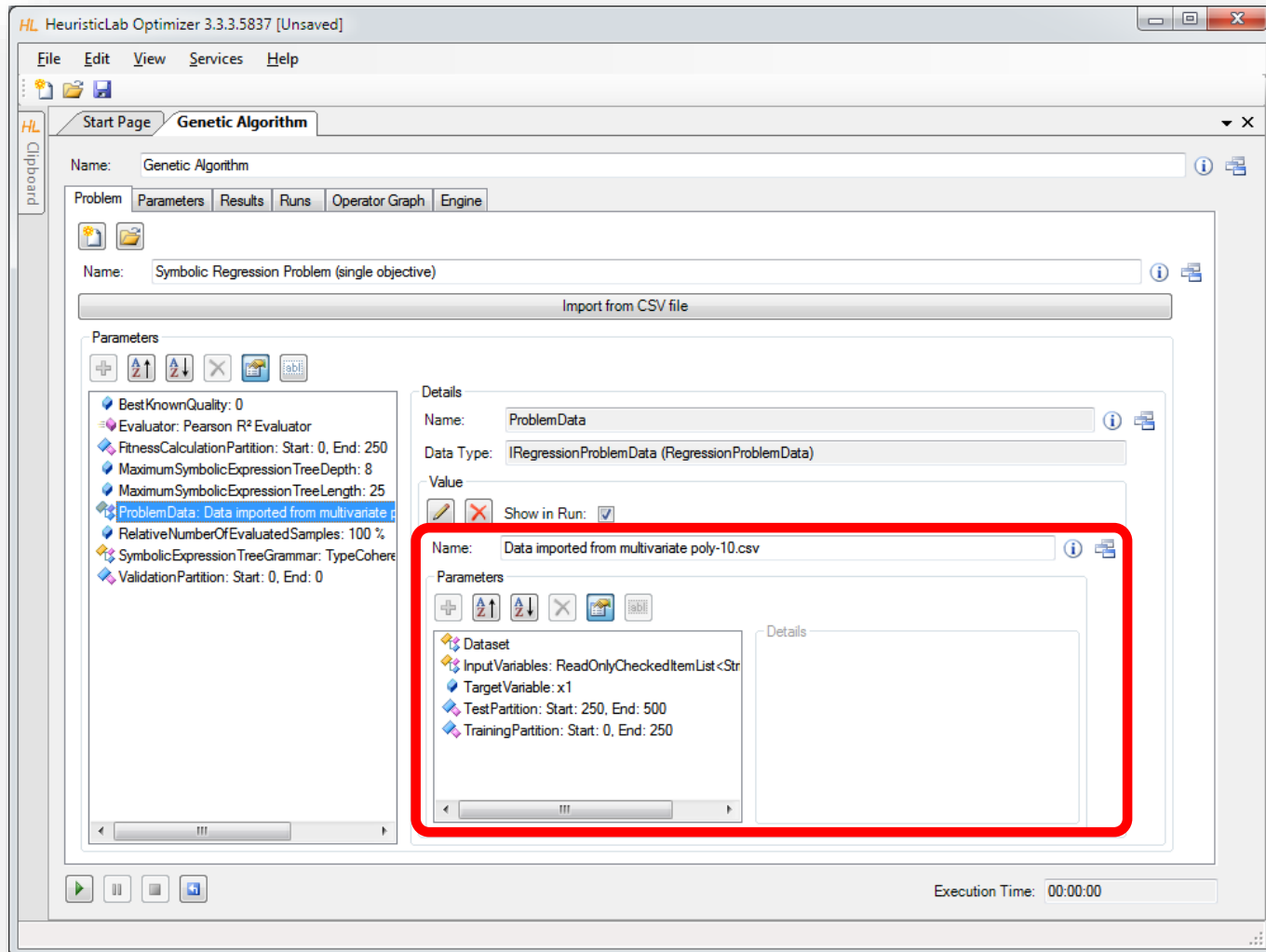
Create New Symbolic Regression Problem



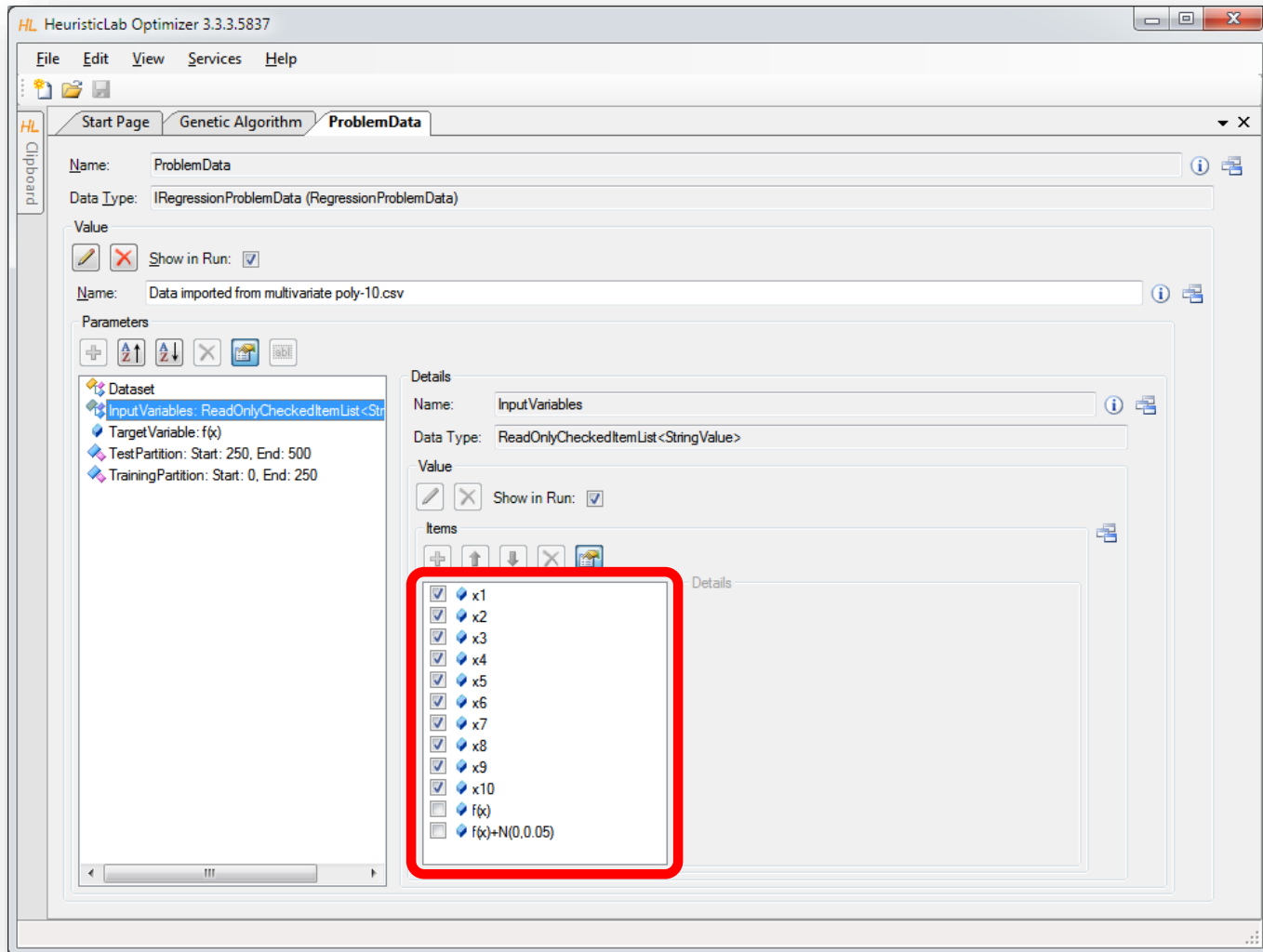
Import Data



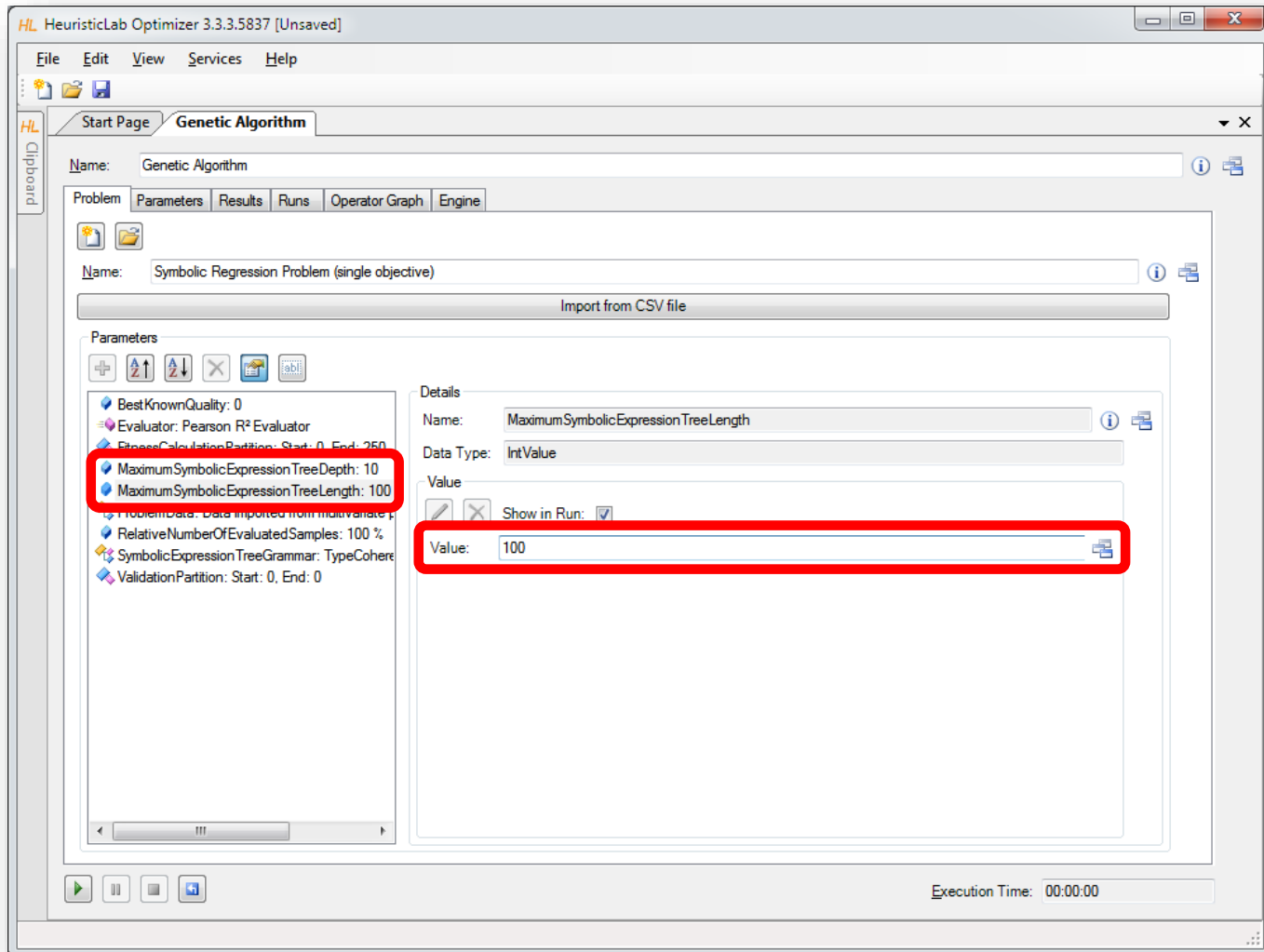
Inspect Data and Configure Dataset



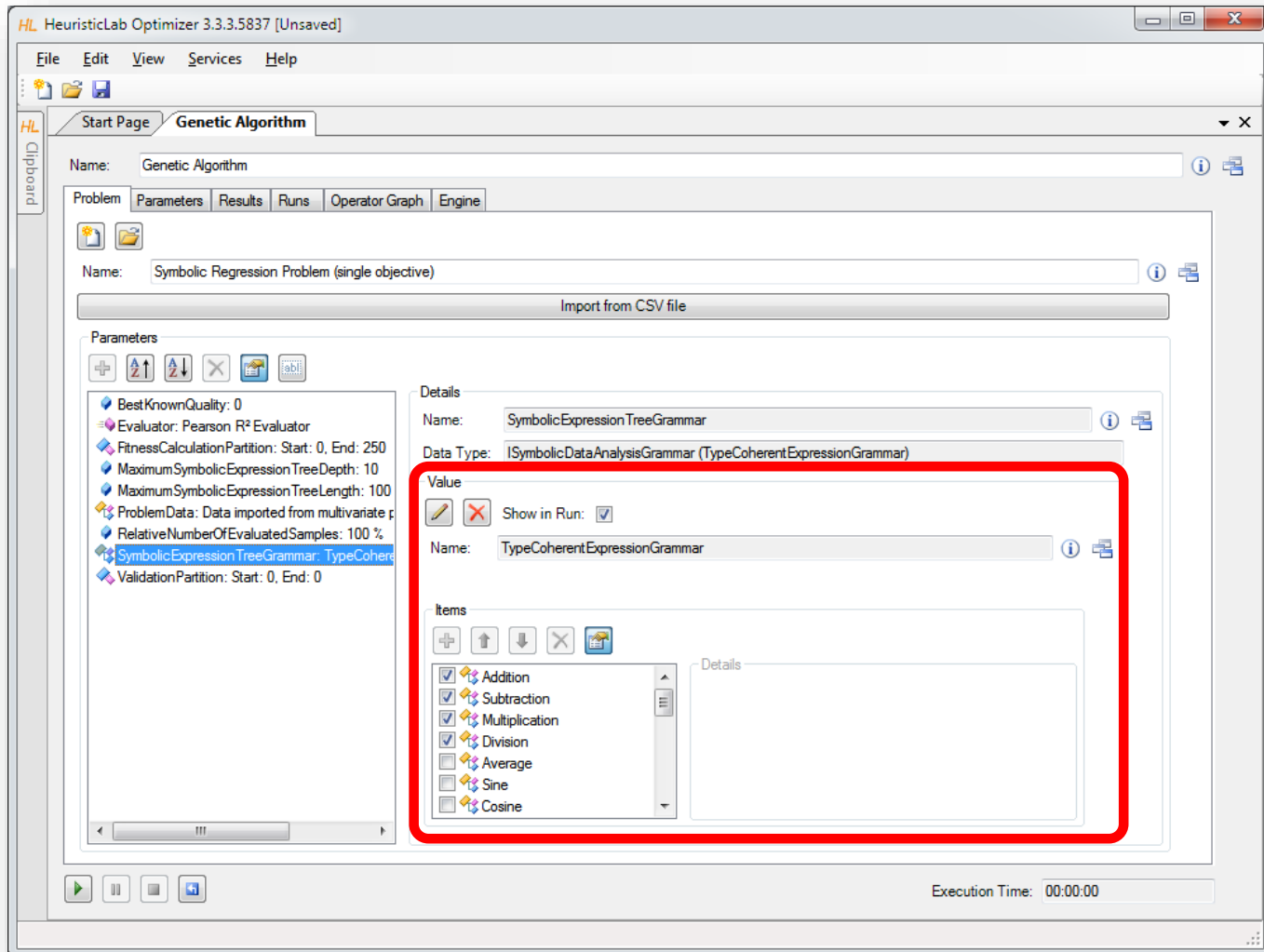
Set Target and Input Variables



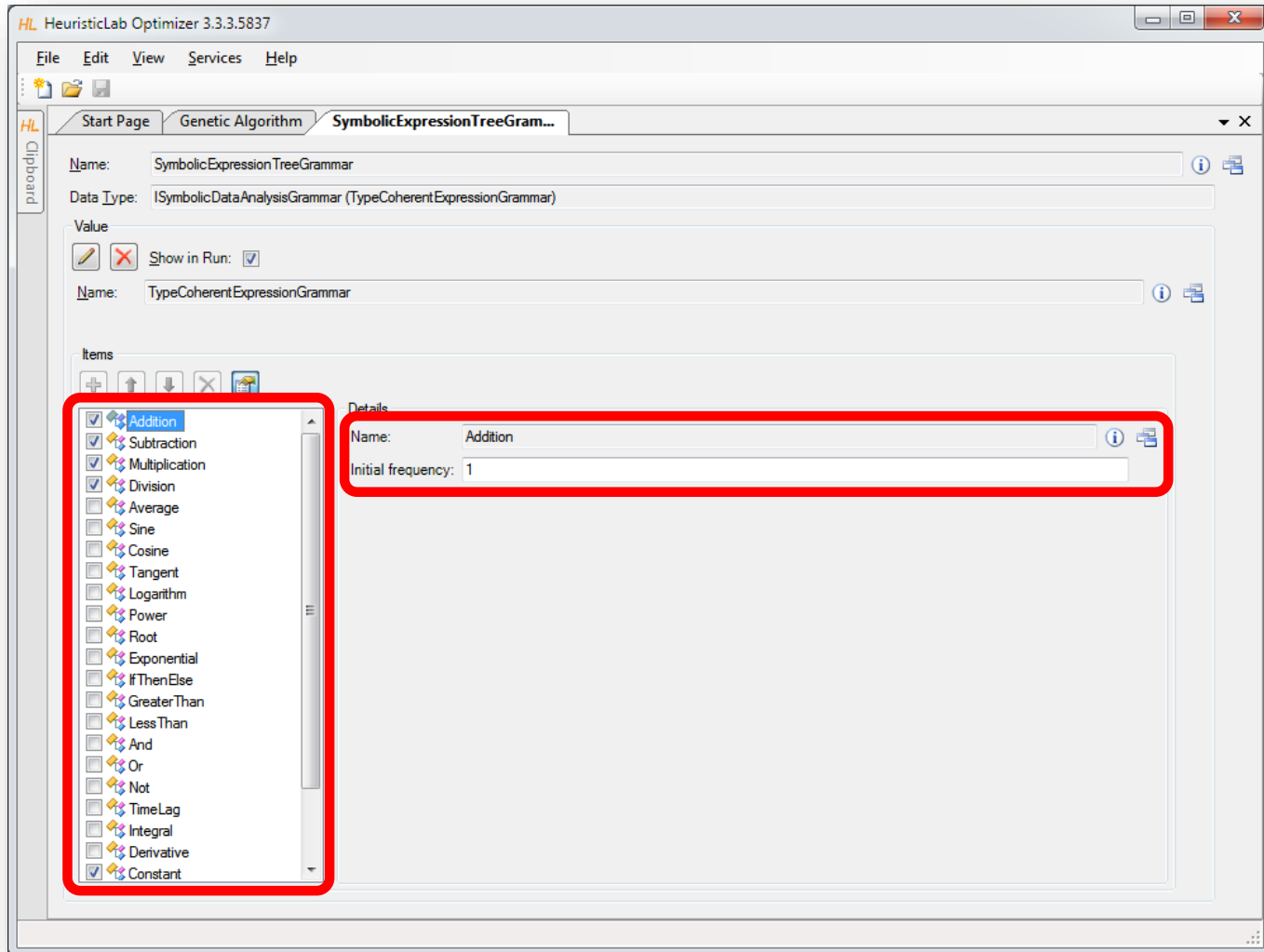
Configure Maximal Model Depth and Length



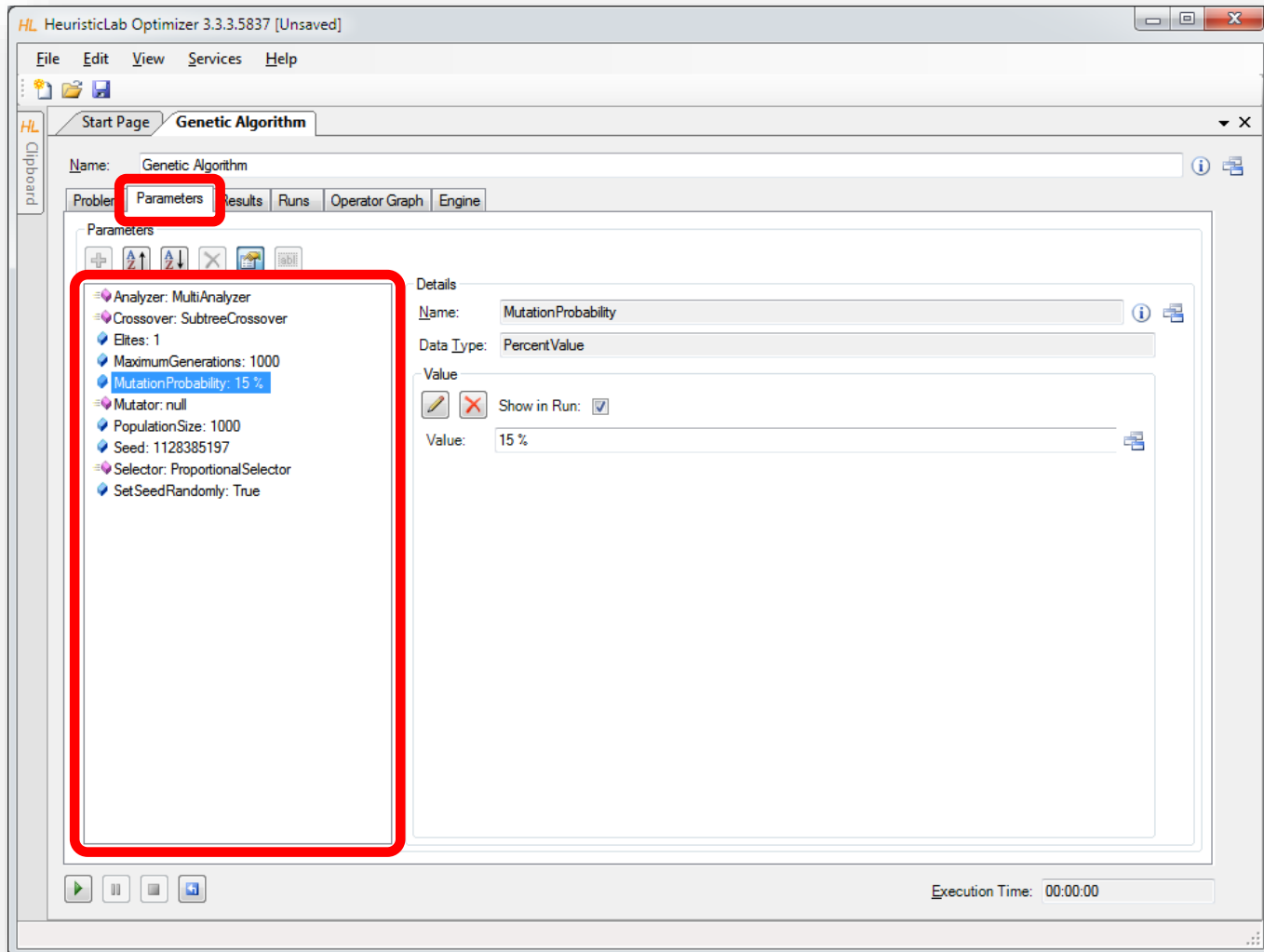
Configure Function Set (Grammar)



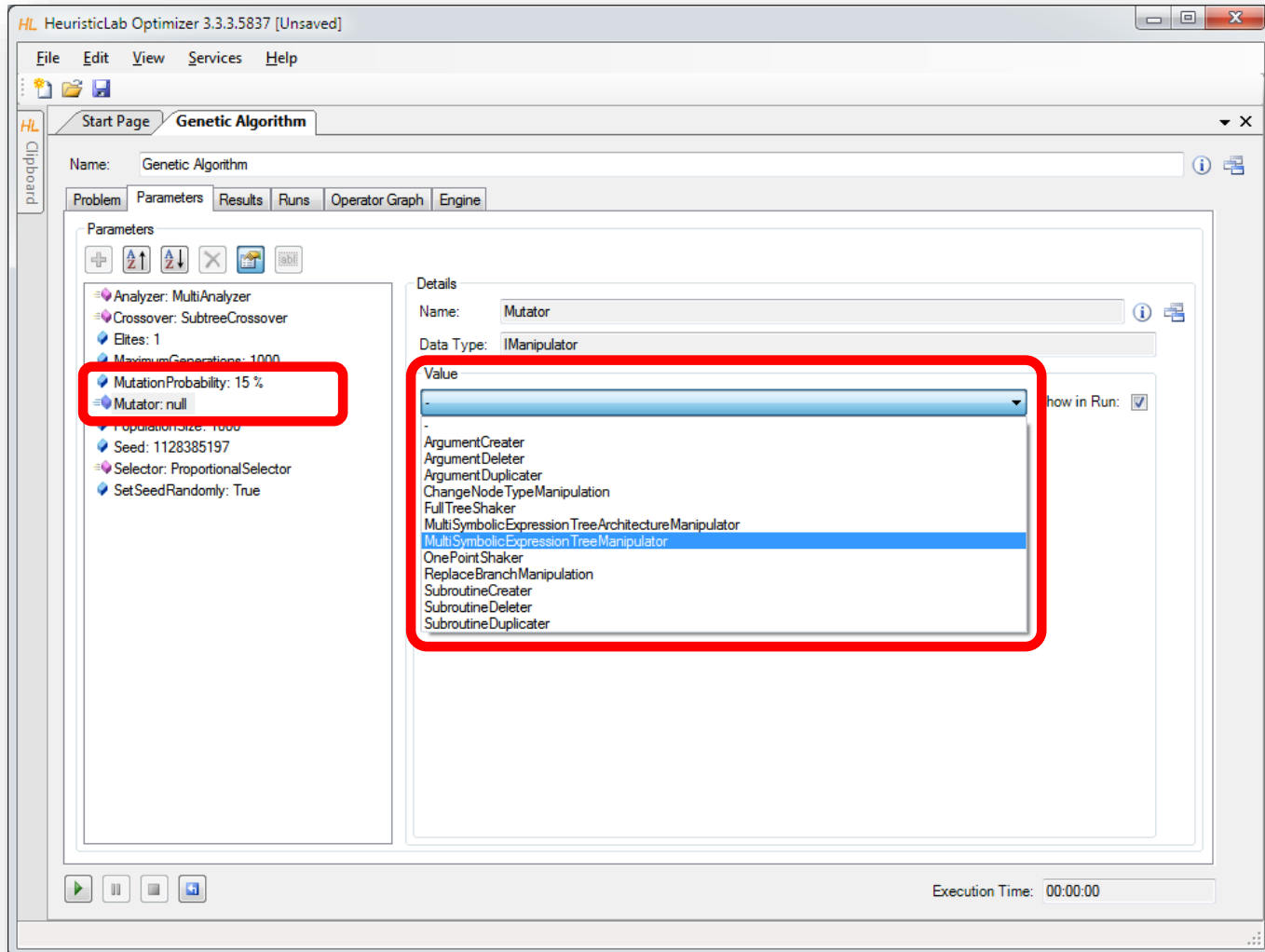
Configure Function Set (Grammar)



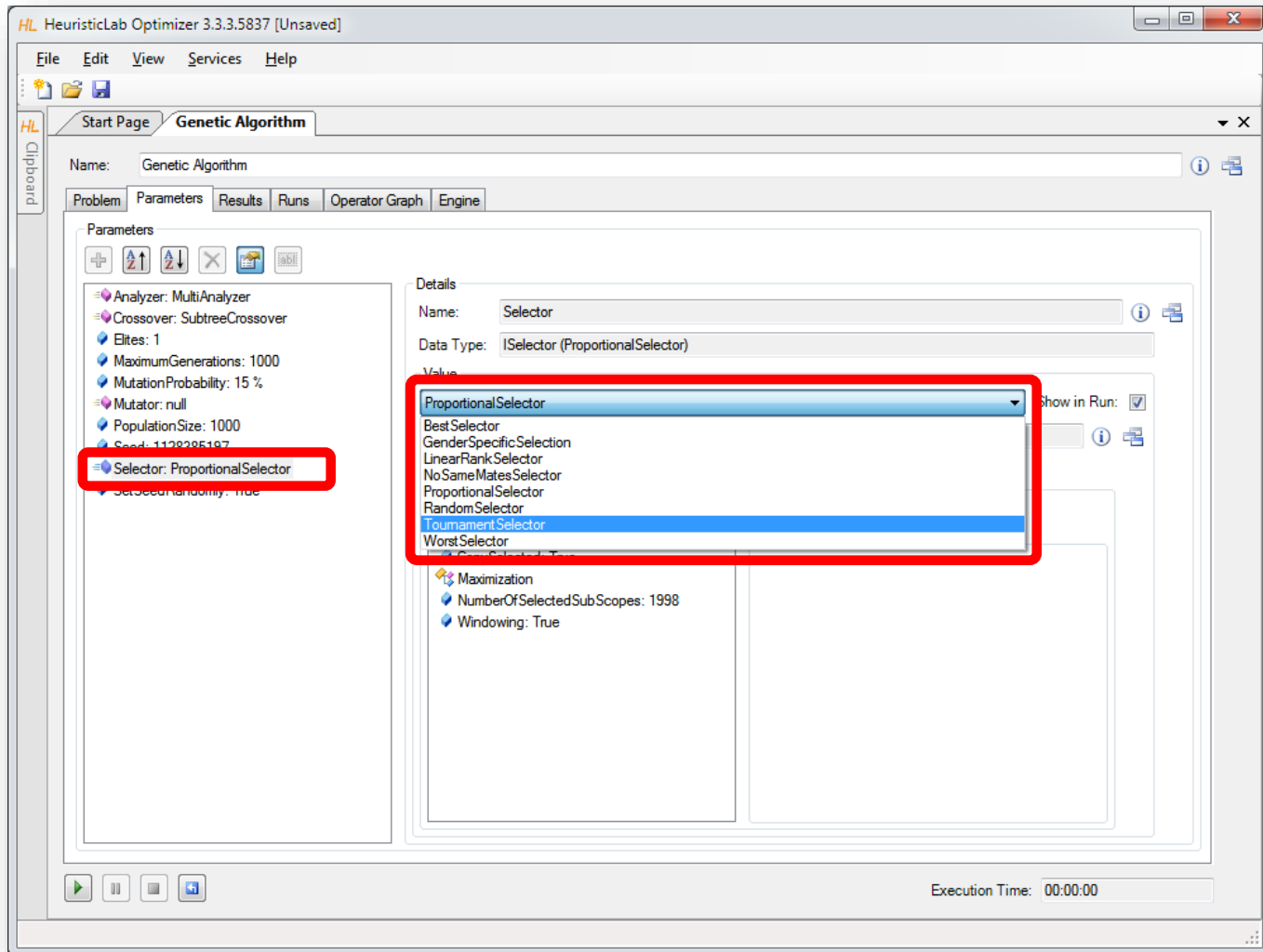
Configure Algorithm Parameters



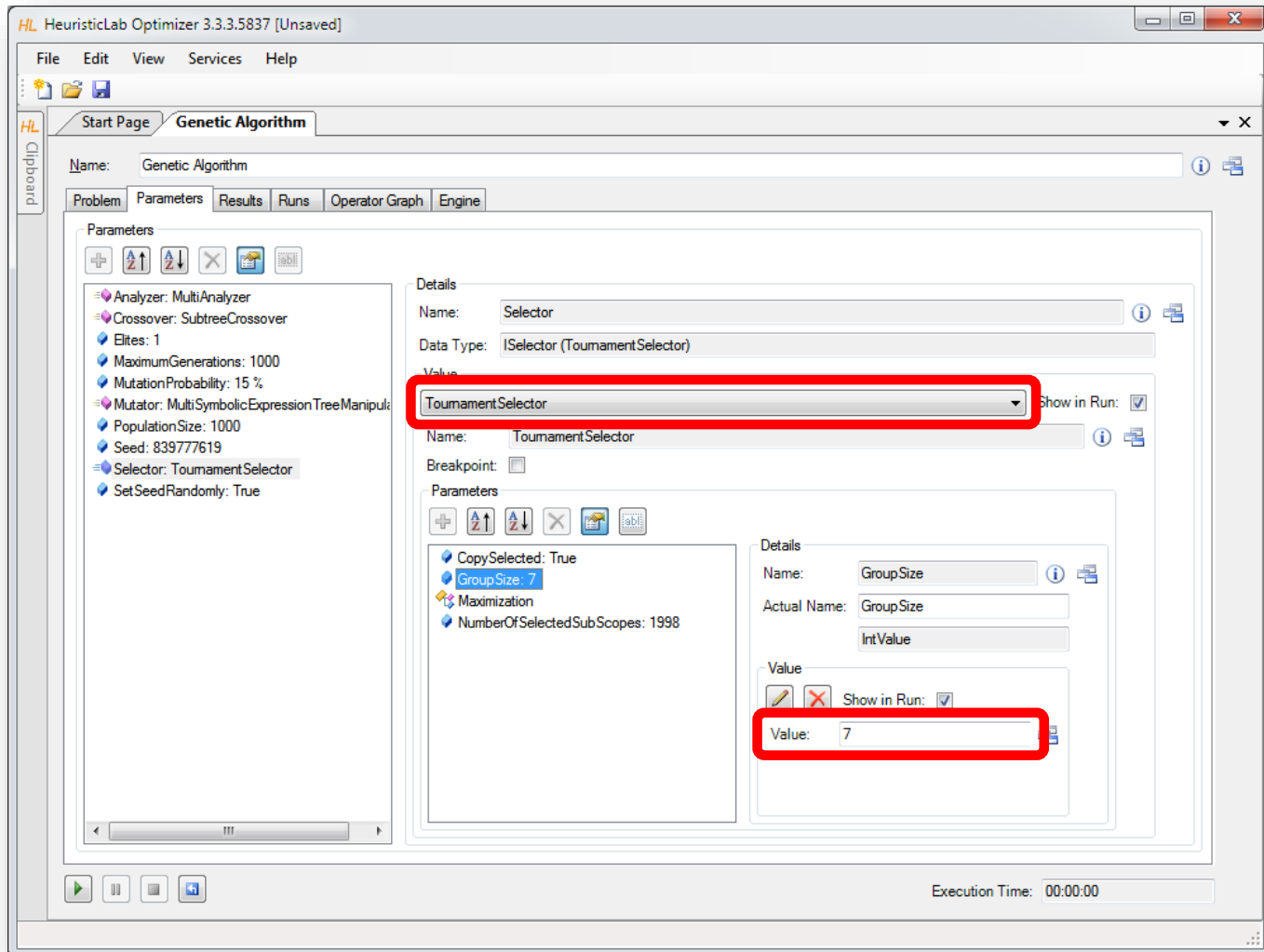
Configure Mutation Operator



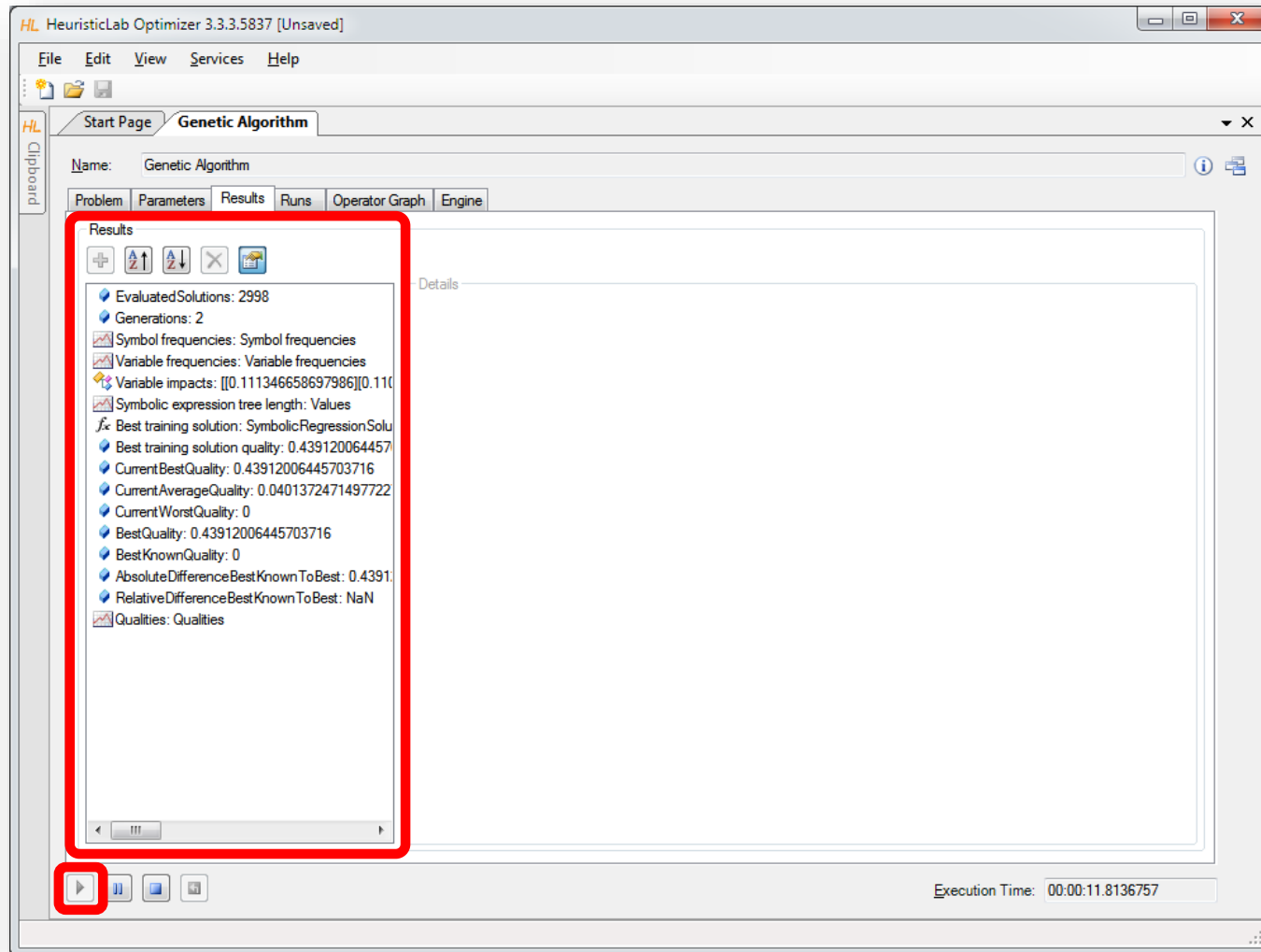
Configure Selection Operator



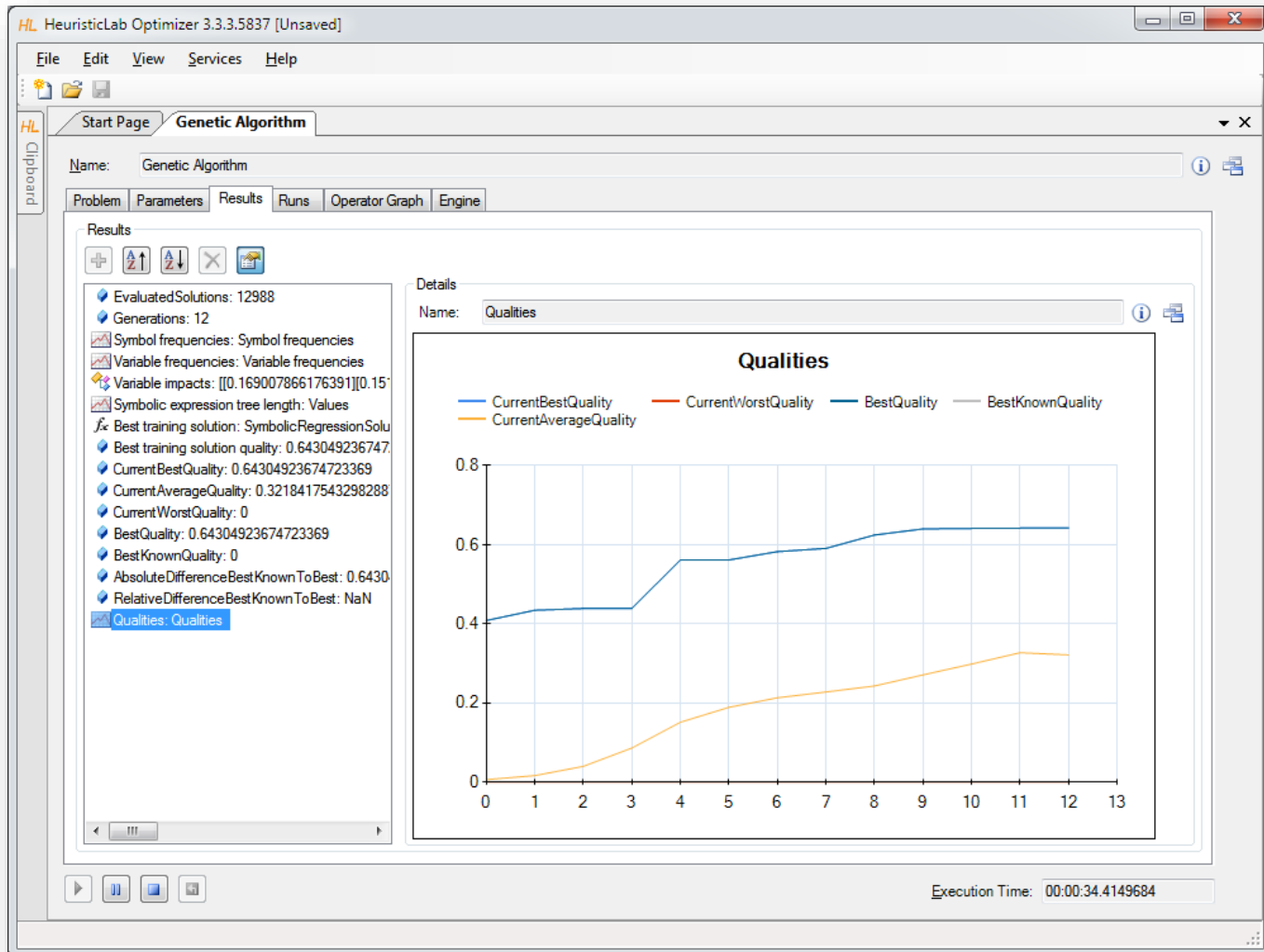
Configure Tournament Group Size



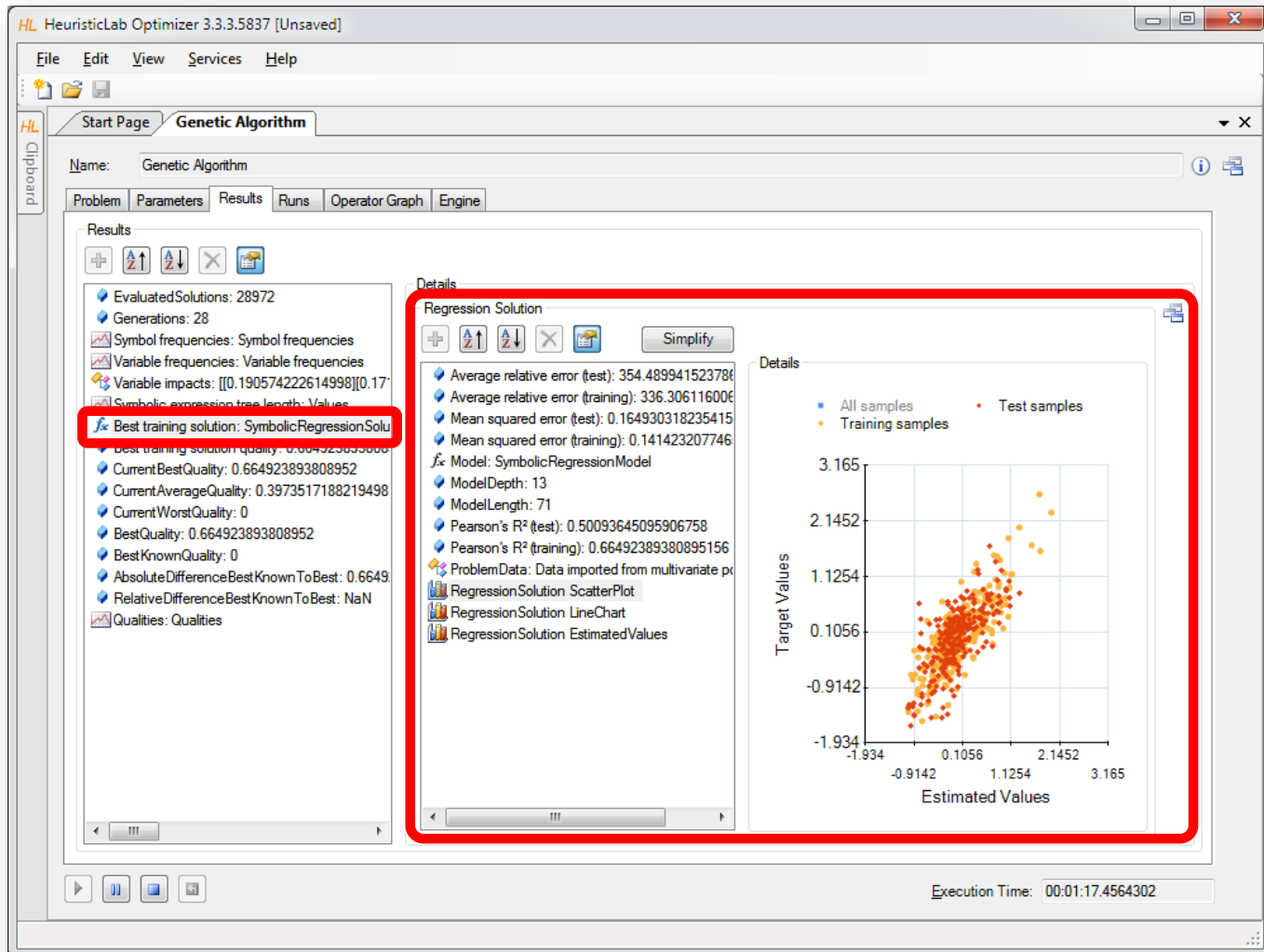
Start Algorithm and Inspect Results



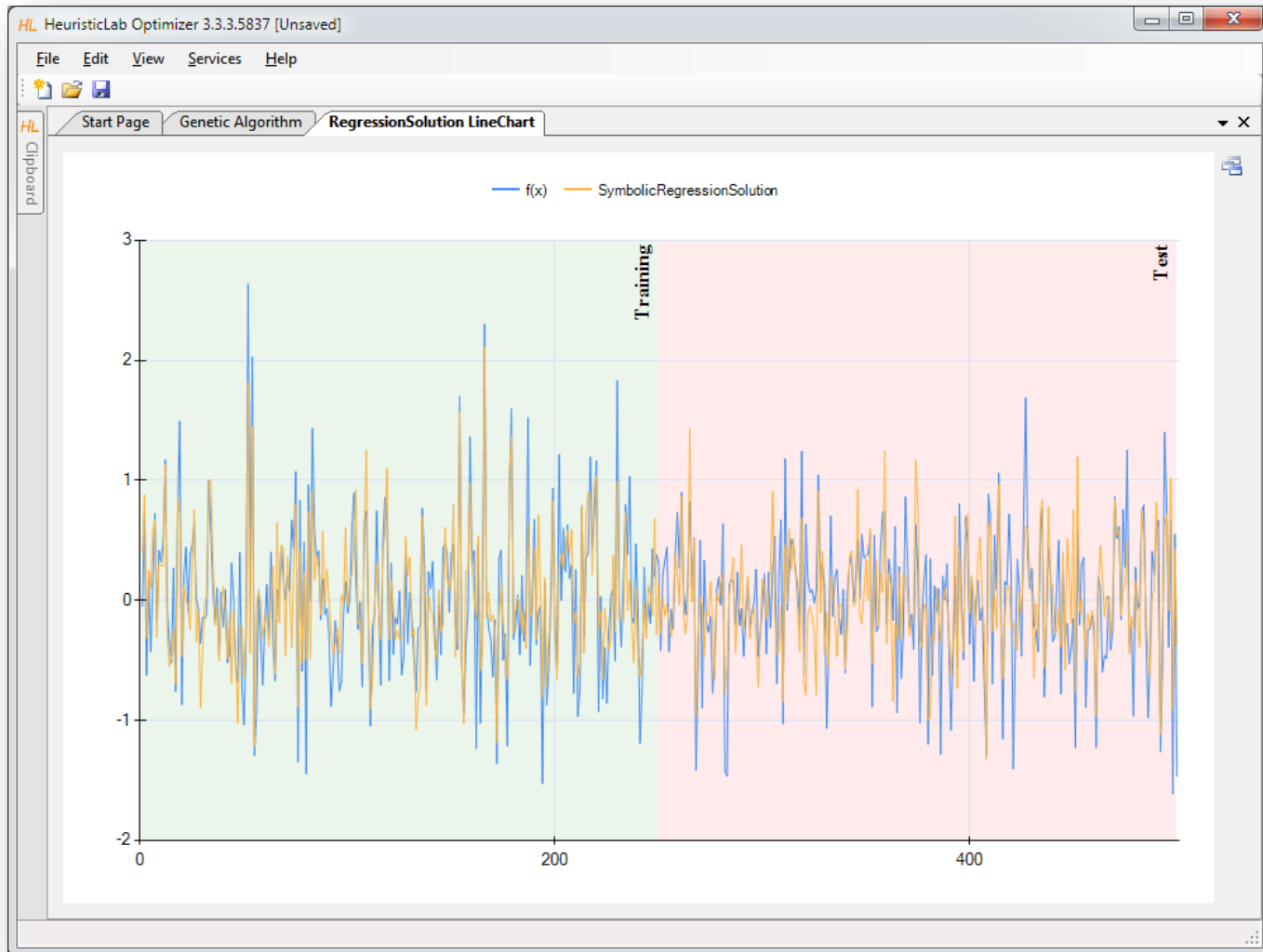
Inspect Quality Chart



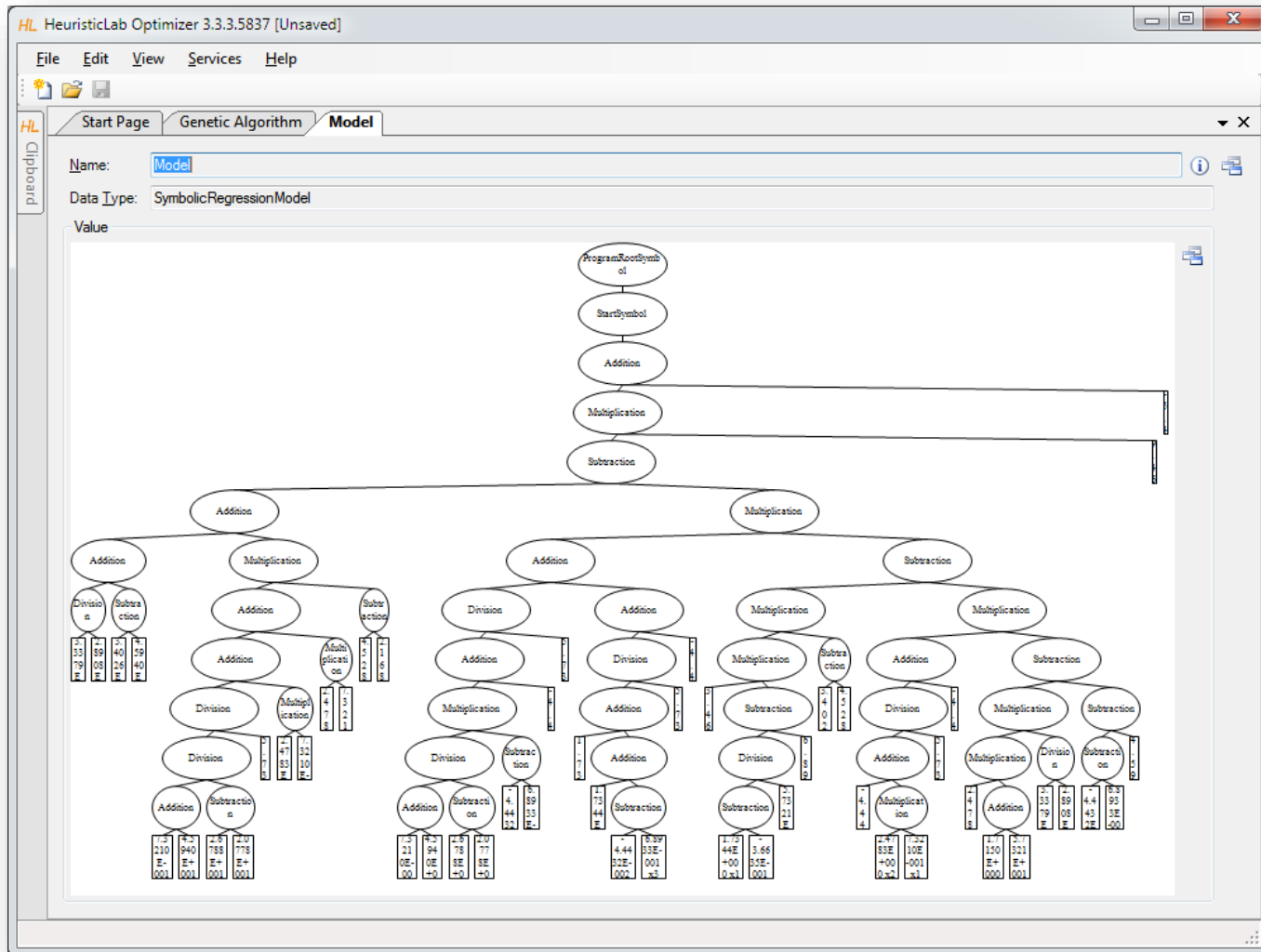
Inspect Best Model on Training Partition



Inspect Linechart of Best Model on Training Partition

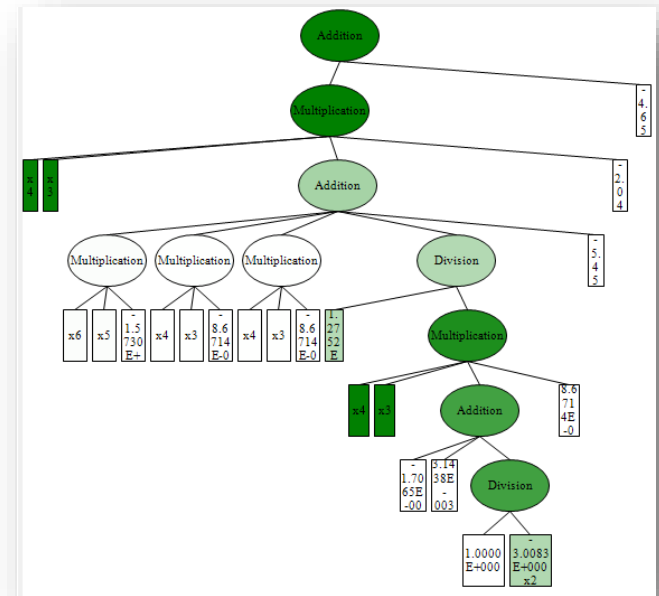


Inspect Structure of Best Model on Training Partition



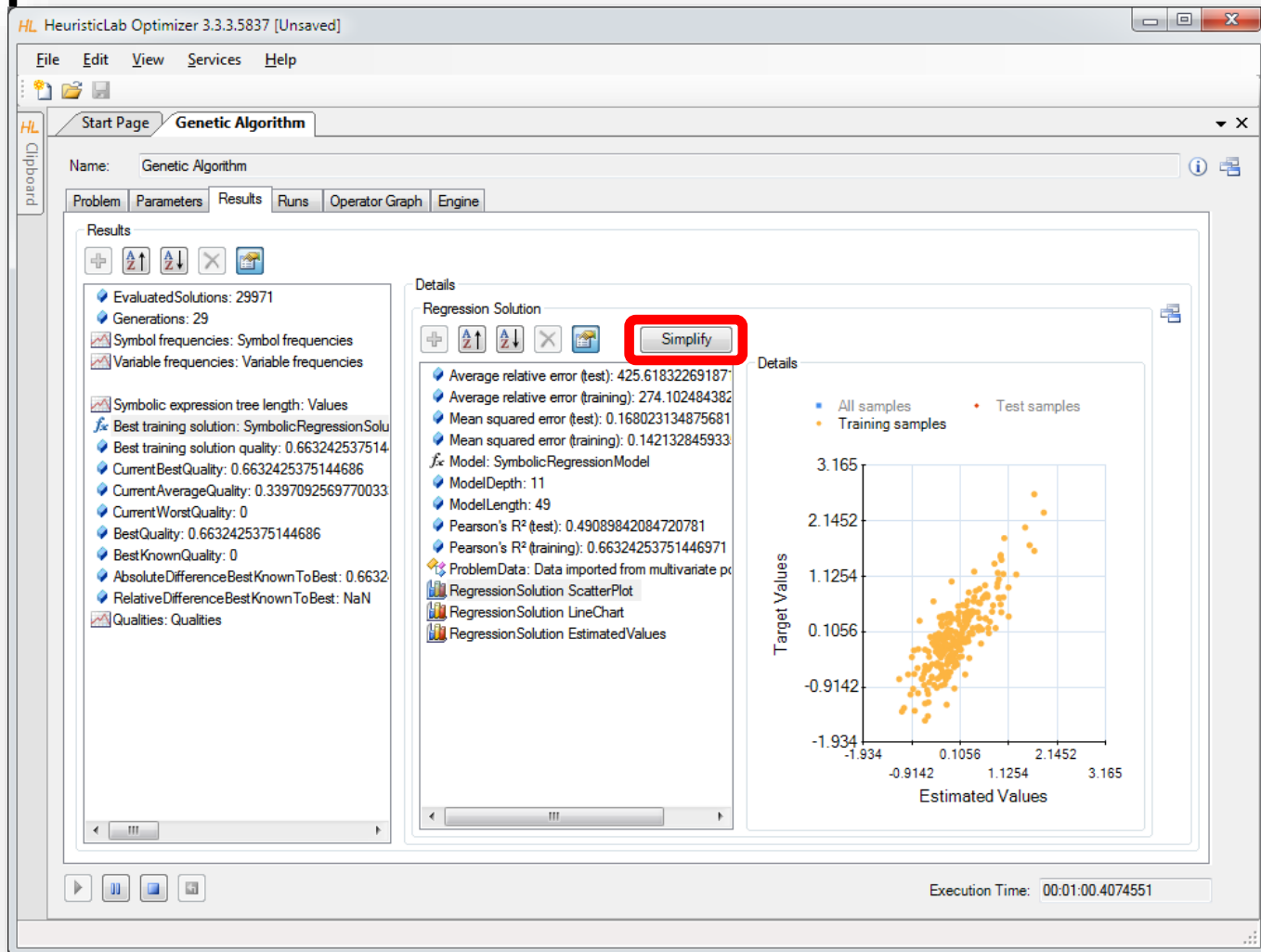
Model Simplification and Export

- Demonstration
 - automatic simplification
 - visualization of node impacts
 - manual simplification
 - online update of results
 - model export
 - Excel
 - MATLAB
 - LaTeX

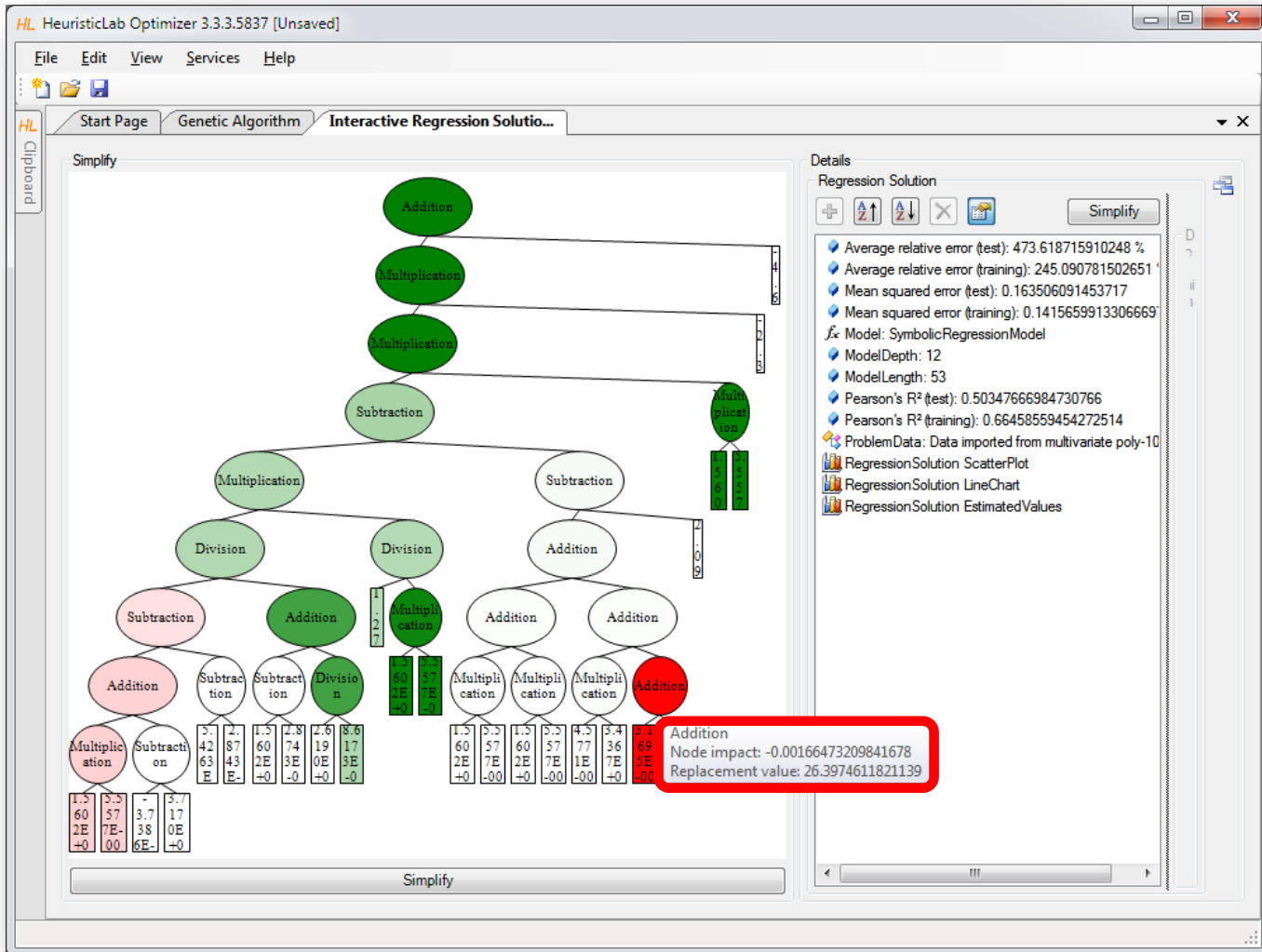


$$\begin{aligned}
 & \text{Result} = x_4(t) \cdot x_3(t) \cdot c_{20} \tag{13} \\
 & \cdot \left(x_6(t) \cdot x_5(t) \cdot c_4 + x_4(t) \cdot x_3(t) \cdot c_7 + x_4(t) \cdot x_3(t) \cdot c_{10} + \frac{c_{11} x_1(t)}{x_4(t) \cdot x_3(t) \cdot \left(c_{14} x_4(t) + c_{15} x_5(t) + \frac{1}{c_{17} x_2(t)} \right) \cdot c_{18}} + c_{19} \right) + c_{21} \\
 & \tag{14}
 \end{aligned}$$

Detailed Model Analysis and Simplification



Symbolic Simplification and Node Impacts



The screenshot shows the HeuristicLab Optimizer interface with a symbolic regression tree. The tree structure is as follows:

- Root: Addition (green)
- Level 1: Multiplication (green)
- Level 2: Multiplication (green)
- Level 3: Subtraction (green)
- Level 4: Multiplication (green) and Subtraction (white)
- Level 5: Division (green) and Division (green) under the left Multiplication; Addition (white) under the right Subtraction.
- Level 6: Subtraction (pink) and Addition (green) under the left Division; Addition (white) and Addition (white) under the right Division.
- Level 7: Addition (pink), Subtraction (white), Subtraction (white), and Division (green) under the left Subtraction; Multiplication (white), Multiplication (white), Multiplication (white), and Addition (red) under the right Addition.
- Level 8: Multiplication (pink), Subtraction (white), and Addition (green) under the left Addition; Multiplication (white), Multiplication (white), Multiplication (white), and Addition (red) under the right Multiplication.

Each node is associated with a numerical value. A red box highlights the following data for a specific node:

1.5E+00	5.2E+00	-7.0E+00	3.7E+00
6.0E+00	5.7E+00	3.7E+00	1.7E+00
2.0E+00	7.0E+00	3.8E+00	0.0E+00
1.5E+00	5.2E+00	-7.0E+00	3.7E+00

Details Panel:

Regression Solution

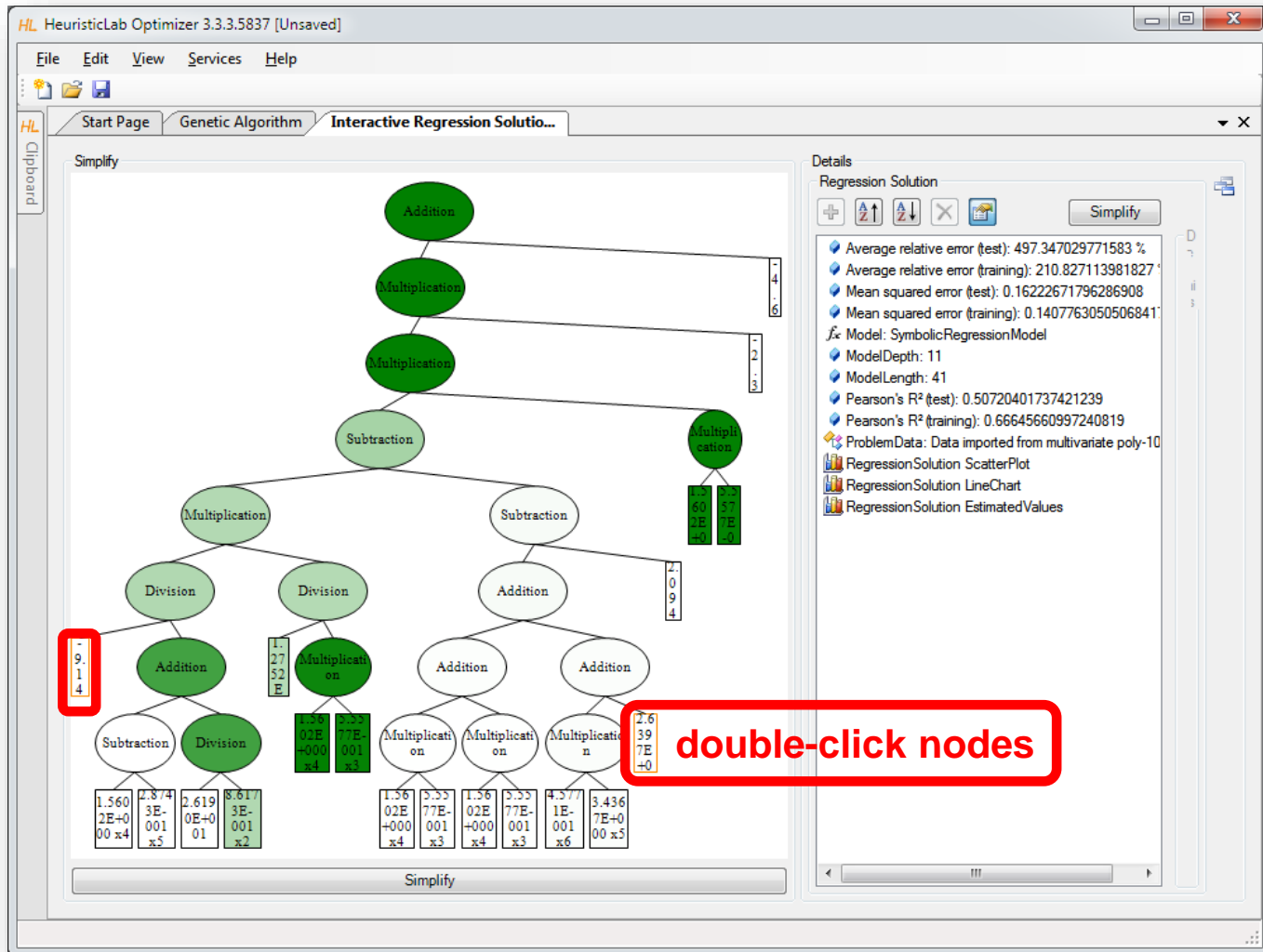
- Average relative error (test): 473.618715910248 %
- Average relative error (training): 245.090781502651 %
- Mean squared error (test): 0.163506091453717
- Mean squared error (training): 0.1415659913306669
- Model: SymbolicRegressionModel
- ModelDepth: 12
- ModelLength: 53
- Pearson's R² (test): 0.50347666984730766
- Pearson's R² (training): 0.66458559454272514
- ProblemData: Data imported from multivariate poly-10
- RegressionSolution ScatterPlot
- RegressionSolution LineChart
- RegressionSolution EstimatedValues

Node Impact Summary:

1.5E+00	5.2E+00	-7.0E+00	3.7E+00
6.0E+00	5.7E+00	3.7E+00	1.7E+00
2.0E+00	7.0E+00	3.8E+00	0.0E+00
1.5E+00	5.2E+00	-7.0E+00	3.7E+00

Node Impact: -0.00166473209841678
Replacement value: 26.3974611821139

Manual Simplification



The screenshot shows the HeuristicLab Optimizer interface. The main window displays a tree diagram representing a regression solution. The tree starts with an 'Addition' node at the top, which branches into 'Multiplication' and 'Subtraction' nodes. Further down, there are more 'Multiplication' and 'Subtraction' nodes, leading to 'Division' and 'Addition' nodes. The bottom level of the tree contains several 'Multiplication' nodes with numerical coefficients and powers of x (e.g., $1.5602E+000x^4$, $4.3774E-001x^5$, etc.). A red box highlights a node with the value -9.14 . Another red box highlights a node with the value $2.6397E+0$ and the text 'double-click nodes' is written next to it. The right-hand side of the window shows a 'Details' panel for the 'Regression Solution' with various statistics and model information.

HL HeuristicLab Optimizer 3.3.3.5837 [Unsaved]

File Edit View Services Help

Start Page Genetic Algorithm Interactive Regression Solution...

Simplify

Clipboard

Details

Regression Solution

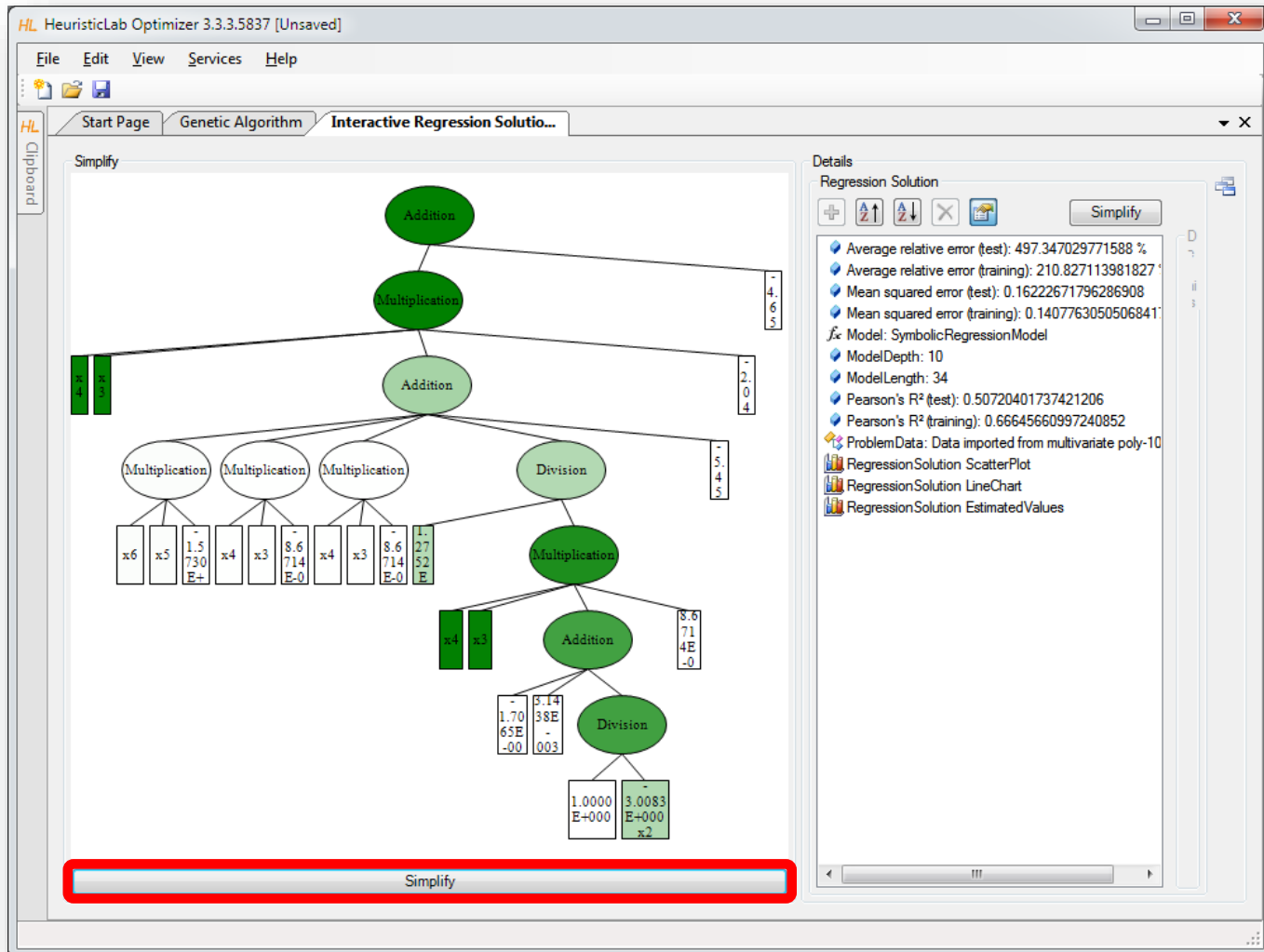
Simplify

- Average relative error (test): 497.347029771583 %
- Average relative error (training): 210.827113981827 %
- Mean squared error (test): 0.16222671796286908
- Mean squared error (training): 0.1407763050506841
- Model: SymbolicRegressionModel
- ModelDepth: 11
- ModelLength: 41
- Pearson's R² (test): 0.50720401737421239
- Pearson's R² (training): 0.66645660997240819
- ProblemData: Data imported from multivariate poly-10
- RegressionSolution ScatterPlot
- RegressionSolution LineChart
- RegressionSolution EstimatedValues

double-click nodes

Simplify

Automatic Symbolic Simplification



The screenshot displays the HeuristicLab Optimizer interface. The main window shows an "Interactive Regression Solution" with a "Simplify" button at the bottom, highlighted with a red rectangle. The central area contains a symbolic tree diagram with nodes labeled "Addition", "Multiplication", and "Division". The tree structure is as follows:

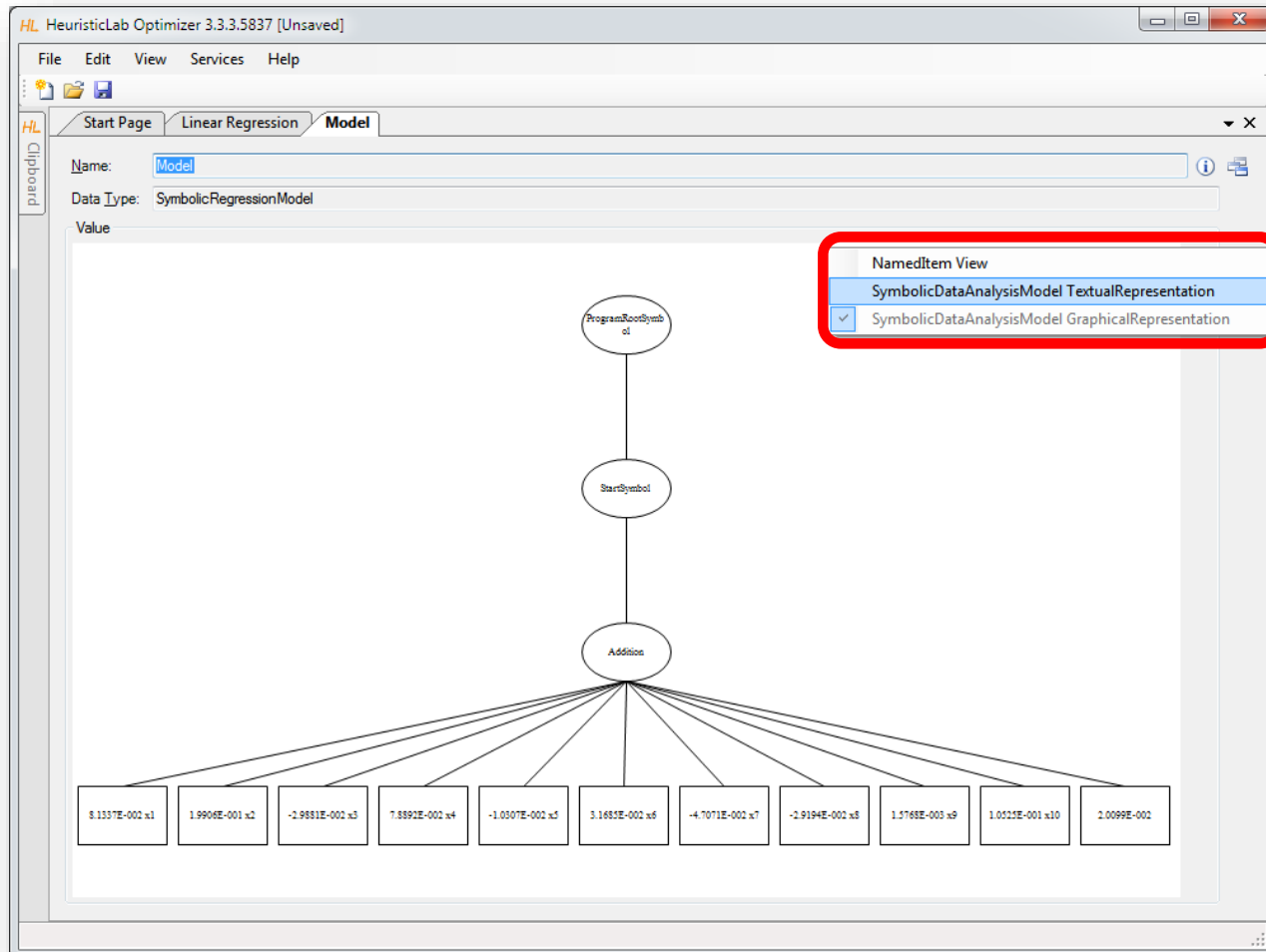
- Root: Addition (value: -4.65)
- Level 1: Multiplication (value: -2.04)
- Level 2: Addition (value: -5.45)
- Level 3: Three Multiplication nodes and one Division node.
- Level 4: Under the first Multiplication node: x6, x5, 1.5730E+, x4, x3, 8.6714E-0, x4, x3, 8.6714E-0, 1.2752E.
- Level 4: Under the second Multiplication node: x4, x3.
- Level 4: Under the third Multiplication node: x4, x3, 8.6714E-0, 1.2752E.
- Level 4: Under the Division node: Multiplication (value: 8.6714E-0)
- Level 5: Under the Multiplication node: Addition (value: 8.6714E-0)
- Level 6: Under the Addition node: Division (value: -0)
- Level 7: Under the Division node: 1.0000E+000, 3.0083E+000, x2.

The right-hand "Details" panel provides the following information:

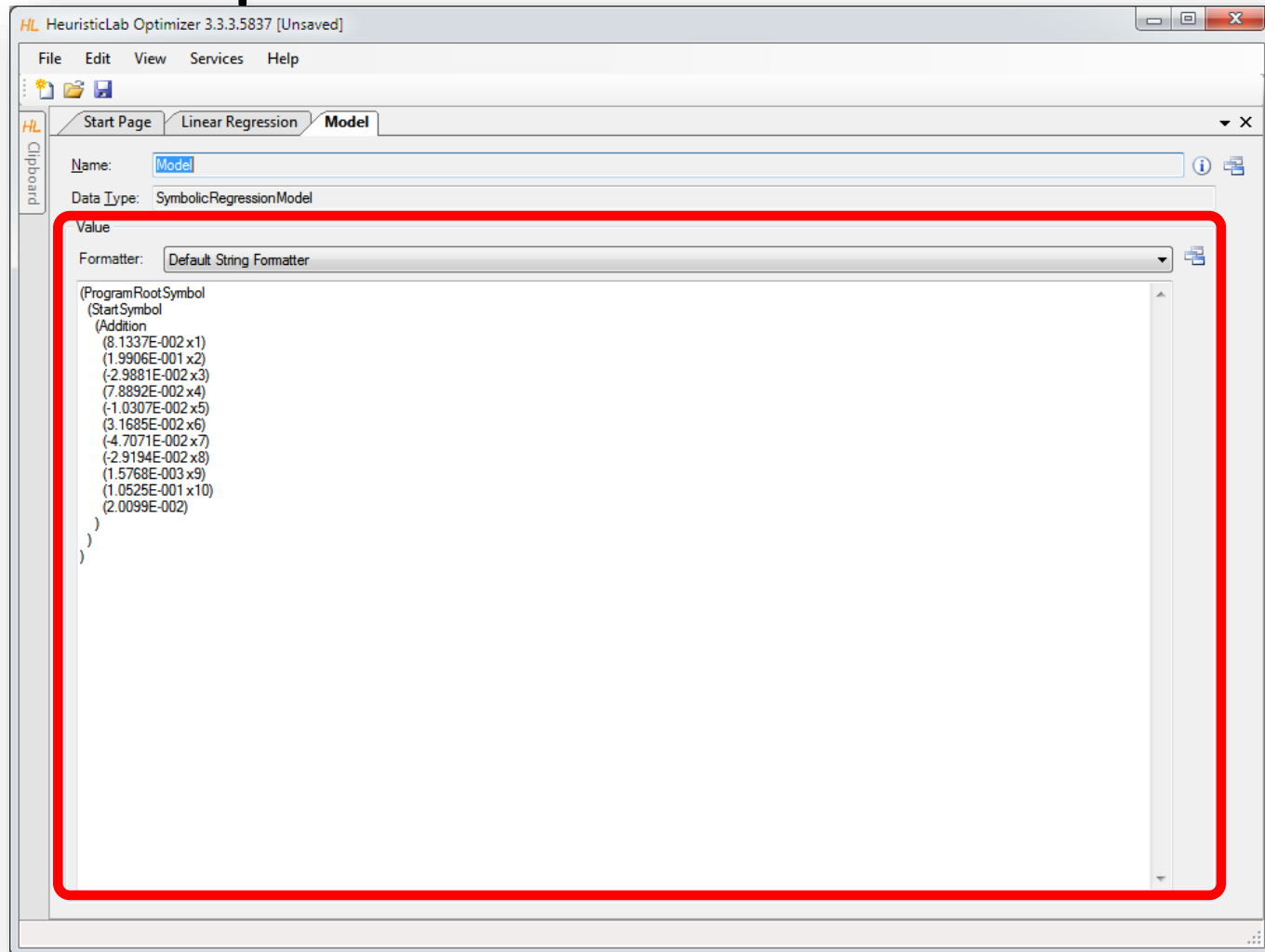
- Regression Solution
- Average relative error (test): 497.347029771588 %
- Average relative error (training): 210.827113981827 %
- Mean squared error (test): 0.16222671796286908
- Mean squared error (training): 0.1407763050506841
- Model: SymbolicRegressionModel
- ModelDepth: 10
- ModelLength: 34
- Pearson's R² (test): 0.50720401737421206
- Pearson's R² (training): 0.66645660997240852
- ProblemData: Data imported from multivariate poly-10
- RegressionSolution ScatterPlot
- RegressionSolution LineChart
- RegressionSolution EstimatedValues

Textual Representations Are Also Available

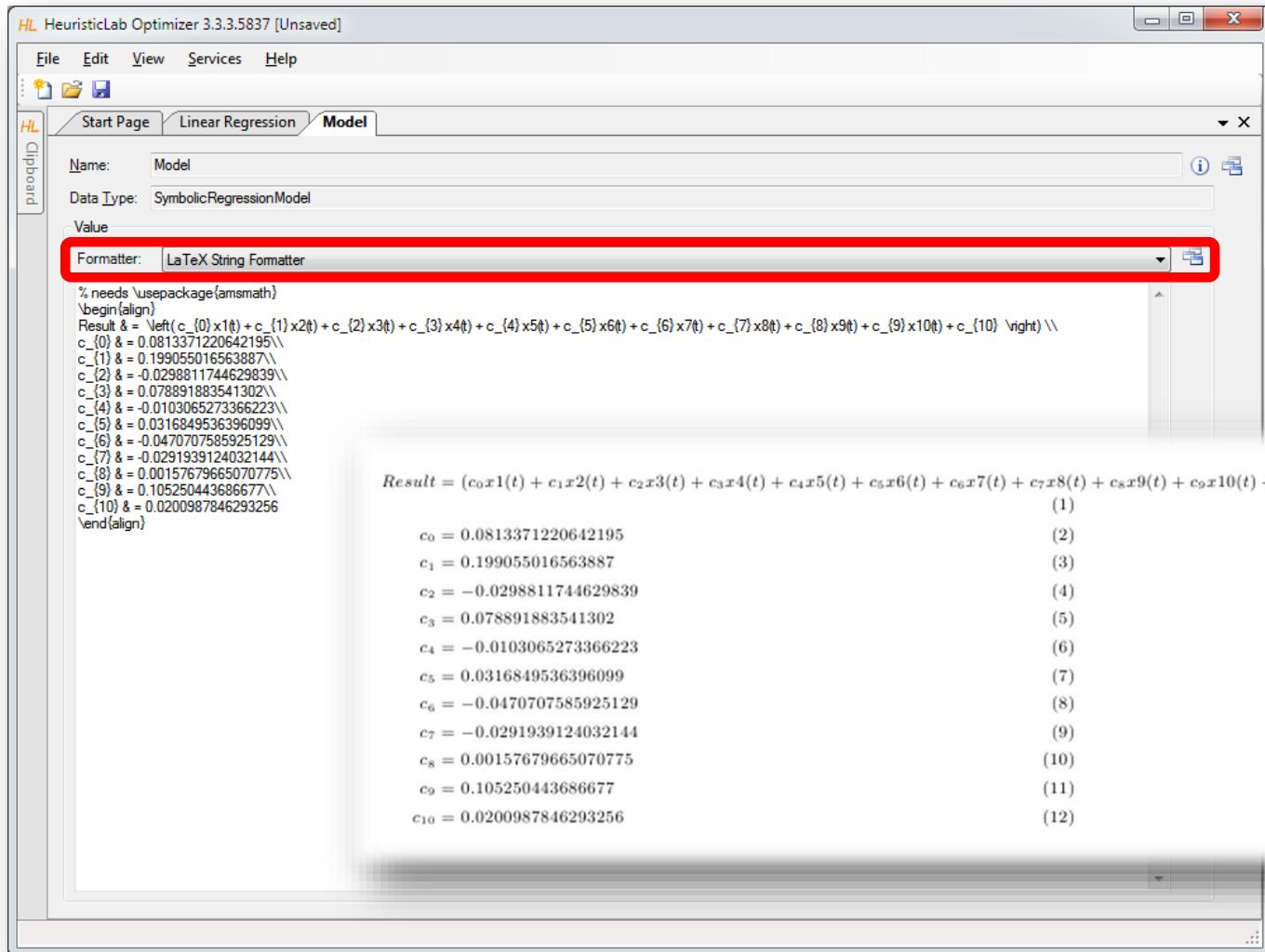
- Use *ViewHost* to switch to textual representation view.



Default Textual Representation for Model Export



Textual Representation for Export to LaTeX



The screenshot shows the HeuristicLab Optimizer interface. The 'Model' tab is active, and the 'Formatter' dropdown is set to 'LaTeX String Formatter'. The main text area contains LaTeX code for a symbolic regression model. A red box highlights the 'Formatter' dropdown. A preview window shows the resulting LaTeX output.

```
% needs \usepackage{amsmath}
\begin{align}
Result &= \left( c_0 x1(t) + c_1 x2(t) + c_2 x3(t) + c_3 x4(t) + c_4 x5(t) + c_5 x6(t) + c_6 x7(t) + c_7 x8(t) + c_8 x9(t) + c_9 x10(t) + c_{10} \right) \\\
c_0 &= 0.0813371220642195 \\\
c_1 &= 0.199055016563887 \\\
c_2 &= -0.0298811744629839 \\\
c_3 &= 0.078891883541302 \\\
c_4 &= -0.0103065273366223 \\\
c_5 &= 0.0316849536396099 \\\
c_6 &= -0.0470707585925129 \\\
c_7 &= -0.0291939124032144 \\\
c_8 &= 0.00157679665070775 \\\
c_9 &= 0.105250443686677 \\\
c_{10} &= 0.0200987846293256
\end{align}
```

Result = $(c_0 x1(t) + c_1 x2(t) + c_2 x3(t) + c_3 x4(t) + c_4 x5(t) + c_5 x6(t) + c_6 x7(t) + c_7 x8(t) + c_8 x9(t) + c_9 x10(t) + c_{10})$

$c_0 = 0.0813371220642195$	(1)
$c_1 = 0.199055016563887$	(2)
$c_2 = -0.0298811744629839$	(3)
$c_3 = 0.078891883541302$	(4)
$c_4 = -0.0103065273366223$	(6)
$c_5 = 0.0316849536396099$	(7)
$c_6 = -0.0470707585925129$	(8)
$c_7 = -0.0291939124032144$	(9)
$c_8 = 0.00157679665070775$	(10)
$c_9 = 0.105250443686677$	(11)
$c_{10} = 0.0200987846293256$	(12)

LaTeX Export

HL HeuristicLab Optimizer 3.3.3.5837 [Unsaved]

File Edit View Services Help

Start Page Genetic Algorithm Interactive Regression Solution S... Model

Name: Model

Data Type: SymbolicRegressionModel

Value

Formatter: LaTeX String Formatter

```

% needs \usepackage{amsmath}
\begin{align}
Result &= \left( c_4 x_4(t) + c_7 x_7(t) + c_{10} x_{10}(t) + c_{13} x_{13}(t) + c_{16} x_{16}(t) + c_{19} x_{19}(t) + c_{21} x_{21}(t) \right) \\
&+ \frac{c_{11} x_1(t)}{x_4(t) \cdot x_3(t) \cdot \left( c_{14} x_4(t) + c_{15} x_5(t) + \frac{1}{c_{17} x_2(t)} \right) \cdot c_{18}} + c_{19} + c_{21} \\
c_4 &= -1.57302367616477 \\
c_7 &= -0.867137925013337 \\
c_{10} &= -0.867137925013337 \\
c_{11} &= 1.27519978915975 \\
c_{14} &= -0.017064976517855 \\
c_{15} &= 0.00314376988160885 \\
c_{17} &= -3.00832012161288 \\
c_{18} &= 0.867137925013337 \\
c_{19} &= -5.45190909899249 \\
c_{20} &= -0.204498330755849 \\
c_{21} &= -0.0465339907207764
\end{align}

```

Result = $x_4(t) \cdot x_3(t) \cdot c_{20}$ (13)

$$\cdot \left(x_6(t) \cdot x_5(t) \cdot c_4 + x_4(t) \cdot x_3(t) \cdot c_7 + x_4(t) \cdot x_3(t) \cdot c_{10} + \frac{c_{11} x_1(t)}{x_4(t) \cdot x_3(t) \cdot \left(c_{14} x_4(t) + c_{15} x_5(t) + \frac{1}{c_{17} x_2(t)} \right) \cdot c_{18}} + c_{19} \right) + c_{21}$$

$c_4 = -1.57302367616477$ (15)

$c_7 = -0.867137925013337$ (16)

$c_{10} = -0.867137925013337$ (17)

$c_{11} = 1.27519978915975$ (18)

$c_{14} = -0.017064976517855$ (19)

$c_{15} = 0.00314376988160885$ (20)

$c_{17} = -3.00832012161288$ (21)

$c_{18} = 0.867137925013337$ (22)

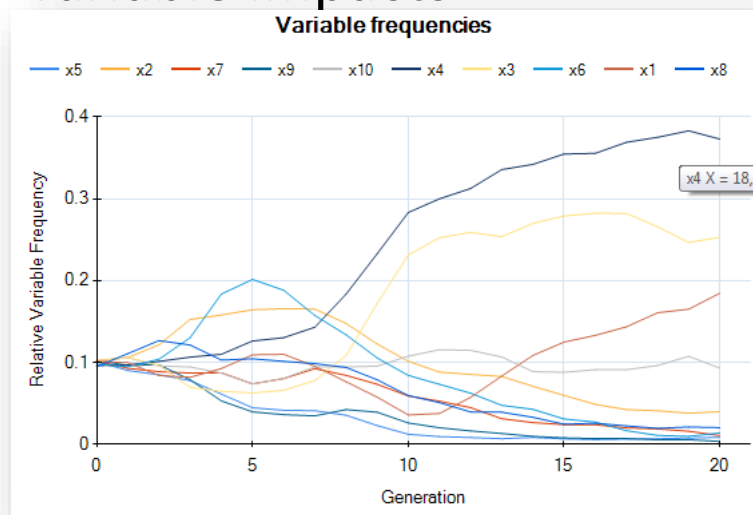
$c_{19} = -5.45190909899249$ (23)

$c_{20} = -0.204498330755849$ (24)

$c_{21} = -0.0465339907207764$ (25)

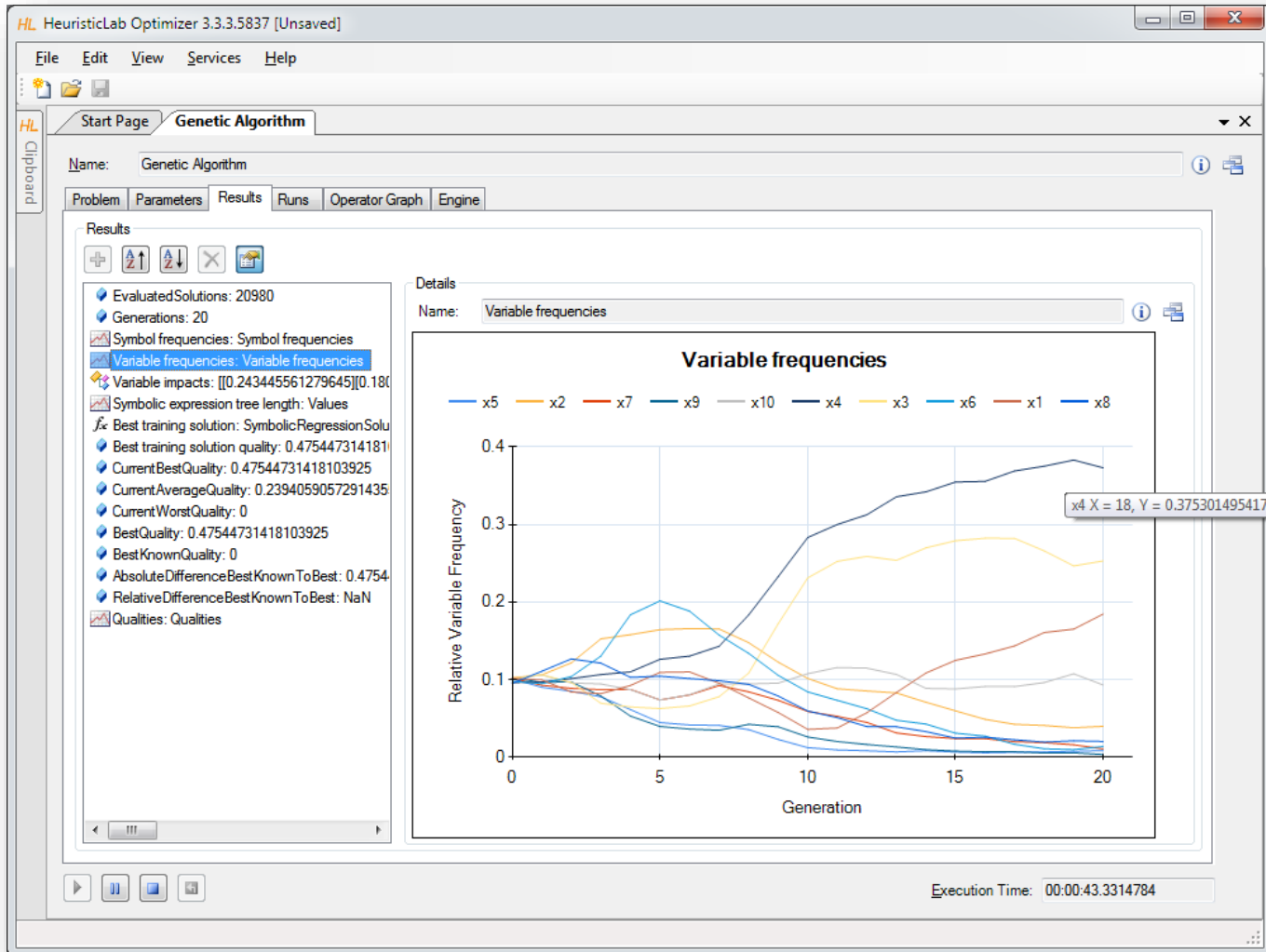
Variable Relevance Analysis

- Which variables are important for correct predictions?
- Demonstration
 - Variable frequency analyzer
 - symbol frequency analyzer
 - variable impacts

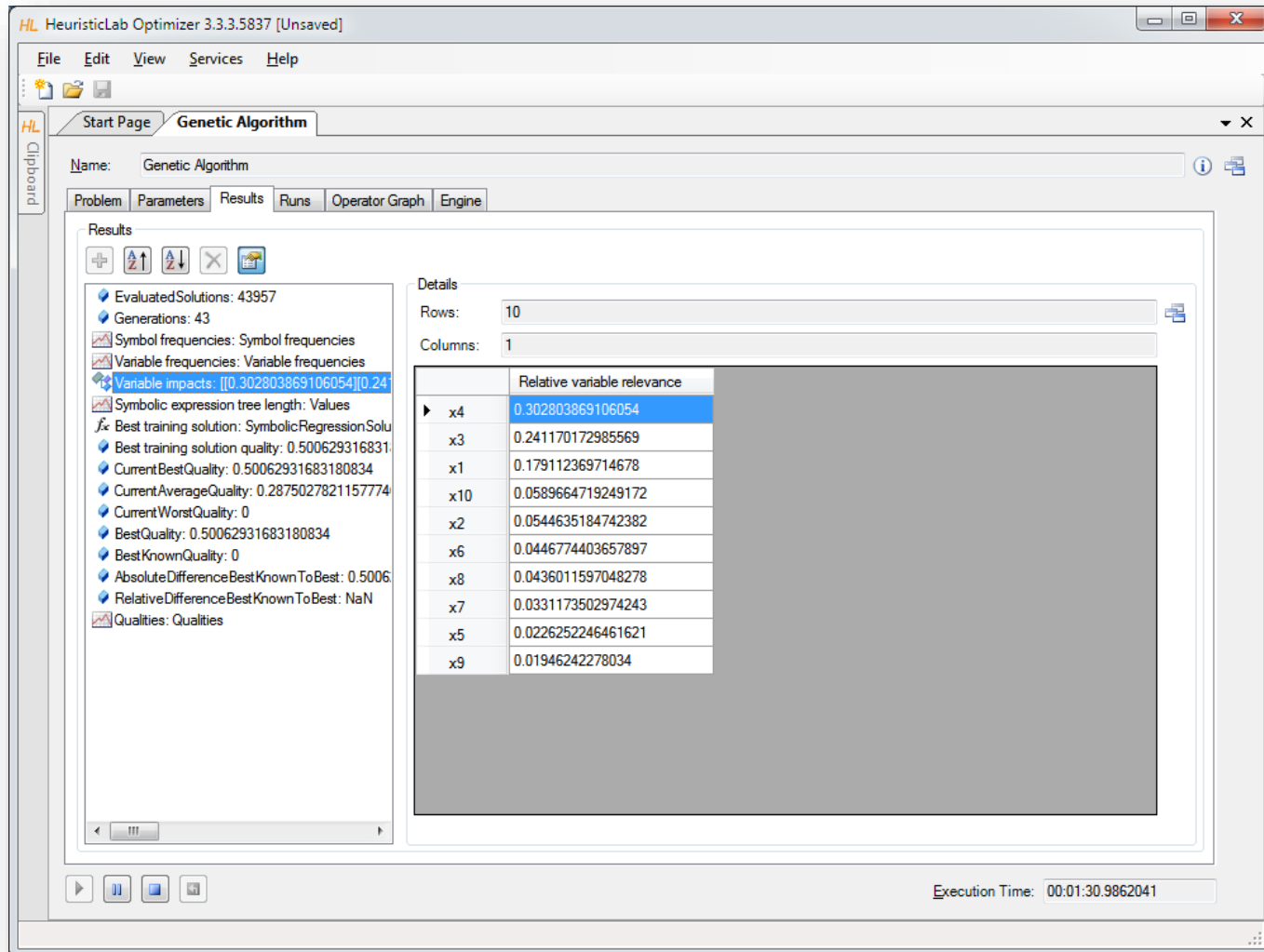


	Relative variable relevance
x4	0.302803869106054
x3	0.241170172985569
x1	0.179112369714678
x10	0.0589664719249172
x2	0.0544635184742382
x6	0.0446774403657897
x8	0.0436011597048278
x7	0.0331173502974243
x5	0.0226252246461621
x9	0.01946242278034

Inspect Variable Frequency Chart



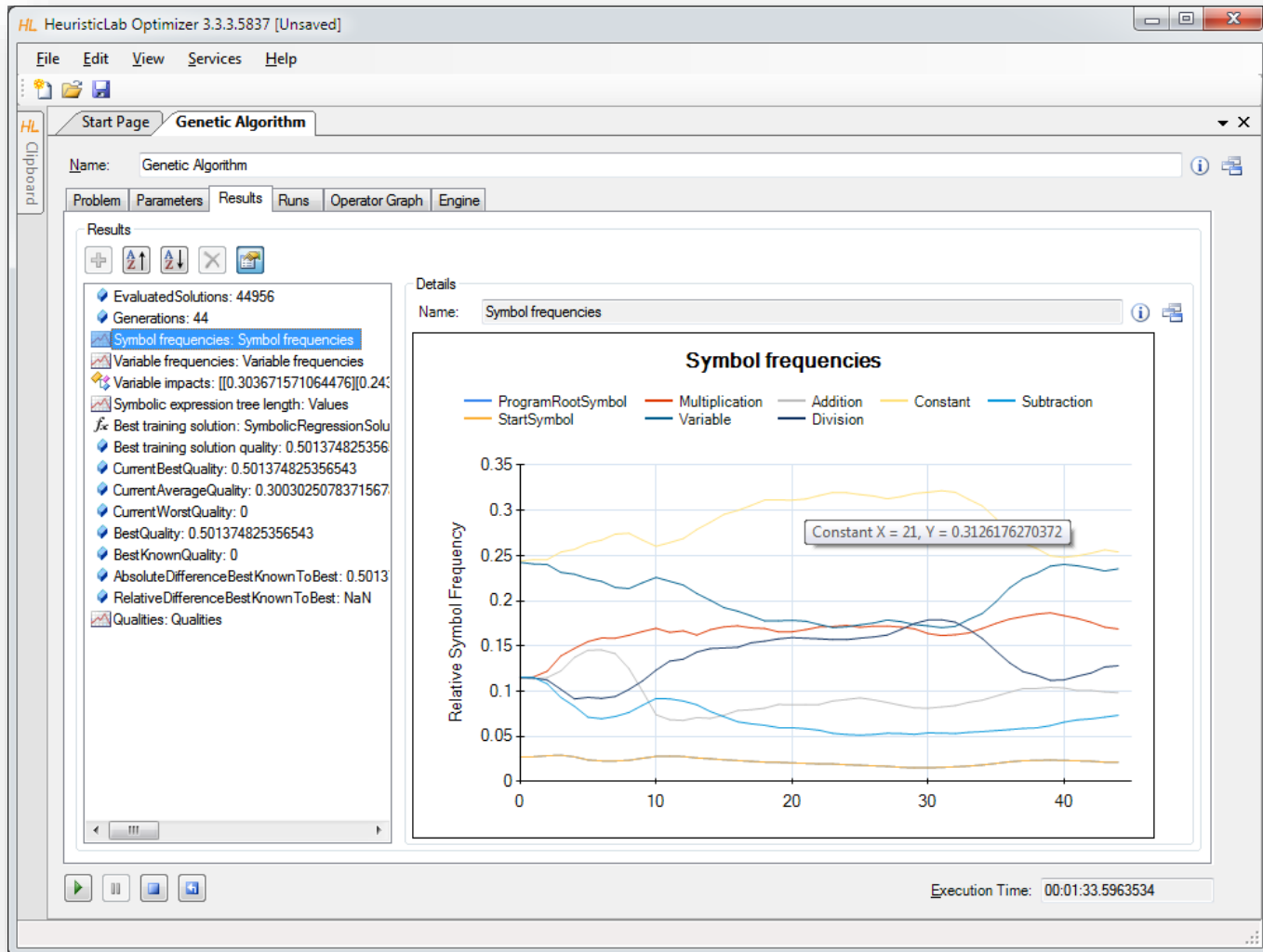
Inspect Variable Impacts



The screenshot shows the HeuristicLab Optimizer interface. The 'Results' tab is active, displaying a list of results on the left and a table of variable impacts on the right. The table is titled 'Relative variable relevance' and lists variables x1 through x10 with their corresponding relevance values. Variable x4 has the highest relevance at 0.302803869106054.

Variable	Relative variable relevance
x4	0.302803869106054
x3	0.241170172985569
x1	0.179112369714678
x10	0.0589664719249172
x2	0.0544635184742382
x6	0.0446774403657897
x8	0.0436011597048278
x7	0.0331173502974243
x5	0.0226252246461621
x9	0.01946242278034

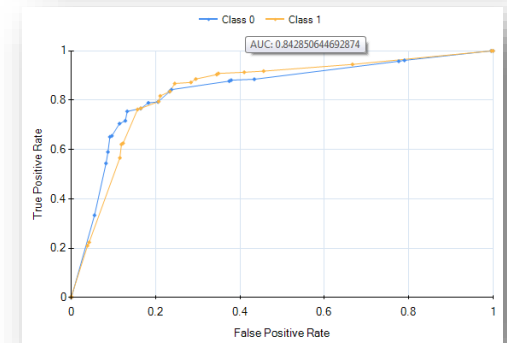
Inspect Symbol Frequencies



Classification with HeuristicLab



- Symbolic classification
 - evolve discriminating function using GP
 - find thresholds to assign classes
- Demonstration
 - real world medical application
 - model accuracy
 - visualization of model output
 - discriminating function output
 - ROC-curve
 - confusion matrix

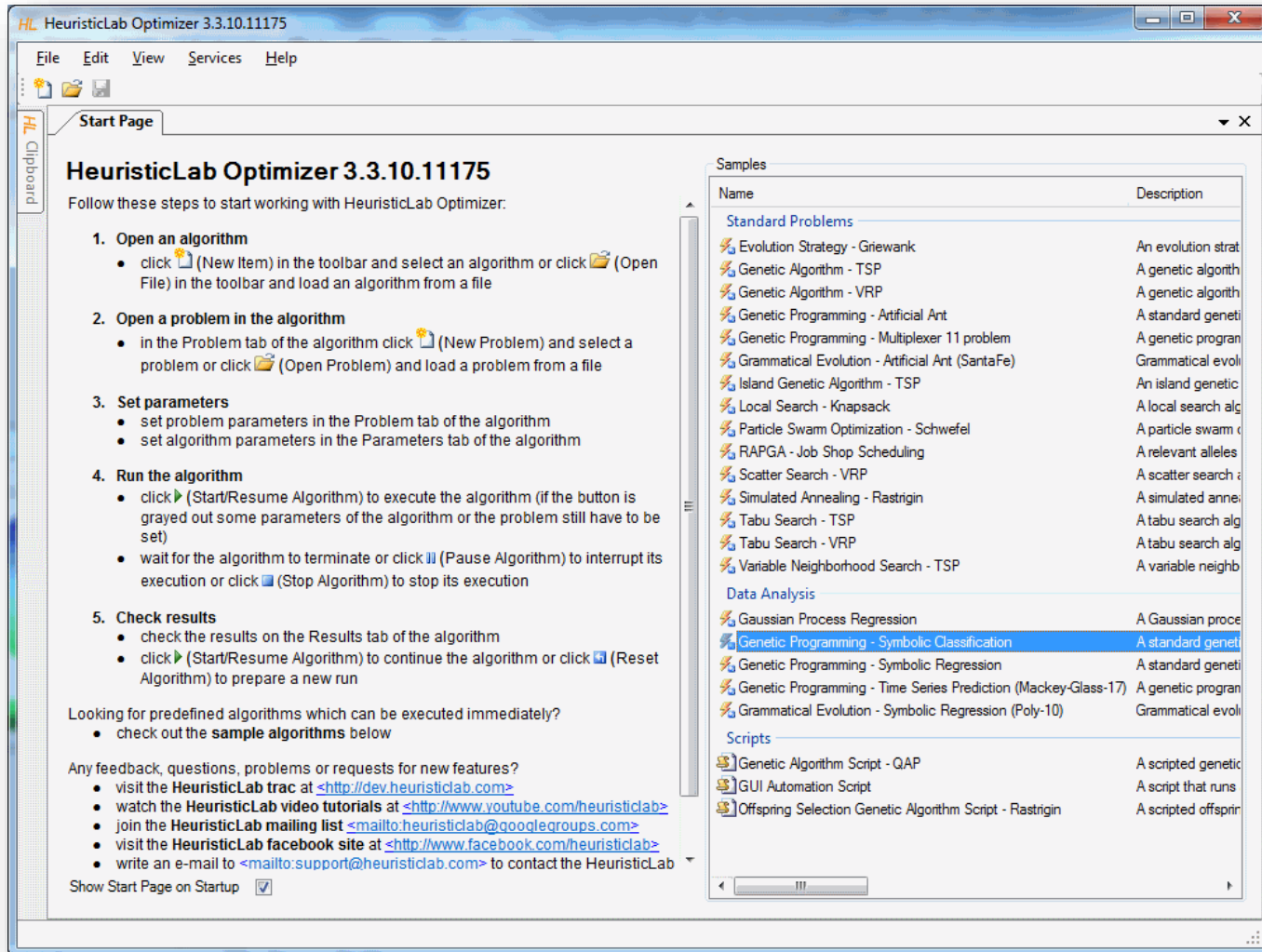


	Actual Class 0	Actual Class 1
Predicted Class 0	197	29
Predicted Class 1	64	190

Case Study: Classification

- Real world medical dataset (*Mammographic Mass*) from UCI Machine Learning Repository
 - data from non-invasive mammography screening
 - variables:
 - patient age
 - visual features of inspected mass lesions: shape, margin, density
 - target variable: severity (malignant, benign)
 - available as a benchmark problem instance in HeuristicLab

Open Sample



The screenshot shows the HeuristicLab Optimizer 3.3.10.11175 application window. The main area displays a 'Start Page' with a 'HeuristicLab Optimizer 3.3.10.11175' title and a list of five numbered steps for starting work with the optimizer. A 'Samples' panel on the right lists various optimization problems and scripts, with 'Genetic Programming - Symbolic Classification' selected. The interface includes a menu bar (File, Edit, View, Services, Help) and a toolbar with icons for opening files and starting algorithms.

HeuristicLab Optimizer 3.3.10.11175

Follow these steps to start working with HeuristicLab Optimizer:

- 1. Open an algorithm**
 - click (New Item) in the toolbar and select an algorithm or click (Open File) in the toolbar and load an algorithm from a file
- 2. Open a problem in the algorithm**
 - in the Problem tab of the algorithm click (New Problem) and select a problem or click (Open Problem) and load a problem from a file
- 3. Set parameters**
 - set problem parameters in the Problem tab of the algorithm
 - set algorithm parameters in the Parameters tab of the algorithm
- 4. Run the algorithm**
 - click (Start/Resume Algorithm) to execute the algorithm (if the button is grayed out some parameters of the algorithm or the problem still have to be set)
 - wait for the algorithm to terminate or click (Pause Algorithm) to interrupt its execution or click (Stop Algorithm) to stop its execution
- 5. Check results**
 - check the results on the Results tab of the algorithm
 - click (Start/Resume Algorithm) to continue the algorithm or click (Reset Algorithm) to prepare a new run

Looking for predefined algorithms which can be executed immediately?

- check out the **sample algorithms** below

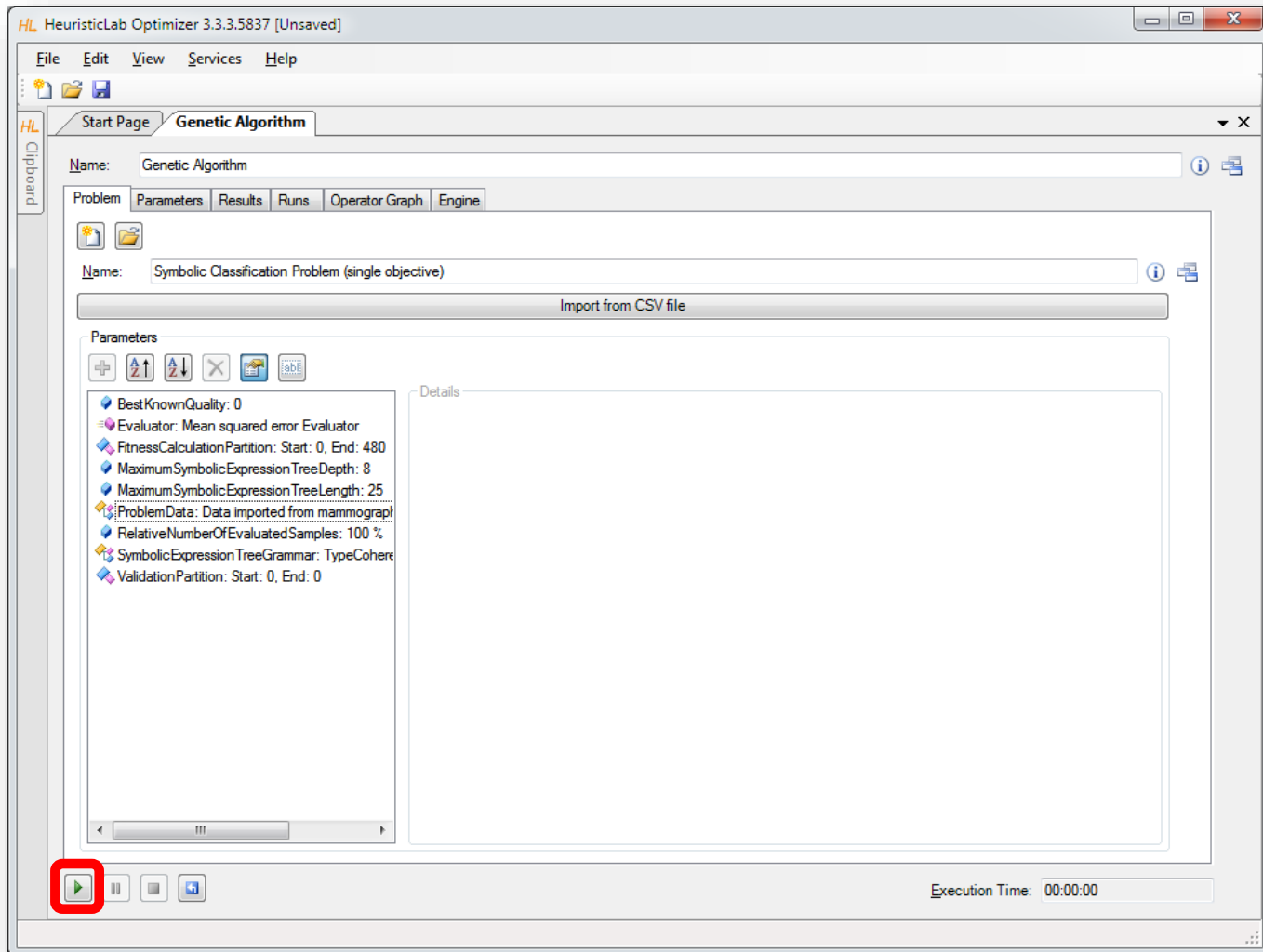
Any feedback, questions, problems or requests for new features?

- visit the **HeuristicLab trac** at <http://dev.heuristiclab.com>
- watch the **HeuristicLab video tutorials** at <http://www.youtube.com/heuristiclab>
- join the **HeuristicLab mailing list** <mailto:heuristiclab@googlegroups.com>
- visit the **HeuristicLab facebook site** at <http://www.facebook.com/heuristiclab>
- write an e-mail to <mailto:support@heuristiclab.com> to contact the HeuristicLab

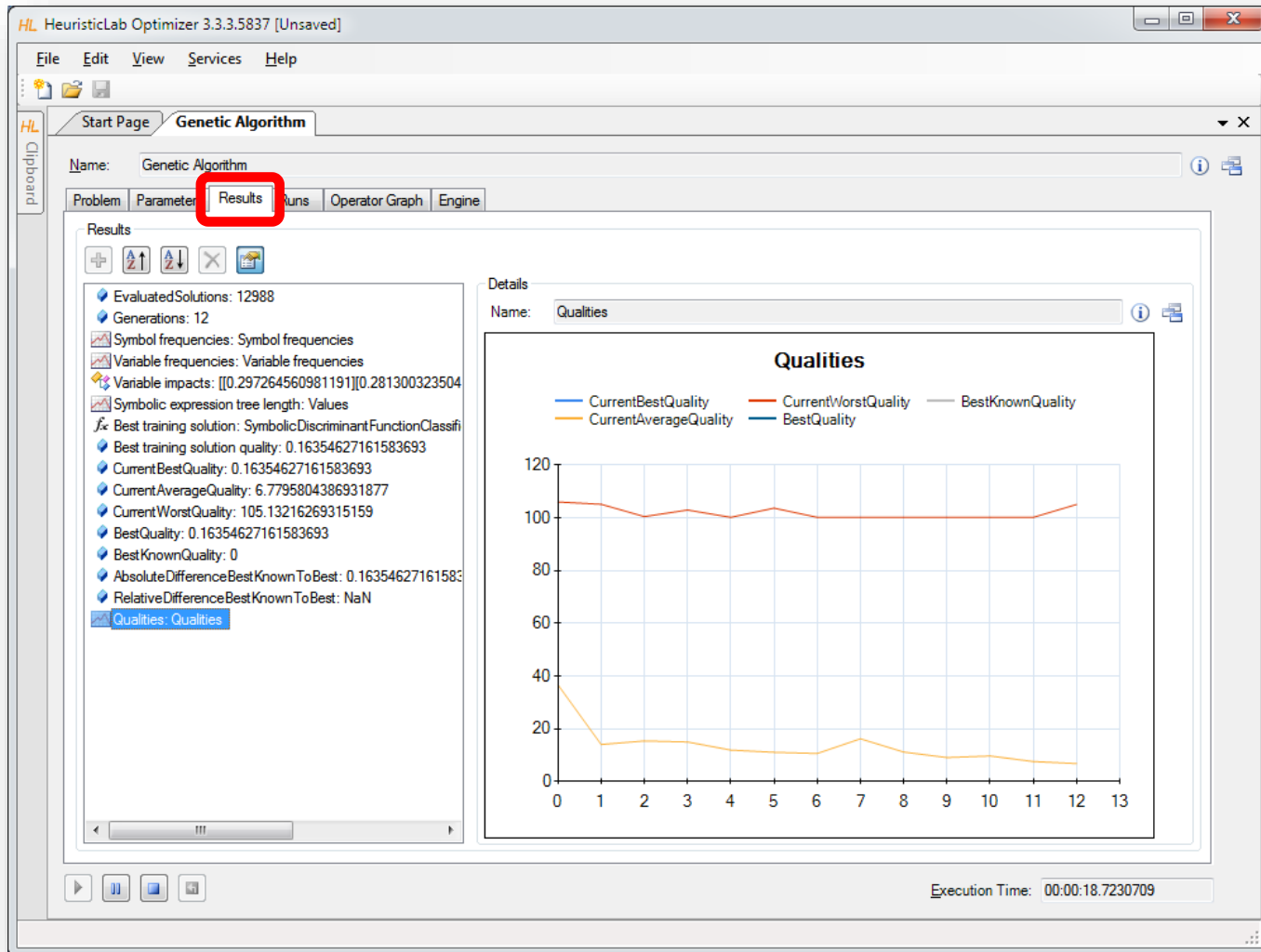
Show Start Page on Startup

Name	Description
Standard Problems	
Evolution Strategy - Griewank	An evolution strat
Genetic Algorithm - TSP	A genetic algorithm
Genetic Algorithm - VRP	A genetic algorithm
Genetic Programming - Artificial Ant	A standard geneti
Genetic Programming - Multiplexer 11 problem	A genetic program
Grammatical Evolution - Artificial Ant (SantaFe)	Grammatical evoli
Island Genetic Algorithm - TSP	An island genetic
Local Search - Knapsack	A local search alg
Particle Swarm Optimization - Schwefel	A particle swam c
RAPGA - Job Shop Scheduling	A relevant alleles
Scatter Search - VRP	A scatter search a
Simulated Annealing - Rastrigin	A simulated anne
Tabu Search - TSP	A tabu search alg
Tabu Search - VRP	A tabu search alg
Variable Neighborhood Search - TSP	A variable neighb
Data Analysis	
Gaussian Process Regression	A Gaussian proce
Genetic Programming - Symbolic Classification	A standard geneti
Genetic Programming - Symbolic Regression	A standard geneti
Genetic Programming - Time Series Prediction (Mackey-Glass-17)	A genetic program
Grammatical Evolution - Symbolic Regression (Poly-10)	Grammatical evoli
Scripts	
Genetic Algorithm Script - QAP	A scripted genetic
GUI Automation Script	A script that runs
Offspring Selection Genetic Algorithm Script - Rastrigin	A scripted offsprin

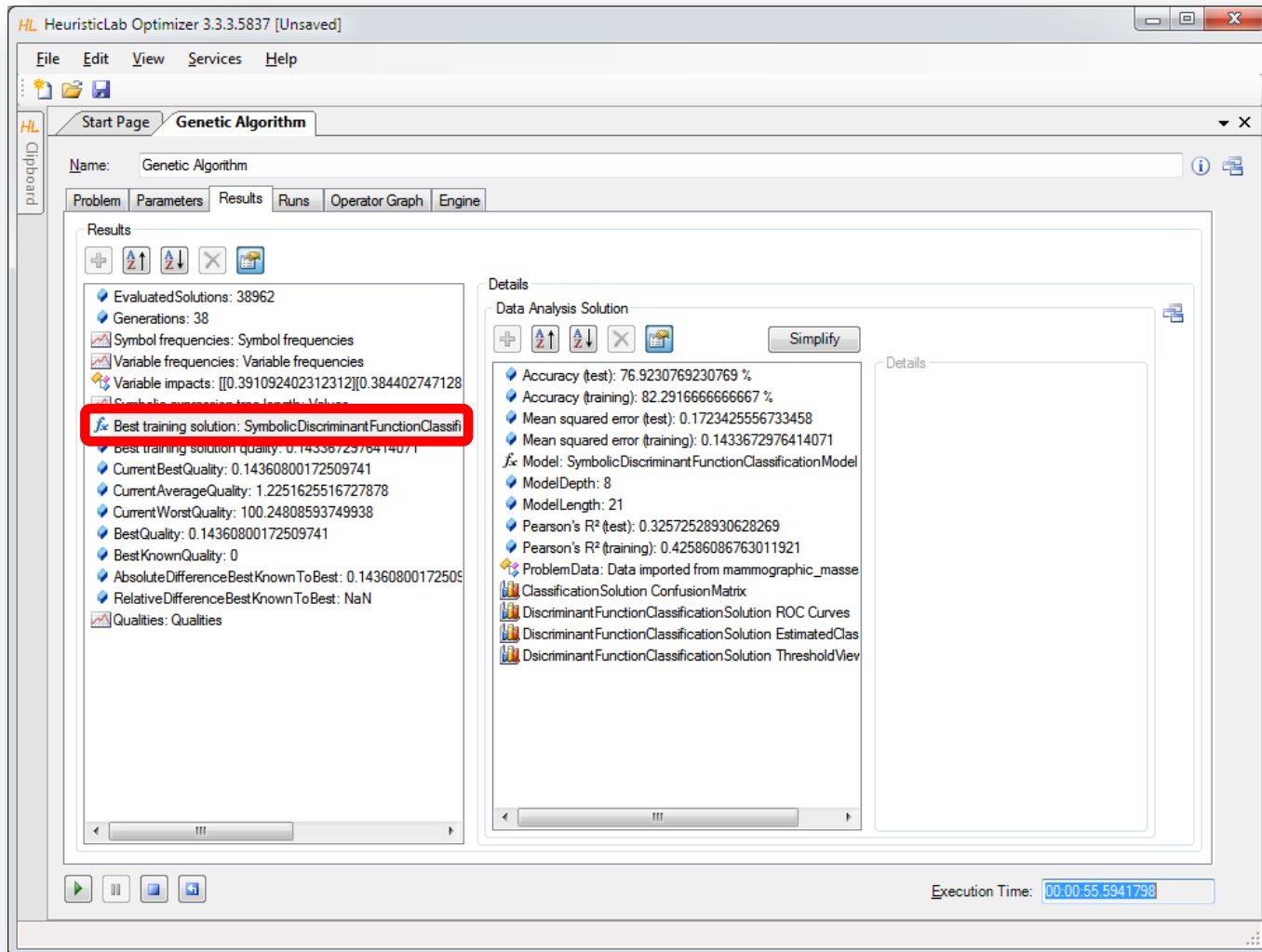
Configure and Run Algorithm



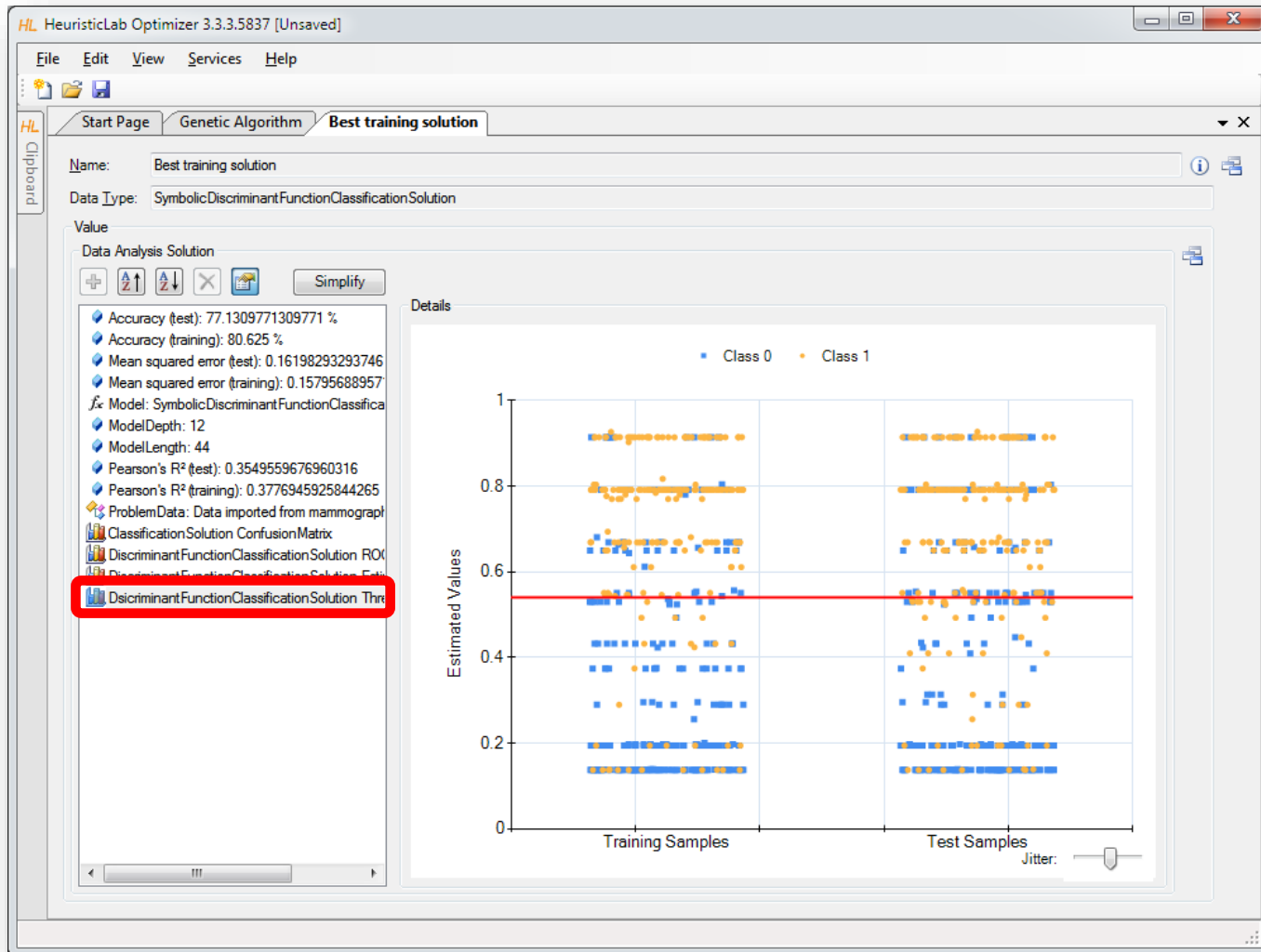
Inspect Quality Linechart



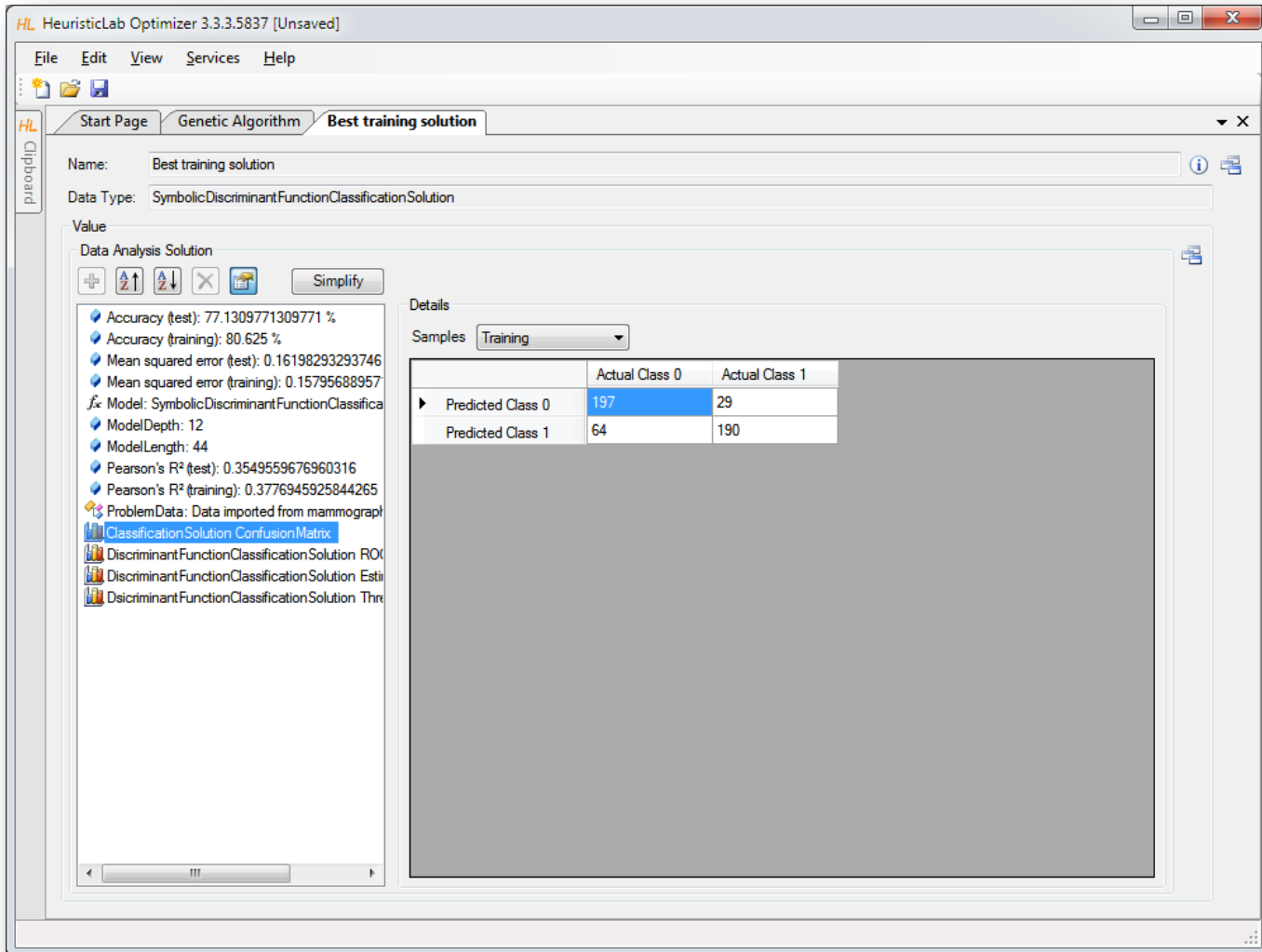
Inspect Best Training Solution



Inspect Model Output and Thresholds



Inspect Confusion Matrix



The screenshot shows the HeuristicLab Optimizer interface. The main window displays the 'Best training solution' for a Genetic Algorithm. The 'Value' section shows the 'Data Analysis Solution' with various performance metrics. The 'Details' section shows a confusion matrix for the 'Training' samples.

Name: Best training solution
Data Type: SymbolicDiscriminantFunctionClassificationSolution

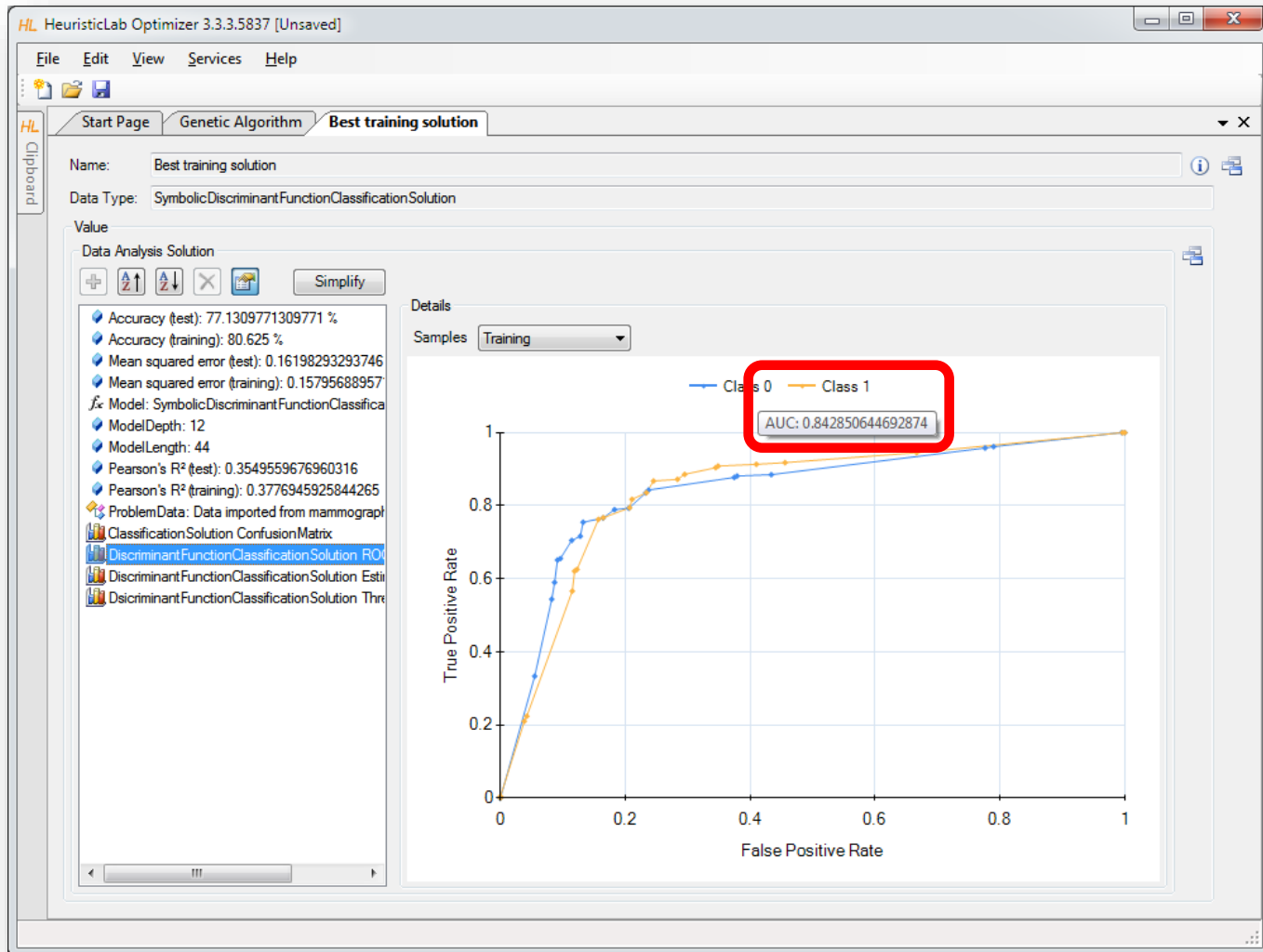
Value
Data Analysis Solution

- Accuracy (test): 77.1309771309771 %
- Accuracy (training): 80.625 %
- Mean squared error (test): 0.16198293293746
- Mean squared error (training): 0.15795688957
- Model: SymbolicDiscriminantFunctionClassificationSolution
- ModelDepth: 12
- ModelLength: 44
- Pearson's R² (test): 0.3549559676960316
- Pearson's R² (training): 0.3776945925844265
- ProblemData: Data imported from mammograph
- ClassificationSolution ConfusionMatrix
- DiscriminantFunctionClassificationSolution RO
- DiscriminantFunctionClassificationSolution Esti
- DiscriminantFunctionClassificationSolution Thre

Details
Samples: Training

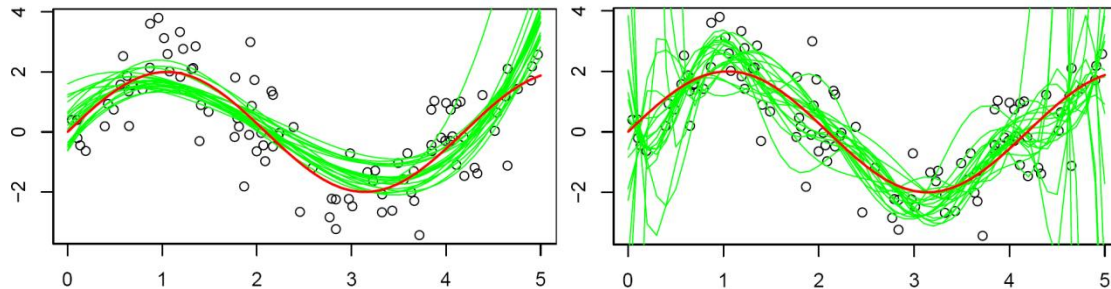
	Actual Class 0	Actual Class 1
Predicted Class 0	197	29
Predicted Class 1	64	190

Inspect ROC Curve



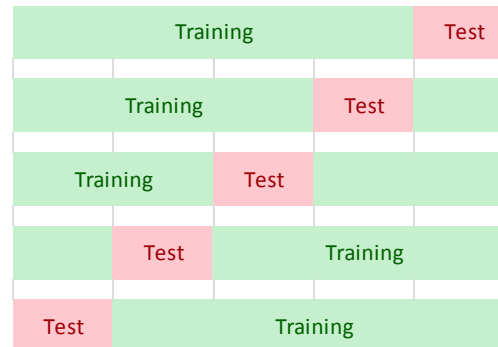
Validation of Results

- Overfitting = memorizing data



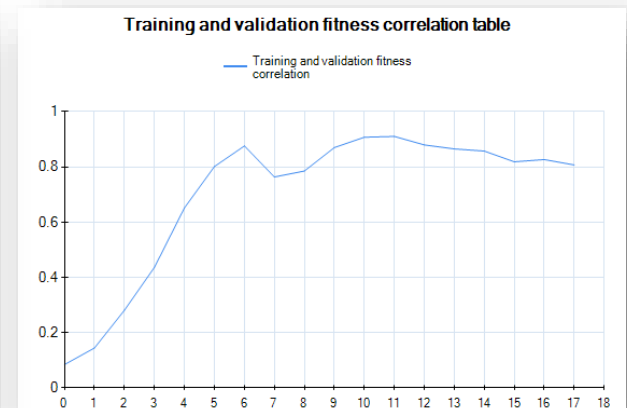
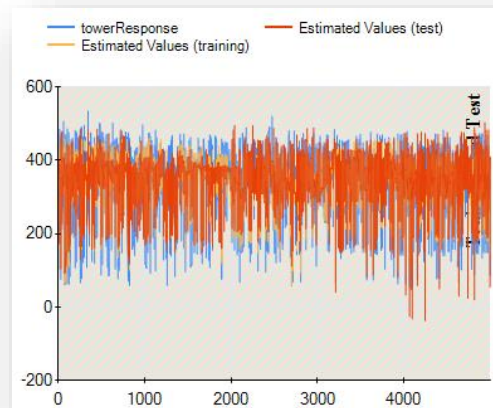
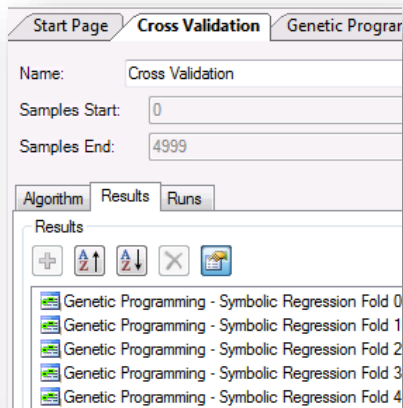
- Strategies to reduce overfitting

- validation partition
- cross-validation

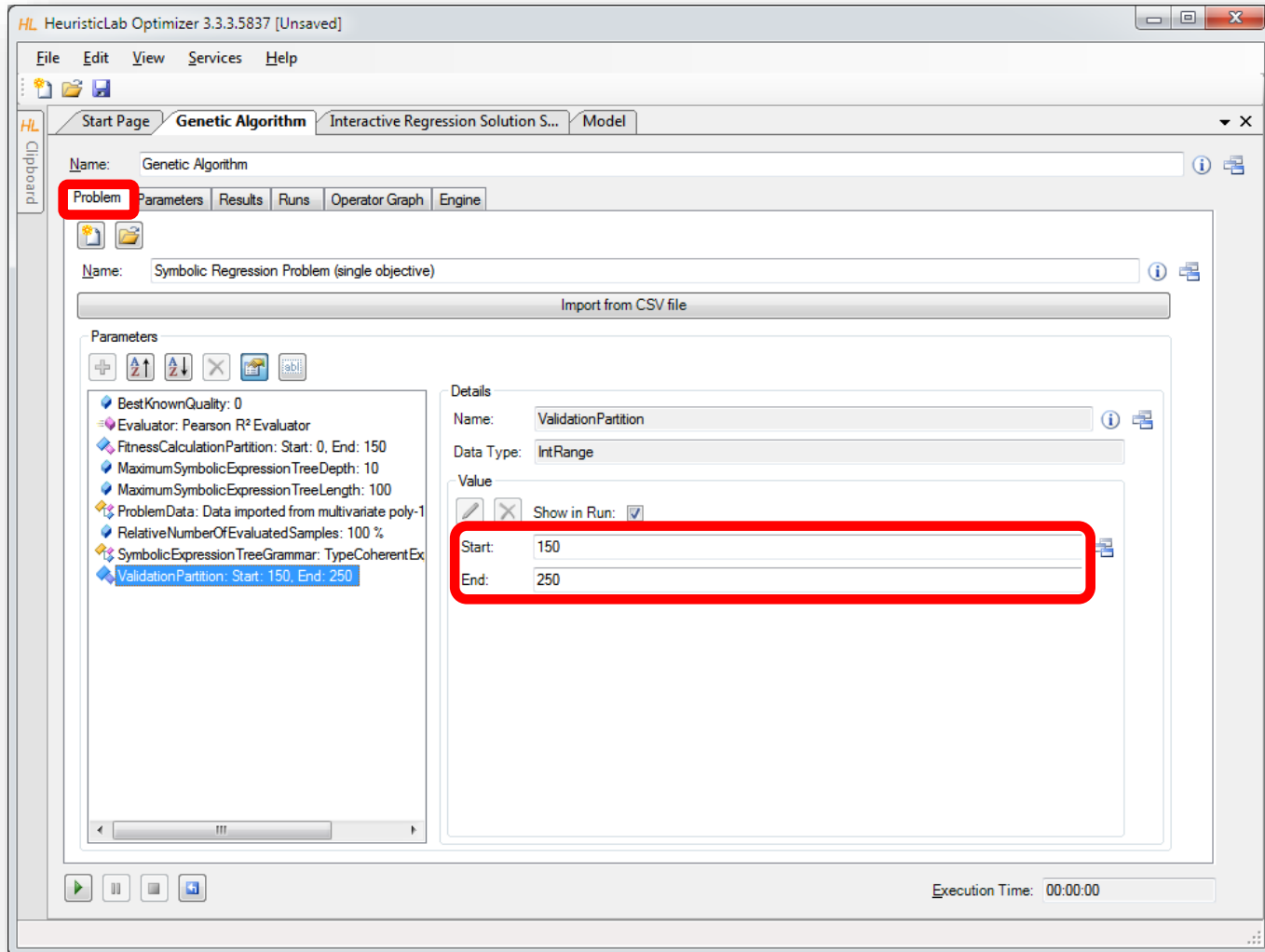


Validation of Results

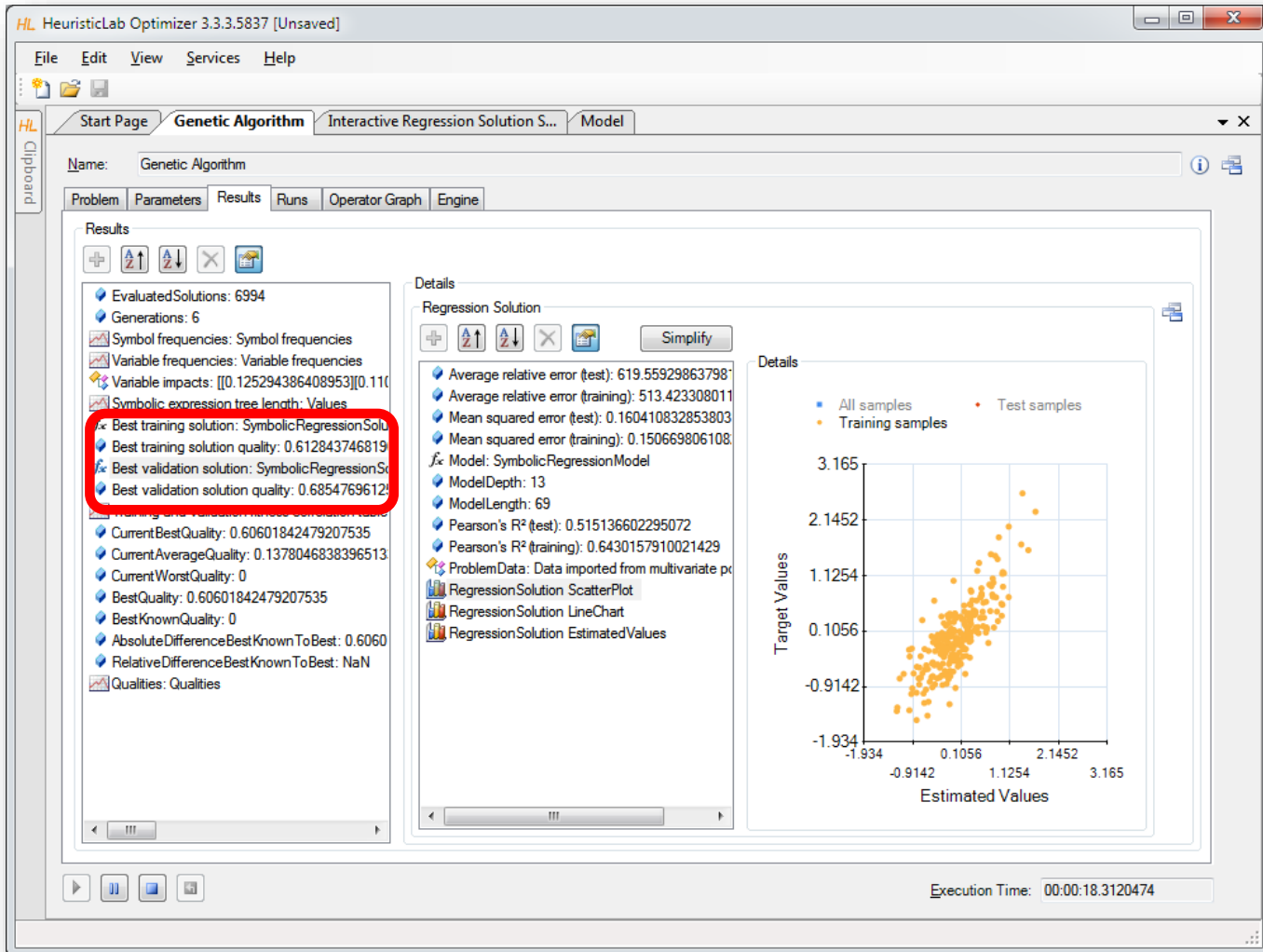
- Demonstration
 - Configuration of a validation set
 - Inspection of best solution on validation set
 - Analysis of training- and validation fitness correlation
 - Cross-validation
 - Configuration
 - Analysis of results



Configuration of Validation Partition



Inspect Best Model on Validation Partition



The screenshot displays the HeuristicLab Optimizer interface. The main window is titled "HL HeuristicLab Optimizer 3.3.3.5837 [Unsaved]". The "Results" tab is active, showing the following information:

- Evaluated Solutions: 6994
- Generations: 6
- Symbol frequencies: Symbol frequencies
- Variable frequencies: Variable frequencies
- Variable impacts: $[[0.125294386408953][0.110...]]$
- Symbolic expression tree length: Values
- Best training solution: SymbolicRegressionSol...
- Best training solution quality: 0.612843746819
- Best validation solution: SymbolicRegressionS...
- Best validation solution quality: 0.6854769612...

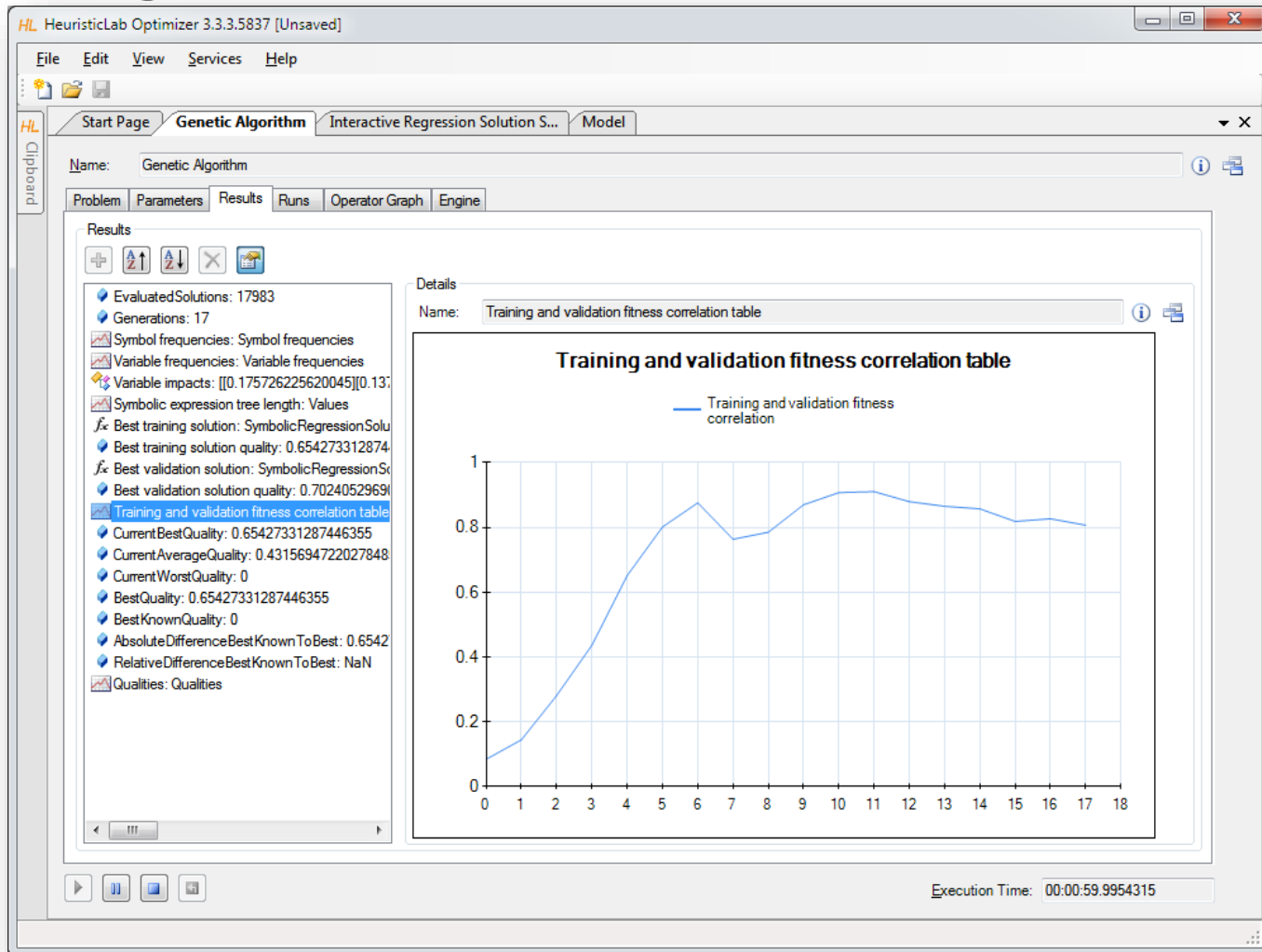
The "Details" tab is also active, showing the following information:

- Regression Solution
- Average relative error (test): 619.55929863798
- Average relative error (training): 513.423308011
- Mean squared error (test): 0.160410832853803
- Mean squared error (training): 0.150669806108
- Model: SymbolicRegressionModel
- ModelDepth: 13
- ModelLength: 69
- Pearson's R² (test): 0.515136602295072
- Pearson's R² (training): 0.6430157910021429
- ProblemData: Data imported from multivariate p...
- RegressionSolution ScatterPlot
- RegressionSolution LineChart
- RegressionSolution EstimatedValues

A scatter plot titled "Target Values" vs "Estimated Values" is shown on the right. The plot displays two data series: "All samples" (blue dots) and "Training samples" (orange dots). The x-axis is labeled "Estimated Values" and ranges from -1.934 to 3.165. The y-axis is labeled "Target Values" and ranges from -1.934 to 3.165. The training samples are clustered around the diagonal line, indicating a good fit to the training data.

Execution Time: 00:00:18.3120474

Inspect Linechart of Correlation of Training and Validation Fitness



Agenda



- Objectives of the Tutorial
- Introduction
- Where to get HeuristicLab?
- Plugin Infrastructure
- Graphical User Interface
- Available Algorithms & Problems
- **Demonstration Part I: Working with HeuristicLab**
- **Demonstration Part II: Data-based Modeling**
- Some Additional Features
- Planned Features
- Team
- Suggested Readings
- Bibliography
- Questions & Answers

Some Additional Features

- HeuristicLab Hive
 - parallel and distributed execution of algorithms and experiments on many computers in a network
- Optimization Knowledge Base (OKB)
 - database to store algorithms, problems, parameters and results
 - open to the public
 - open for other frameworks
 - analyze and store characteristics of problem instances and problem classes
- External solution evaluation and simulation-based optimization
 - interface to couple HeuristicLab with other applications (MATLAB, Simulink, SciLab, AnyLogic, ...)
 - supports different protocols (command line parameters, TCP, ...)
- Parameter grid tests and meta-optimization
 - automatically create experiments to test large ranges of parameters
 - apply heuristic optimization algorithms to find optimal parameter settings for heuristic optimization algorithms



Planned Features

- Algorithms & Problems
 - steady-state genetic algorithm
 - unified tabu search for vehicle routing
 - estimation of distribution algorithms
 - evolution of arbitrary code (Robocode, controller, etc.)
 - ...
- Cloud Computing
 - port HeuristicLab Hive to Windows Azure
- Statistics
 - implement statistical tests and automated statistical analysis
- Have a look at the HeuristicLab roadmap
 - <http://dev.heuristiclab.com/trac.fcgi/roadmap>
- Any other ideas, requests or recommendations?
 - join our HeuristicLab Google group heuristiclab@googlegroups.com
 - write an e-mail to support@heuristiclab.com

HeuristicLab Team



Heuristic and Evolutionary Algorithms Laboratory (HEAL)
School of Informatics, Communications and Media
University of Applied Sciences Upper Austria

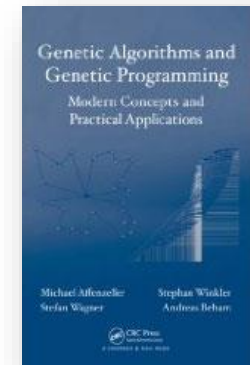
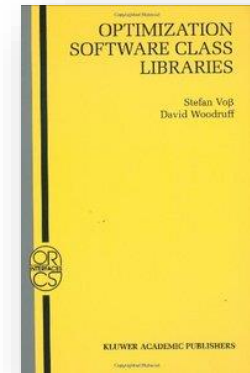
Softwarepark 11
A-4232 Hagenberg
AUSTRIA

WWW: <http://heal.heuristiclab.com>



Suggested Readings

- S. Voß, D. Woodruff (Edts.)
Optimization Software Class Libraries
Kluwer Academic Publishers, 2002
- M. Affenzeller, S. Winkler, S. Wagner, A. Beham
Genetic Algorithms and Genetic Programming
Modern Concepts and Practical Applications
CRC Press, 2009



Bibliography

- S. Wagner, M. Affenzeller
HeuristicLab: A generic and extensible optimization environment
Adaptive and Natural Computing Algorithms, pp. 538-541
Springer, 2005
- S. Wagner, S. Winkler, R. Braune, G. Kronberger, A. Beham, M. Affenzeller
Benefits of plugin-based heuristic optimization software systems
Computer Aided Systems Theory - EUROCAST 2007, Lecture Notes in Computer Science, vol. 4739, pp. 747-754
Springer, 2007
- S. Wagner, G. Kronberger, A. Beham, S. Winkler, M. Affenzeller
Modeling of heuristic optimization algorithms
Proceedings of the 20th European Modeling and Simulation Symposium, pp. 106-111
DIPTEM University of Genova, 2008
- S. Wagner, G. Kronberger, A. Beham, S. Winkler, M. Affenzeller
Model driven rapid prototyping of heuristic optimization algorithms
Computer Aided Systems Theory - EUROCAST 2009, Lecture Notes in Computer Science, vol. 5717, pp. 729-736
Springer, 2009
- S. Wagner
Heuristic optimization software systems - Modeling of heuristic optimization algorithms in the HeuristicLab software environment
Ph.D. thesis, Johannes Kepler University Linz, Austria, 2009.
- S. Wagner, A. Beham, G. Kronberger, M. Kommenda, E. Pitzer, M. Kofler, S. Vonolfen, S. Winkler, V. Dorfer, M. Affenzeller
HeuristicLab 3.3: A unified approach to metaheuristic optimization
Actas del séptimo congreso español sobre Metaheurísticas, Algoritmos Evolutivos y Bioinspirados (MAEB'2010), 2010
- S. Wagner, G. Kronberger, A. Beham, M. Kommenda, A. Scheibenpflug, E. Pitzer, S. Vonolfen, M. Kofler, S. Winkler, V. Dorfer, M. Affenzeller
Architecture and Design of the HeuristicLab Optimization Environment
Advanced Methods and Applications in Computational Intelligence, vol. 6, pp. 197-261, Springer, 2014
- Detailed list of all publications of the HEAL research group: <http://research.fh-ooe.at/de/orgunit/356#showpublications>

Questions & Answers



<http://dev.heuristiclab.com>

heuristiclab@googlegroups.com

<http://www.youtube.com/heuristiclab>

<http://www.facebook.com/heuristiclab>