



# 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

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**HEAL**

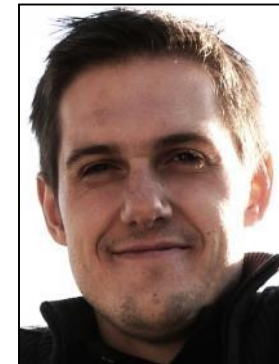
Heuristic and Evolutionary  
Algorithms Laboratory



**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

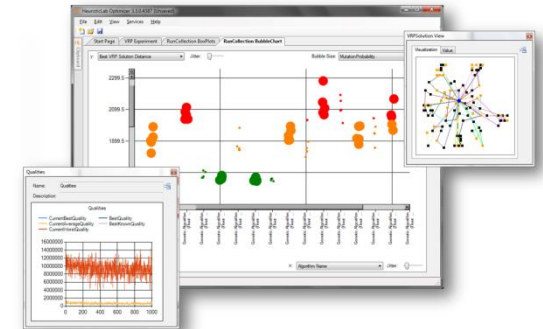
# Objectives of the Tutorial



- 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 3.3.14 "Denver"



# Where to get HeuristicLab?



- Download binaries
  - deployed as ZIP archives
  - latest stable version 3.3.14 "Denver"
    - released on July 24th, 2016
  - daily trunk builds
  - <http://dev.heuristiclab.com/download>
- Check out sources
  - SVN repository
  - HeuristicLab 3.3.14 tag
    - <http://svn.heuristiclab.com/svn/core/tags/3.3.14>
  - Stable development version
    - <http://svn.heuristiclab.com/svn/core/stable>
- License
  - GNU General Public License (Version 3)
- System requirements
  - Microsoft .NET Framework 4.5
  - enough RAM and CPU power ;-)

A screenshot of the HeuristicLab website. The page has a white background with a navigation bar at the top containing links for Home, News, Download, Features, Documentation, Support, and Search. Below the navigation bar is a main content area with a heading 'HeuristicLab' and a sub-heading 'A Paradigm-Independent and Extensible Environment for Heuristic Optimization'. The main content area contains a paragraph of text, a video player titled 'HeuristicLab Tour', a list of features, a download button for version 3.3.14, and a section for 'Research & Publications'. The footer contains a 'Thank you!' message, a logo for ReSharper, and a 'Download in other formats' link.

HeuristicLab  
A Paradigm-Independent and Extensible Environment for Heuristic Optimization

Home News Download Features Documentation Support Search

will: WikiStart Start Page Index History

HeuristicLab is a framework for heuristic and evolutionary algorithms that is developed by members of the **Heuristic and Evolutionary Algorithms Laboratory (HEAL)** since 2002. The developers team of HeuristicLab uses this page to coordinate efforts to improve and extend HeuristicLab.

**HeuristicLab Tour** YouTube

- Graphical User Interface
- Algorithm Prototyping
- Evolutionary Algorithms
- Genetic Programming
- Data Analysis
- Simulation-based Optimization
- Experiment Design and Analysis
- Plugin-based Architecture

**Download HeuristicLab 3.3**  
Version 3.3.14 .NET4 Any CPU  
Changelog

We know that many people are using HeuristicLab in business, research and teaching activities. Please drop us an e-mail, if you're using HeuristicLab in your teaching activities, if you have interesting business cases, or if you would like to get in contact for a research collaboration. See the support section for contact details. It would be great to hear from you!

Research & Publications License Contribute

Join the discussion at the HeuristicLab group  
Email:   
Subscribe Visit group

Imprint: Statement of the ownership/authorship of this webpage plus contact information can be found here.

**Thank you!**

**ReSharper** A big thank you JetBrains for supporting us with a free license of ReSharper every year!

Download in other formats: Plain Text

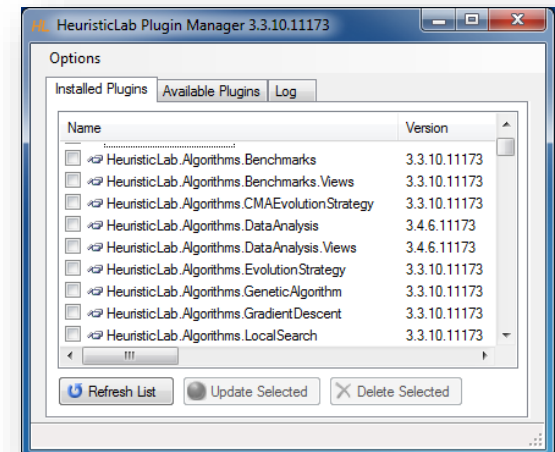
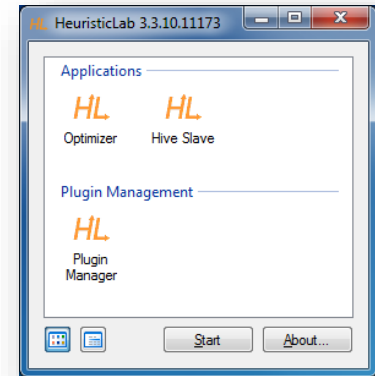
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trac  
Powered by Trac 1.0.1  
By Edgewall Software.

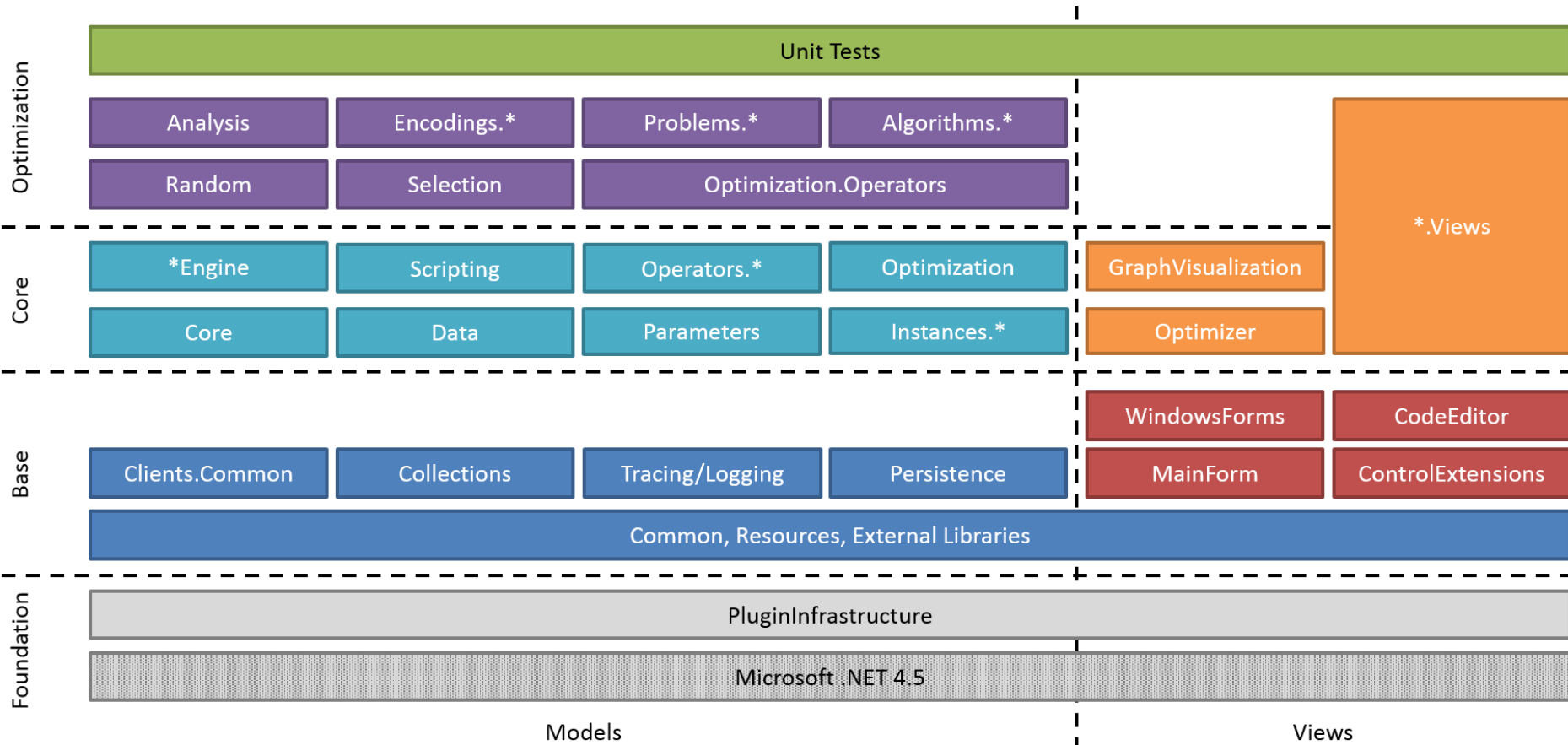
Visit the Trac open source project at <http://trac.edgewall.org/>

# Plugin Infrastructure

- HeuristicLab consists of many assemblies
  - 150+ plugins in HeuristicLab 3.3.14
  - 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



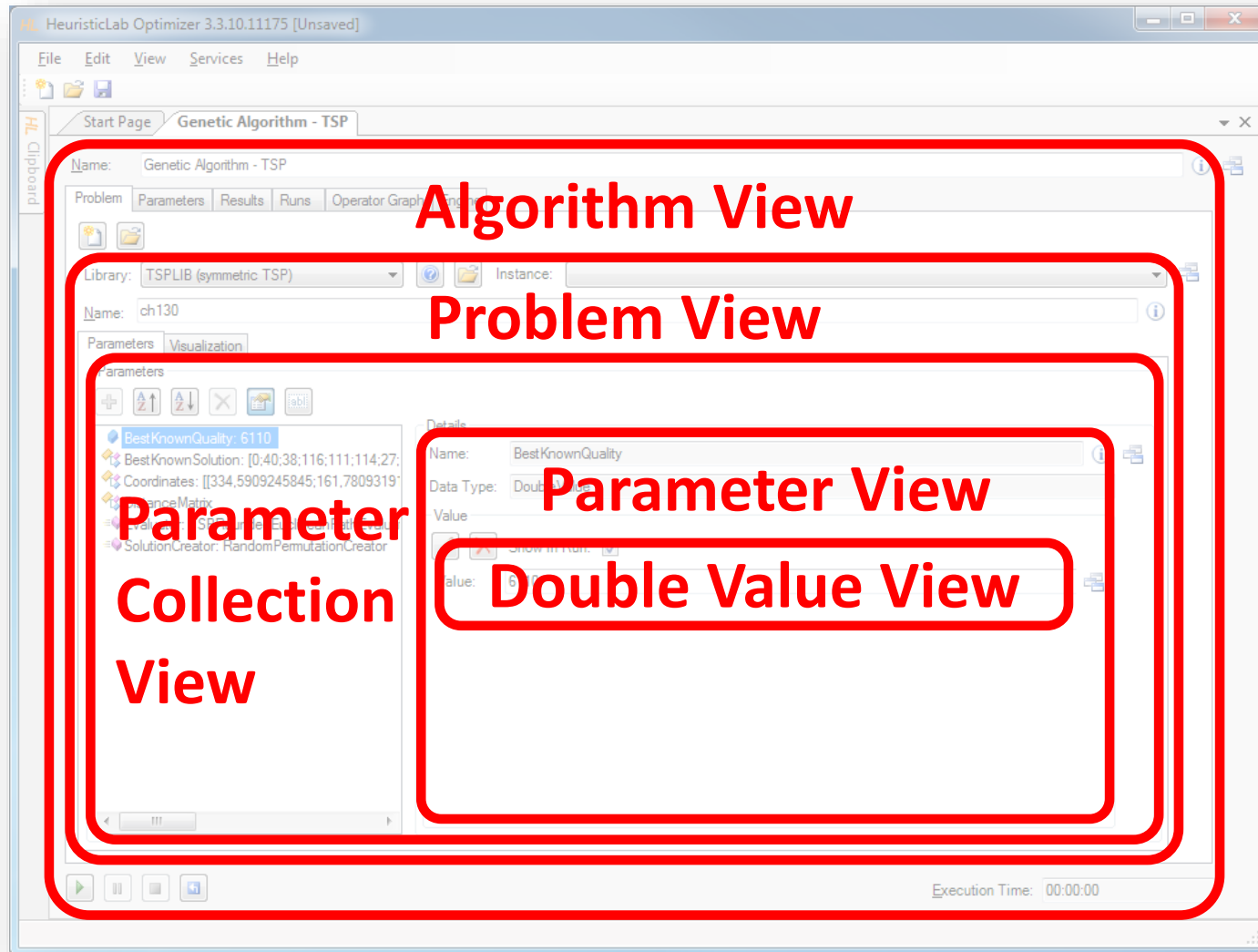


# Graphical User Interface



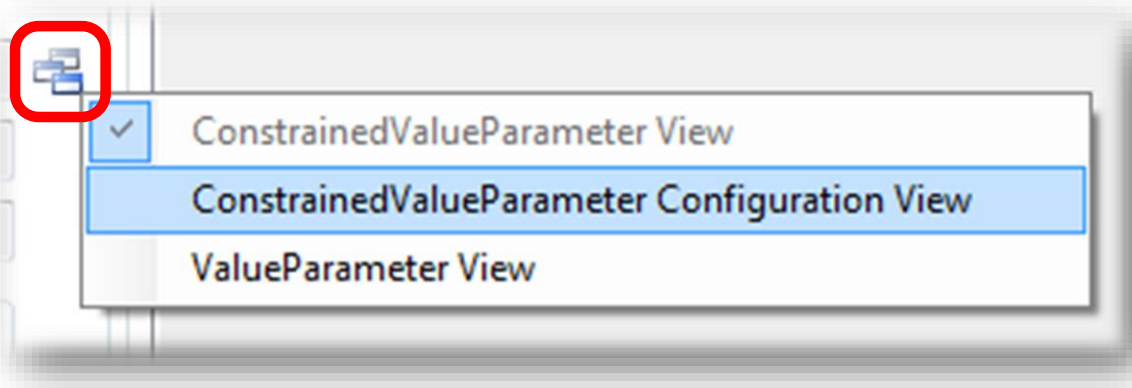
- HeuristicLab GUI is made up of views
  - views are visual representations of content objects
  - views are composed in the same way as their content
  - views and content objects are loosely coupled
  - multiple different views may exist for the same content
- Drag & Drop
  - views support drag & drop 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 (OSGA)
- Island Genetic Algorithm
- Island Offspring Selection Genetic Algorithm
- Parameter-less Population Pyramid (P3)
- SASEGASA
- Relevant Alleles Preserving GA (RAPGA)
- Aged-Layered Population Structure (ALPS)
- 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
- Gradient Boosted Trees
- Gradient Boosted Regression

## Additional Algorithms

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

# Available Problems

## Combinatorial Problems

- Traveling Salesman
- Probabilistic Traveling Salesman
- Vehicle Routing
- Knapsack
- Bin Packing
- NK[P,Q]
- Job Shop Scheduling
- Linear Assignment
- Quadratic Assignment
- OneMax
- Orienteering
- Deceptive trap
- Deceptive trap step
- HIFF

## Genetic Programming Problems

- Test Problems (Even Parity, MUX)
- Symbolic Classification
- Symbolic Regression
- Symbolic Time-Series Prognosis
- Artificial Ant
- Lawn Mower
- Robocode
- Grammatical Evolution

## Additional Problems

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

# Agenda



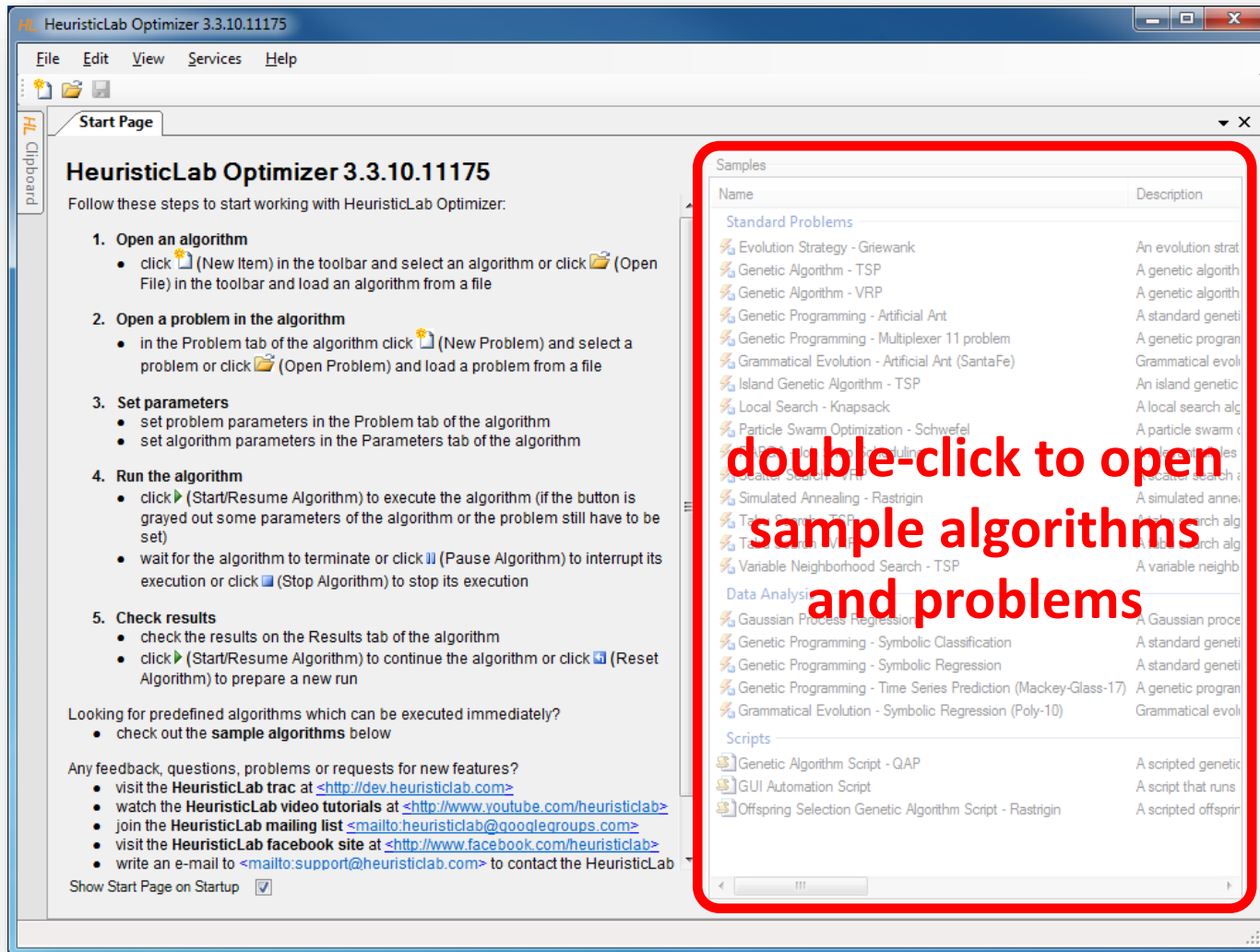
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# Demonstration Part I: Working with HeuristicLab



- 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

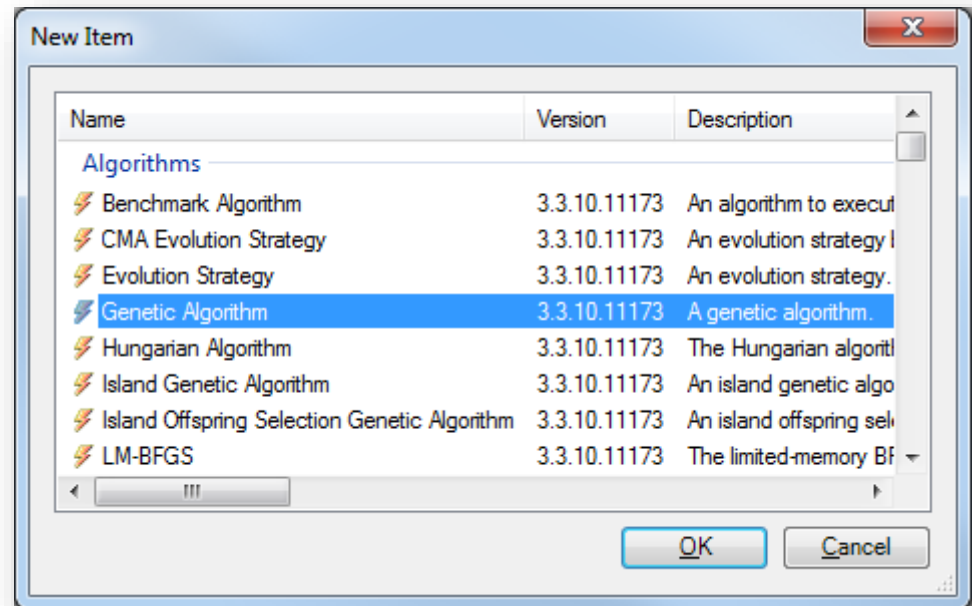
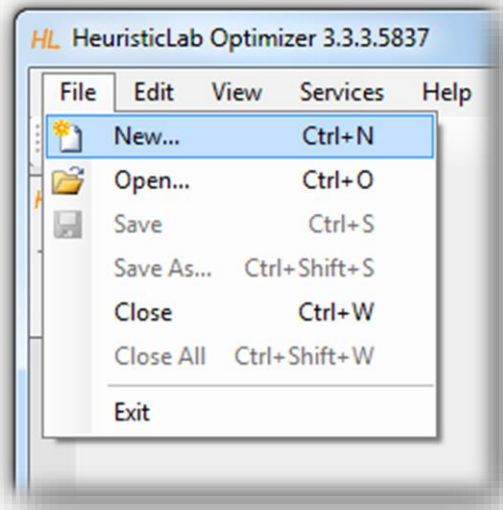
Show Start Page on Startup

Name	Description
<b>Standard Problems</b>	
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
Scatter Search - TSP	A scatter search a
Simulated Annealing - Rastrigin	A simulated anneal
Tabu Search - TSP	A tabu search alg
Variable Neighborhood Search - TSP	A variable neighb
<b>Data Analysis</b>	
Gaussian Process Regression	A Gaussian proces
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
<b>Scripts</b>	
Genetic Algorithm Script - QAP	A scripted genetic
GUI Automation Script	A script that runs
Offspring Selection Genetic Algorithm Script - Rastrigin	A scripted offsprir

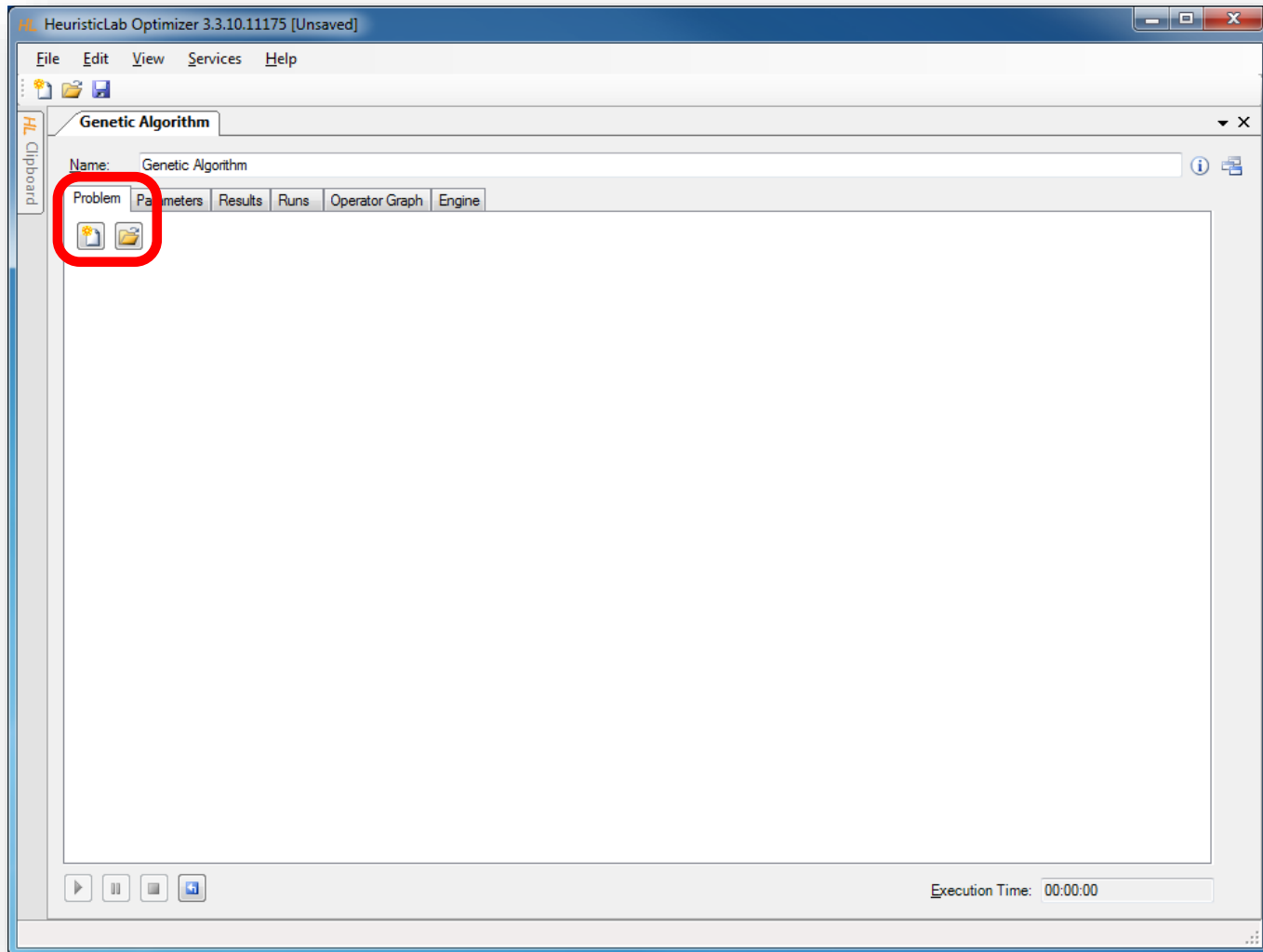
double-click to open  
sample algorithms  
and problems



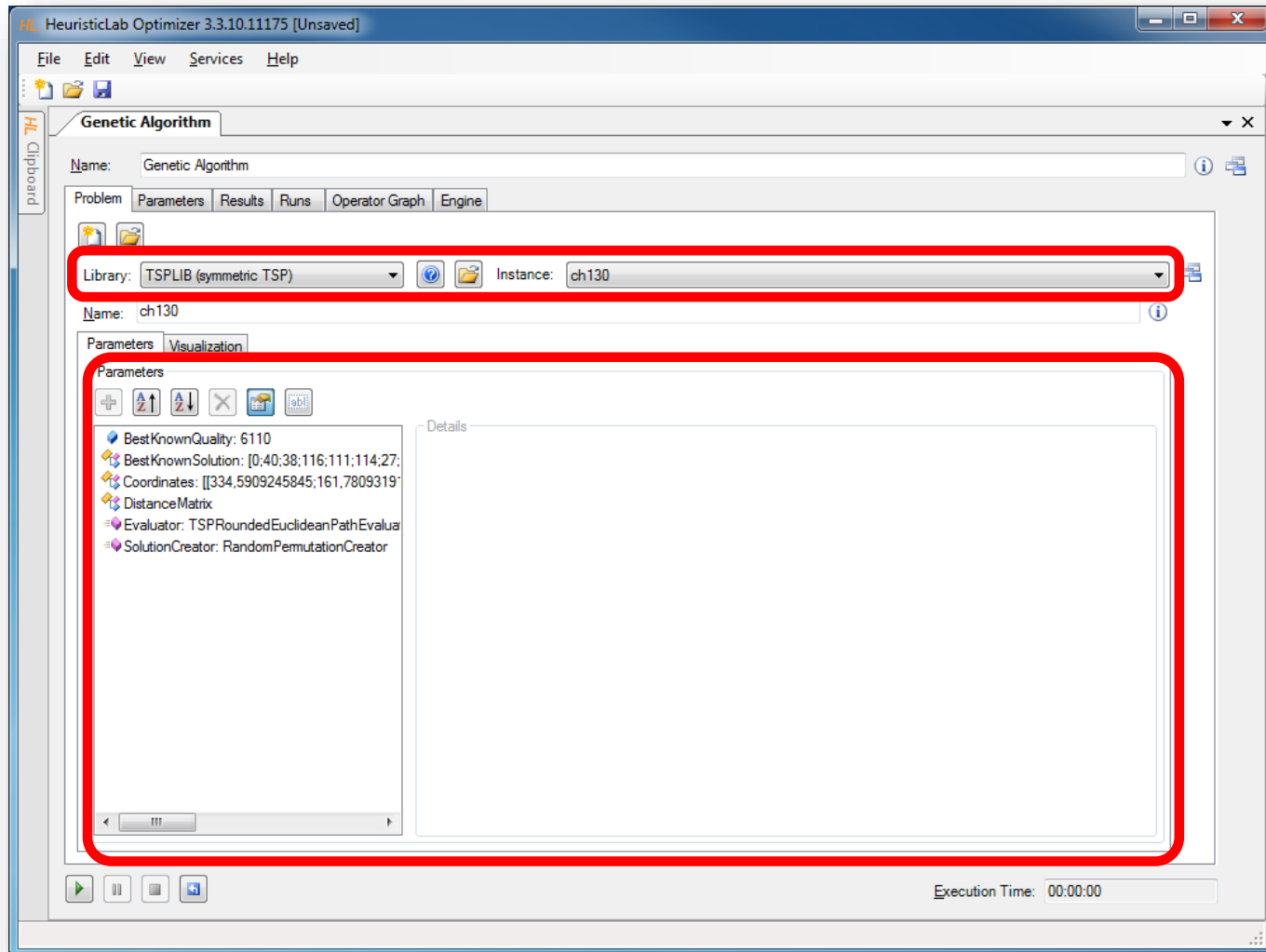
# Create Algorithm



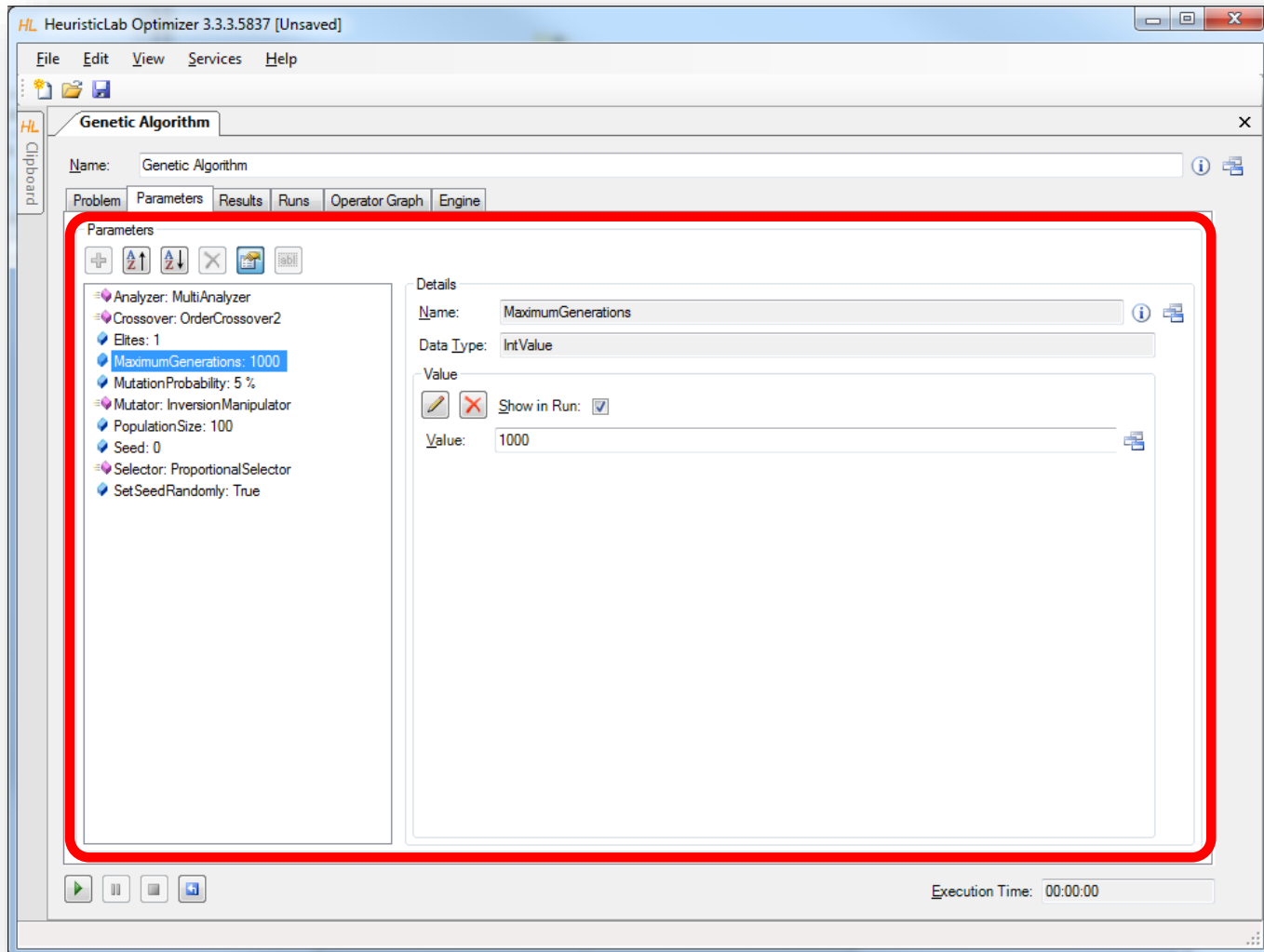
# Create or Load Problem



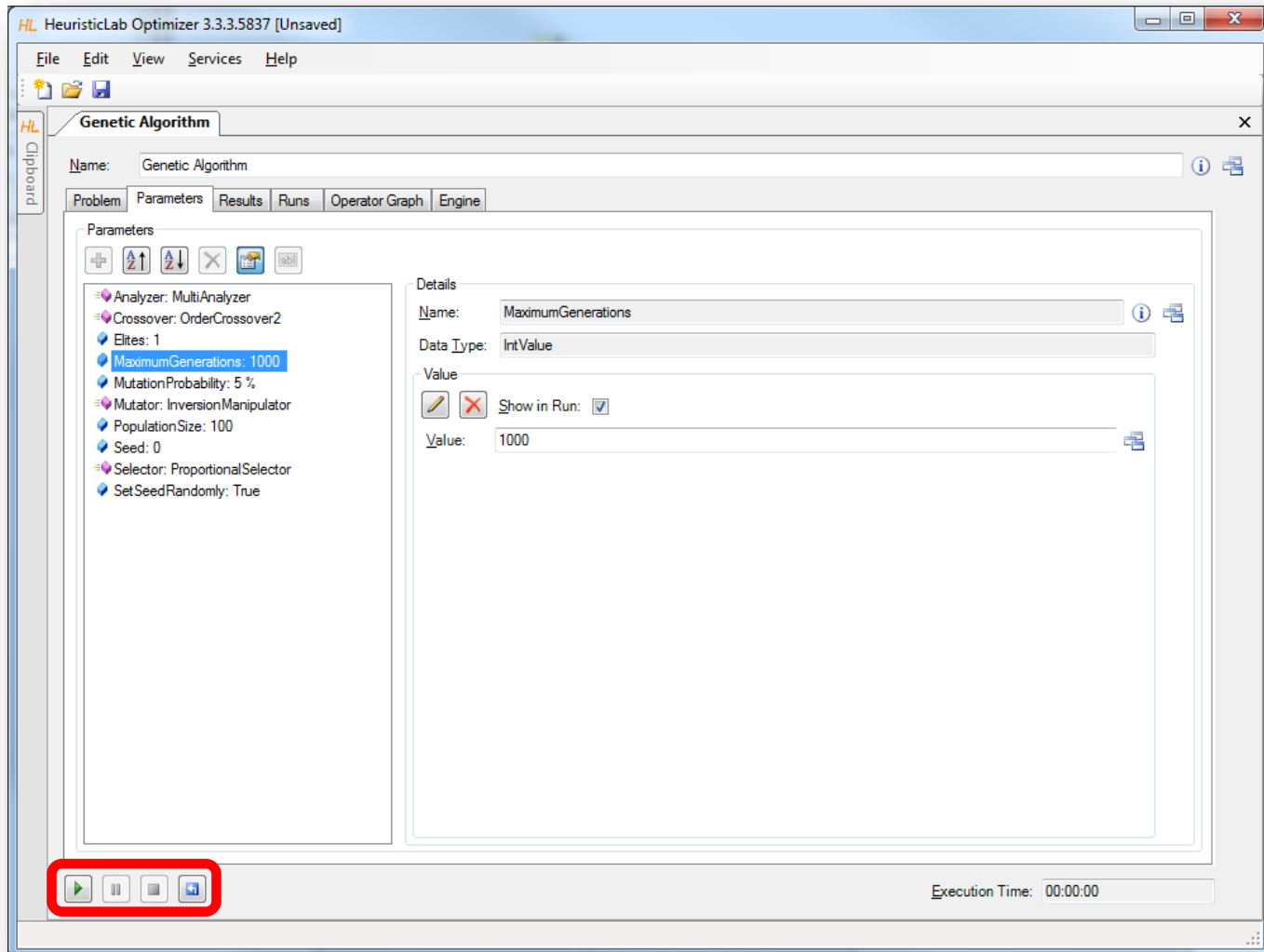
# Import or Parameterize Problem Data



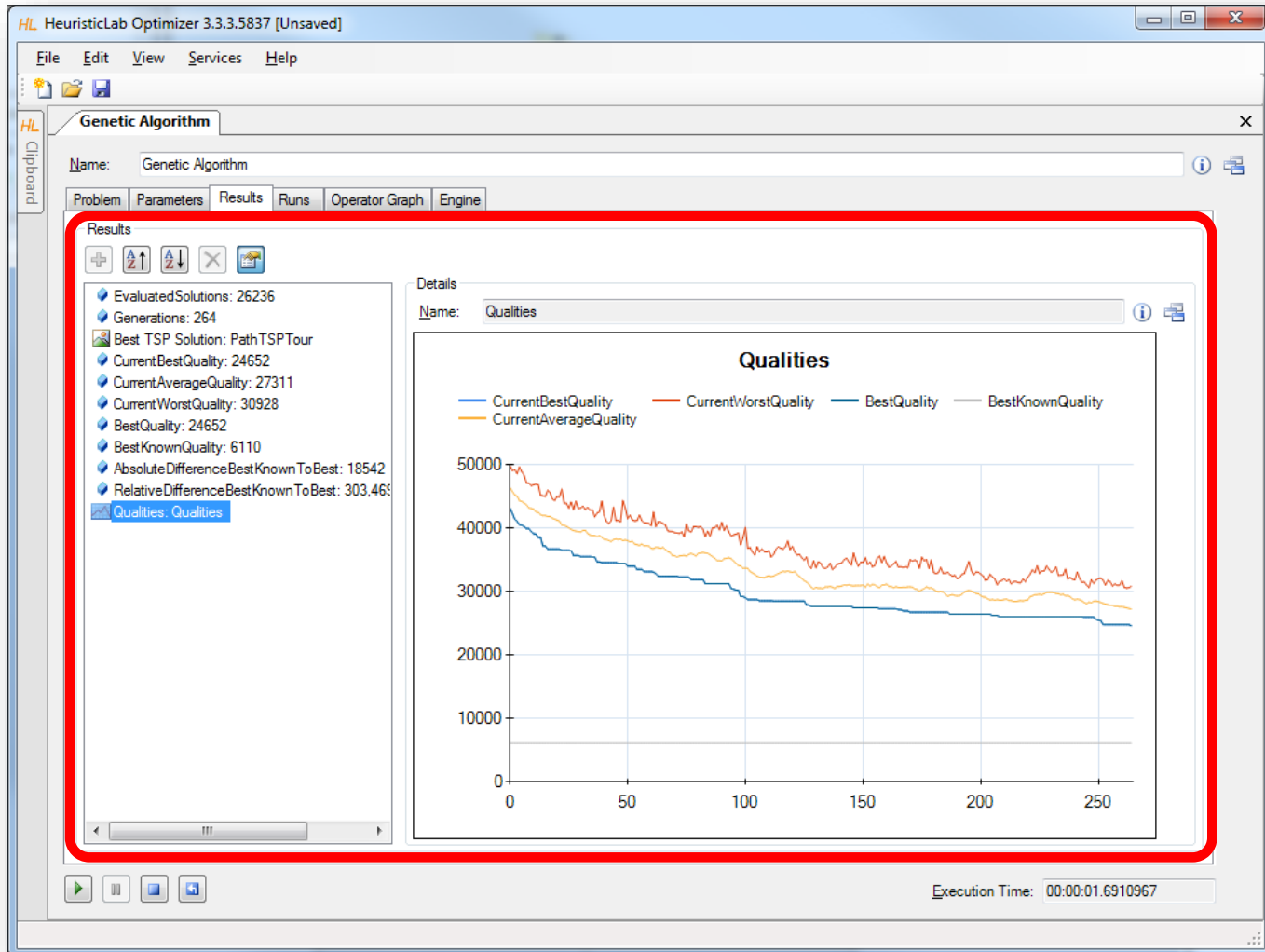
# Parameterize Algorithm



# Start, Pause, Resume, Stop and Reset

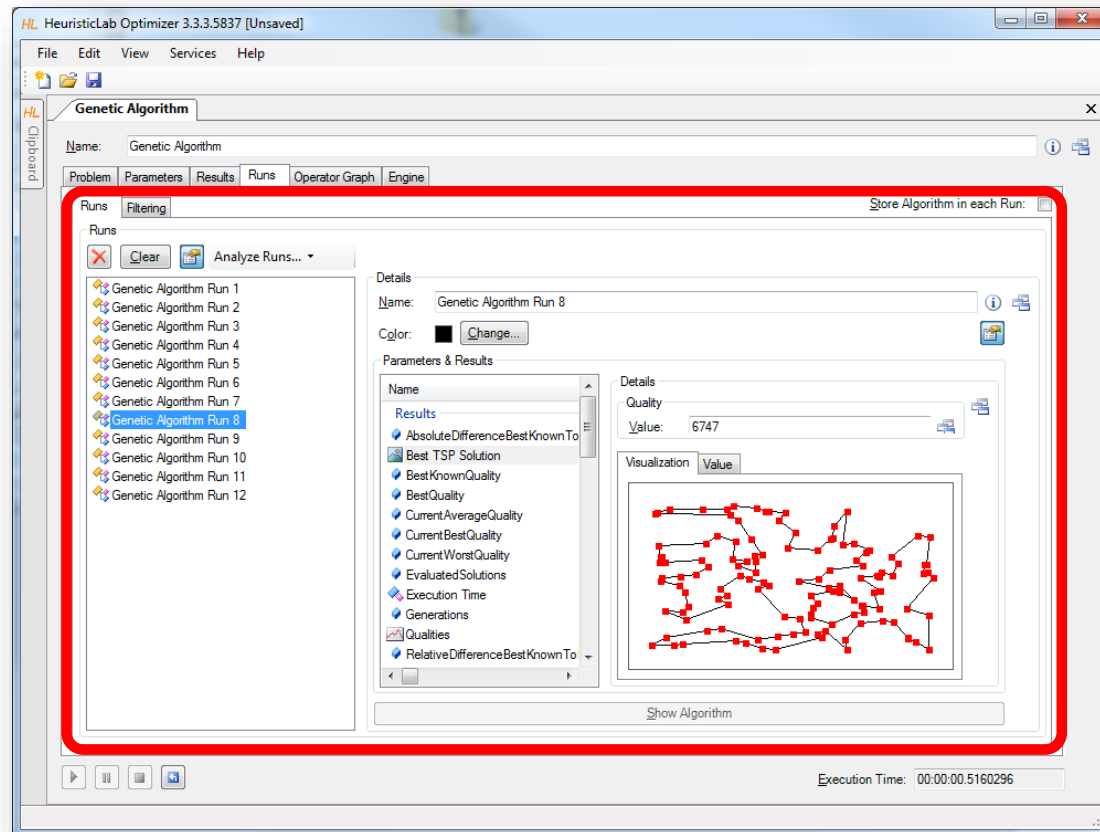


# Inspect Results



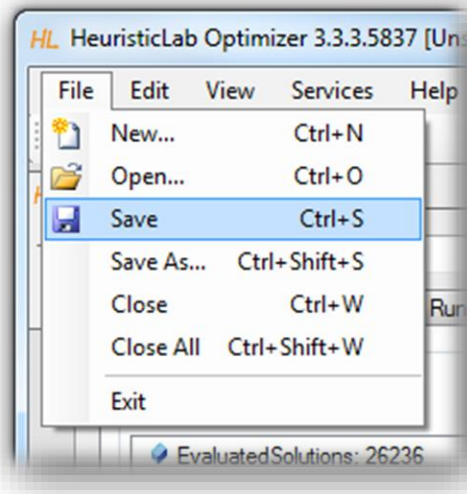
# Compare Runs

- 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

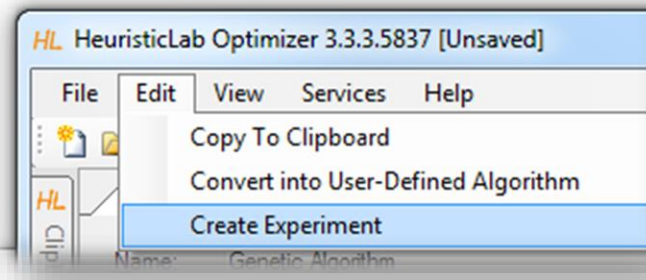
- Save to and load from disk
  - HeuristicLab items (i.e., algorithms, problems, experiments, ...) can be saved to and loaded from a file
  - algorithms can be paused, saved, loaded and resumed
  - data format is custom compressed XML
  - saving and loading files might take several minutes
  - saving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



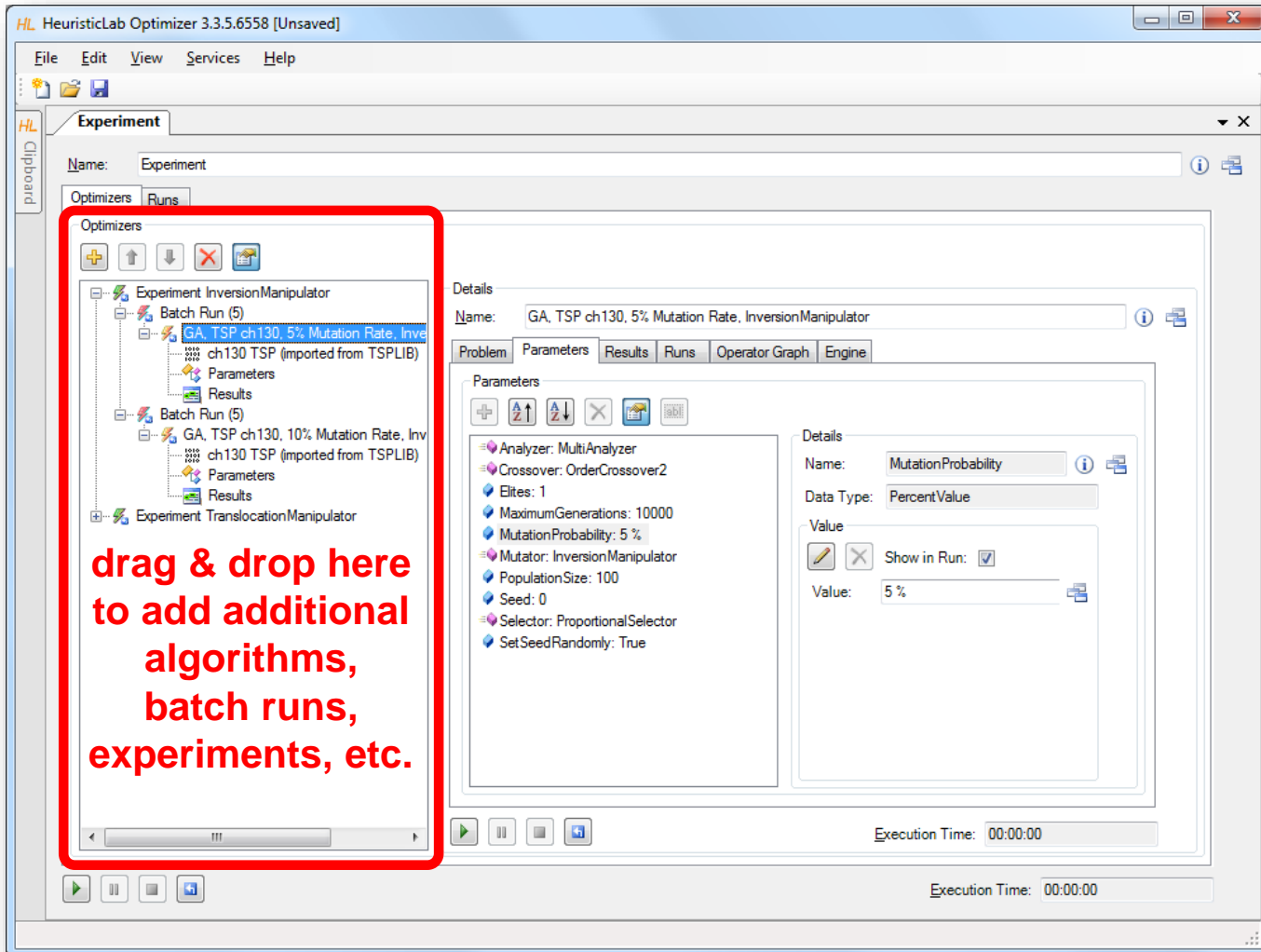


# Create Batch Runs and Experiments

- 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

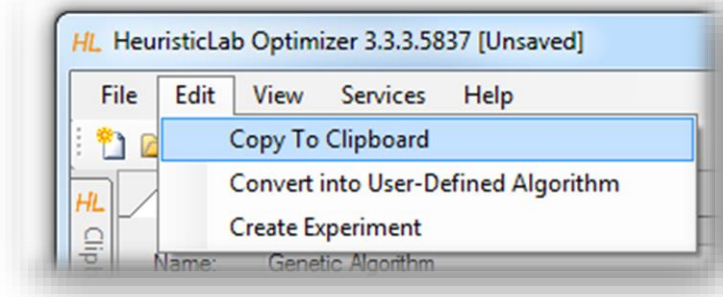


The screenshot displays the HeuristicLab Optimizer interface. The main window is titled "HL HeuristicLab Optimizer 3.3.5.6558 [Unsaved]". The interface is divided into several sections:

- Experiment Section:** Shows the "Experiment" configuration with a name field set to "Experiment". Below it, there are tabs for "Optimizers" and "Runs". The "Optimizers" tab is active, showing a tree view of the experiment structure. A red box highlights this tree view, containing the following text: **drag & drop here to add additional algorithms, batch runs, experiments, etc.**
- Details Section:** Shows the configuration for the selected optimizer, "GA, TSP ch130, 5% Mutation Rate, InversionManipulator". It includes tabs for "Problem", "Parameters", "Results", "Runs", "Operator Graph", and "Engine". The "Parameters" tab is active, showing a list of parameters such as "Analyzer: MultiAnalyzer", "Crossover: OrderCrossover2", "Elites: 1", "MaximumGenerations: 10000", "MutationProbability: 5%", "Mutator: InversionManipulator", "PopulationSize: 100", "Seed: 0", "Selector: ProportionalSelector", and "SetSeedRandomly: True".
- Execution Time:** A field at the bottom right shows "Execution Time: 00:00:00".

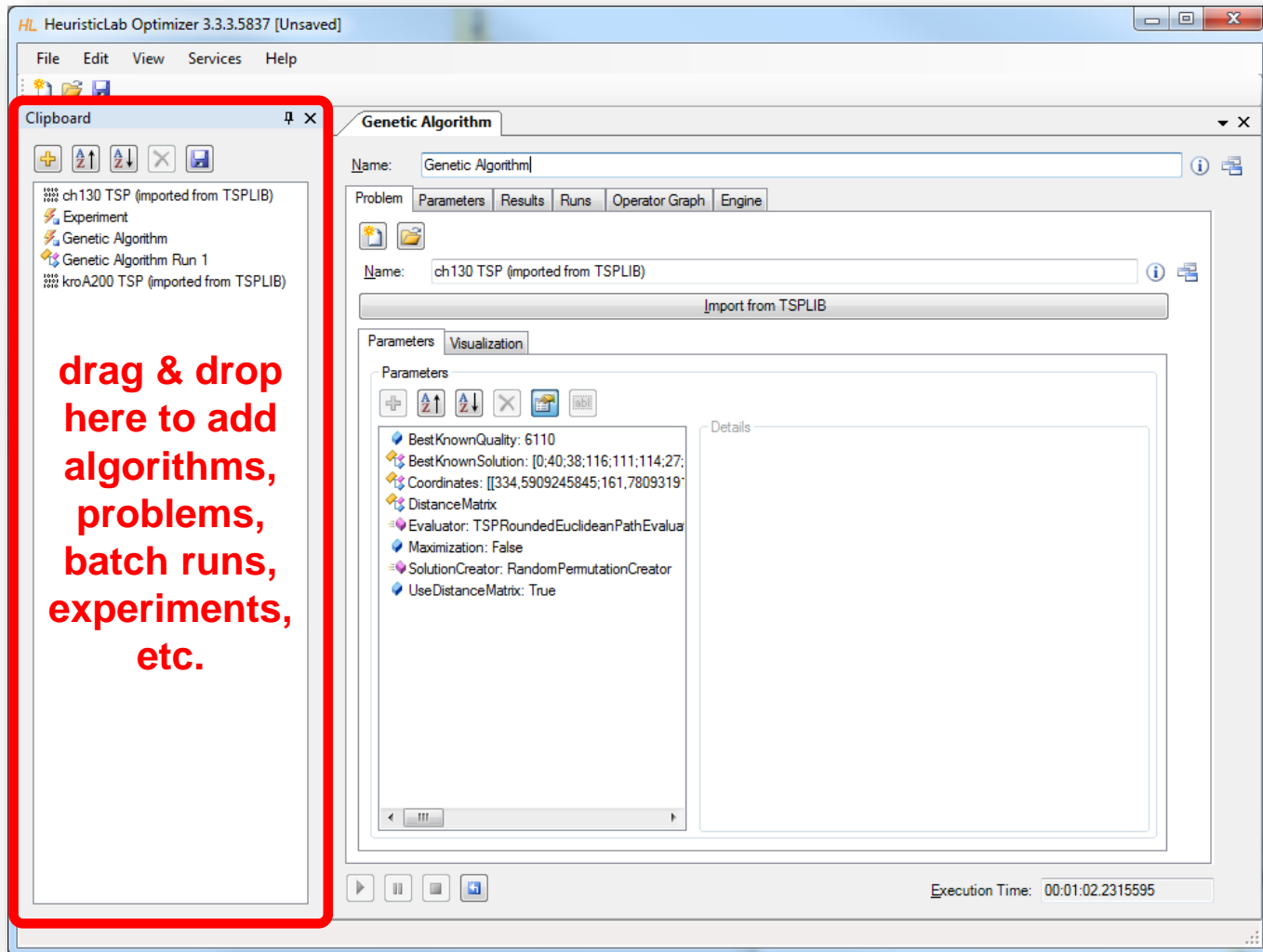
# Clipboard

- 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

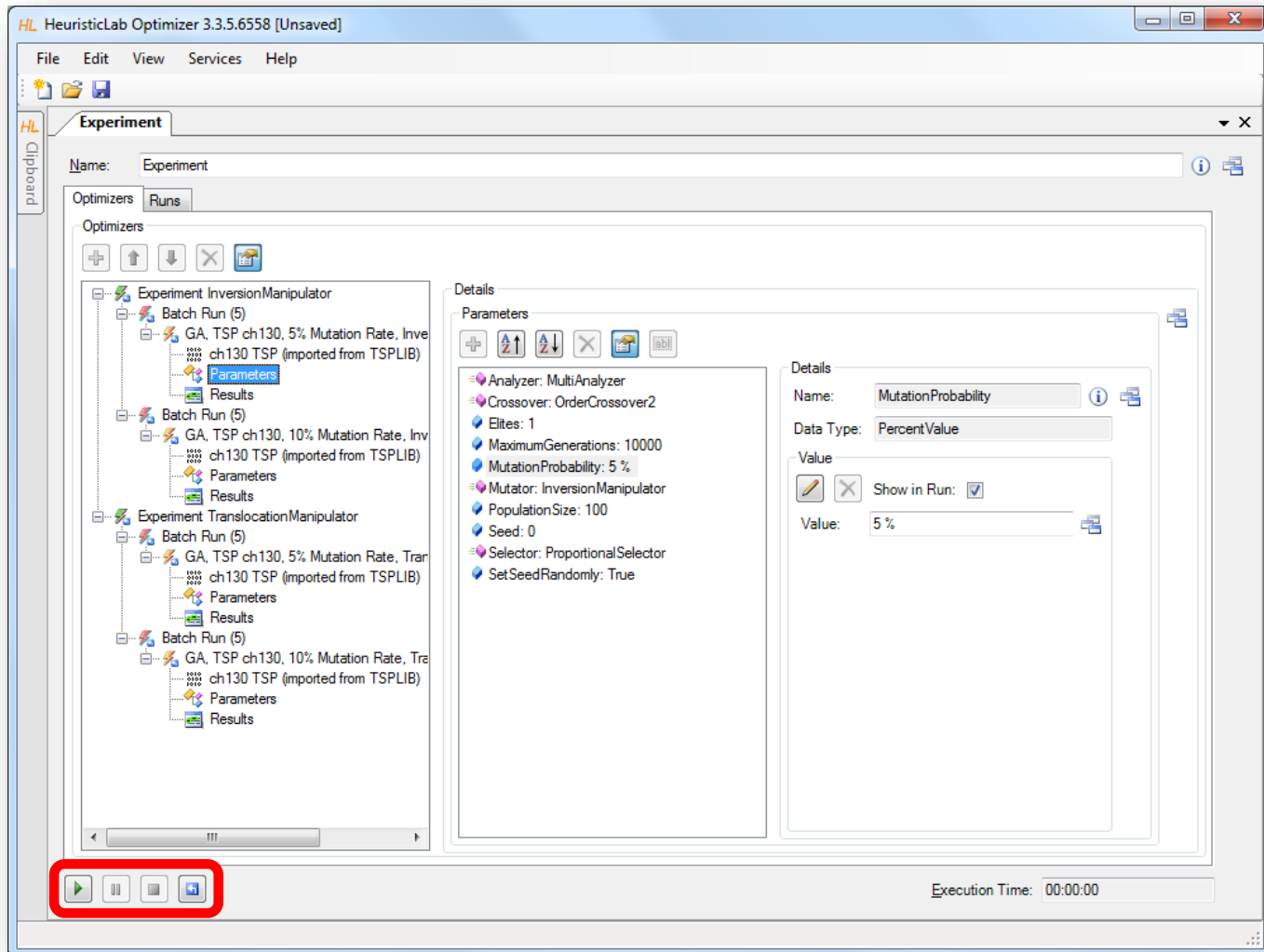


- Show items
  - double-click on an item in the clipboard to show its view
- Save and restore clipboard content
  - click on the save button to write the clipboard content to disk
  - clipboard is automatically restored when HeuristicLab is started the next time

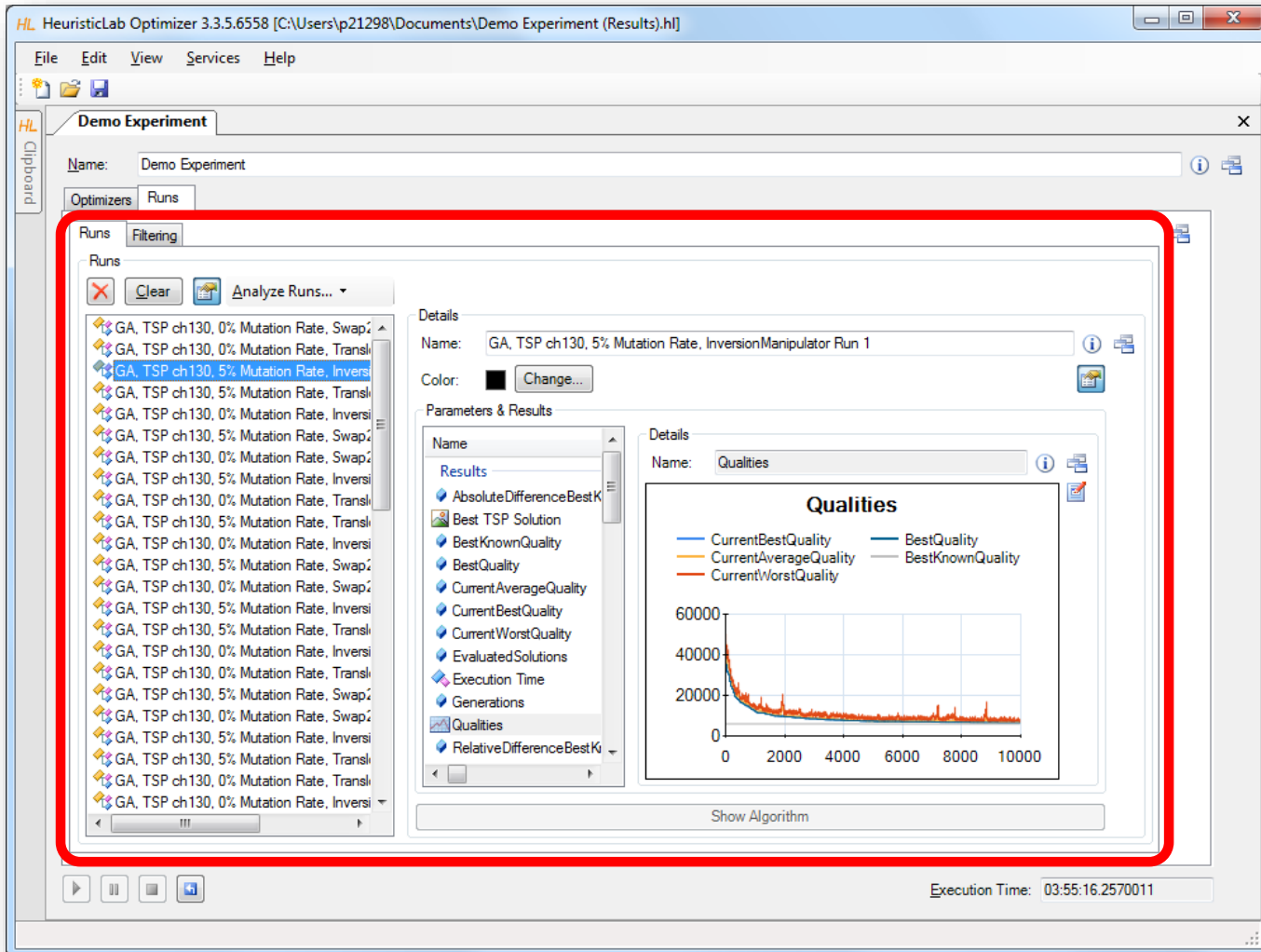
# Clipboard



# Start, Pause, Resume, Stop, Reset



# Compare Runs



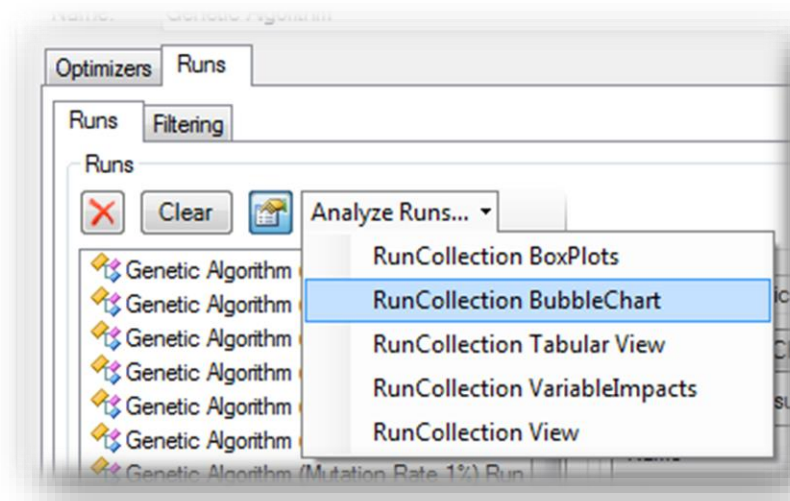
The screenshot displays the HeuristicLab Optimizer interface. The main window is titled "HL HeuristicLab Optimizer 3.3.5.6558 [C:\Users\p21298\Documents\Demo Experiment (Results).hl]". The interface is divided into several sections:

- Runs List:** A list of runs is shown, each with a small icon and a description. The runs are filtered by "GA, TSP ch130, 0% Mutation Rate, Swap?" and "GA, TSP ch130, 5% Mutation Rate, InversionManipulator Run 1".
- Details Panel:** The selected run is "GA, TSP ch130, 5% Mutation Rate, InversionManipulator Run 1". The "Color" is set to black. The "Parameters & Results" section shows a list of results, with "Qualities" selected.
- Qualities Graph:** A line graph titled "Qualities" plots the performance of the run 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 and CurrentAverageQuality lines start at approximately 60,000 and rapidly decrease, stabilizing around 10,000 after about 2,000 generations. The CurrentWorstQuality line starts at approximately 40,000 and also decreases, stabilizing around 10,000. The BestKnownQuality line is a horizontal line at approximately 10,000.

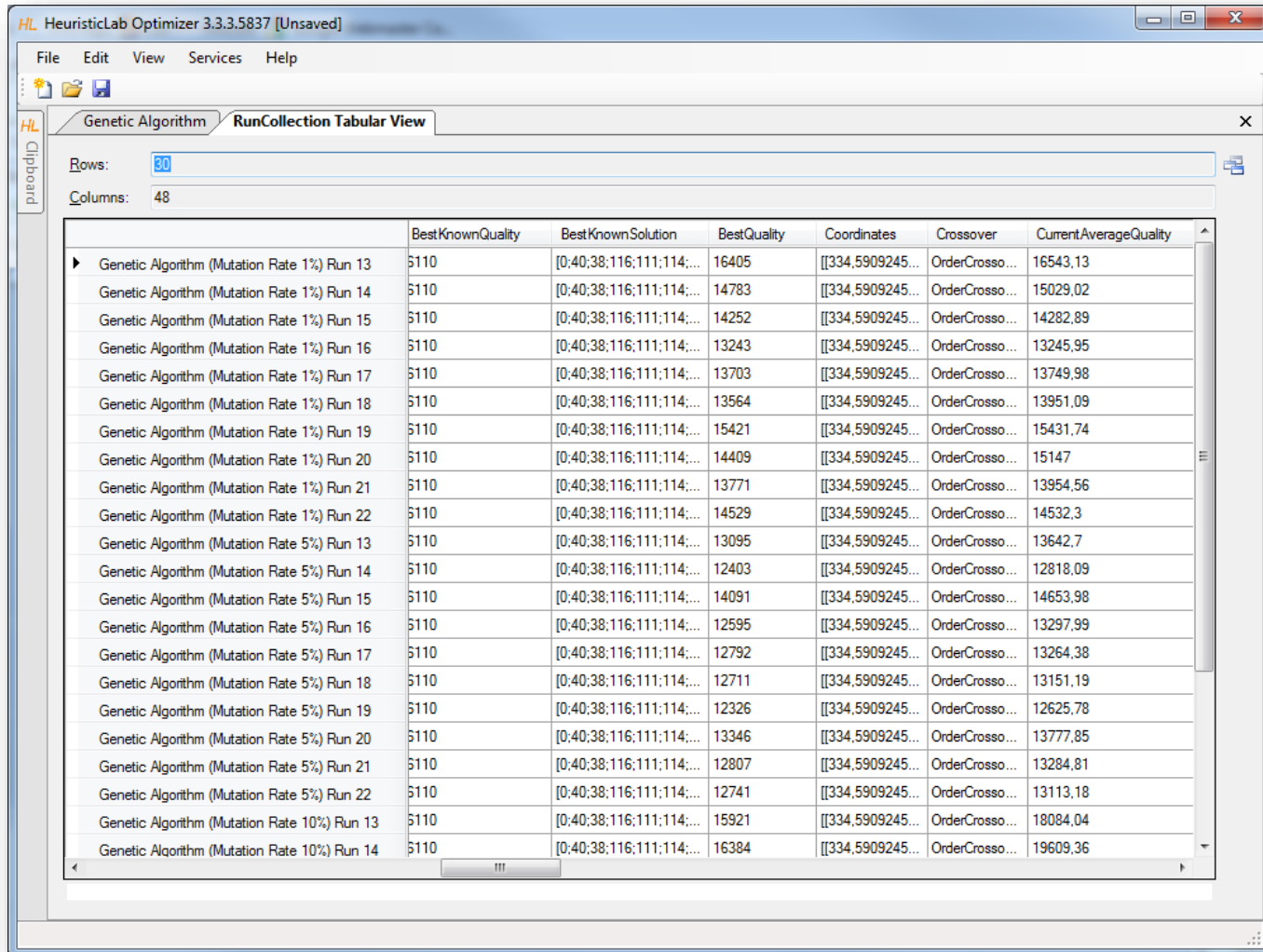
At the bottom of the window, the "Execution Time" is displayed as "03:55:16.2570011".

# 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

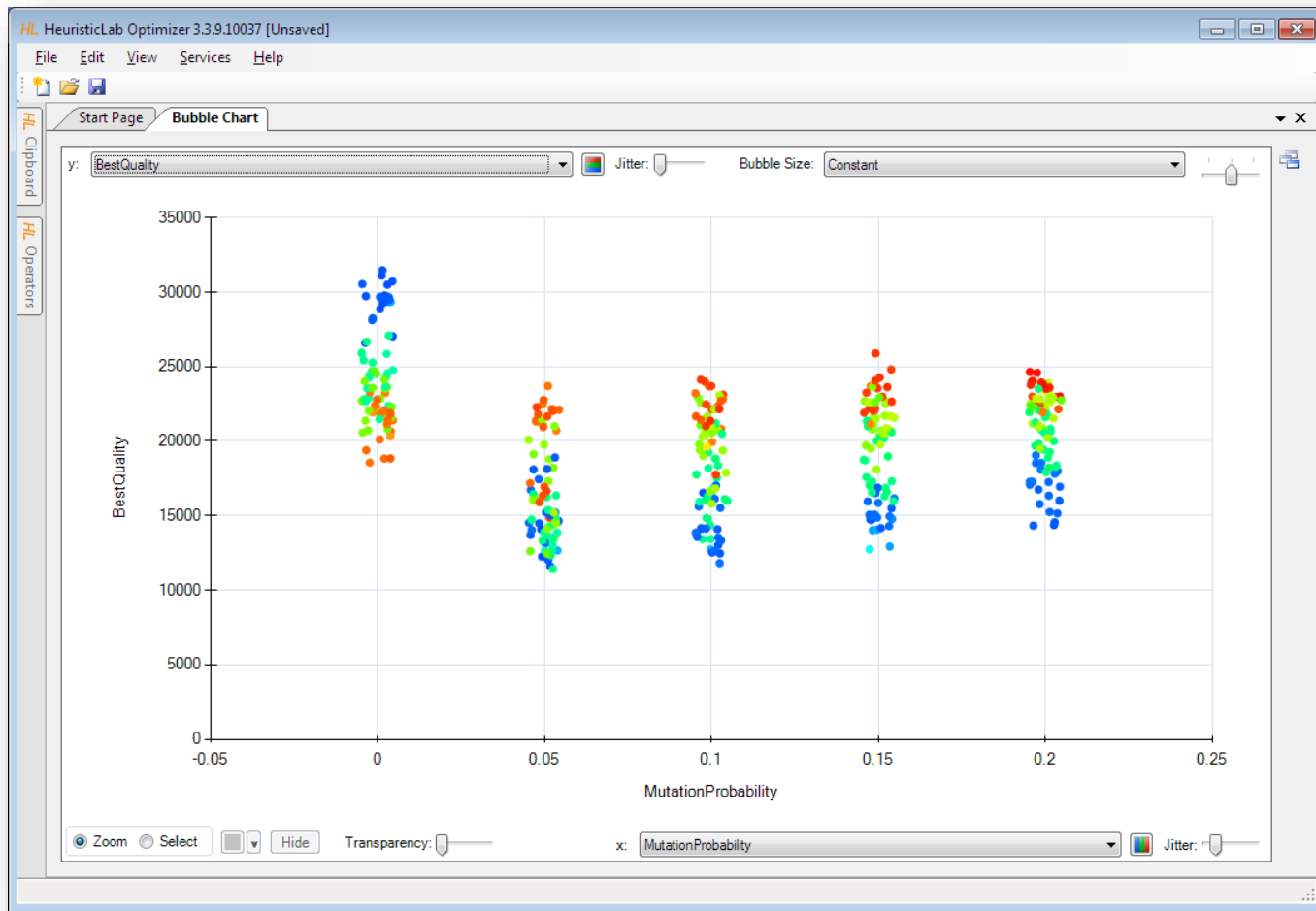


# Runs – Tabular View



- 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

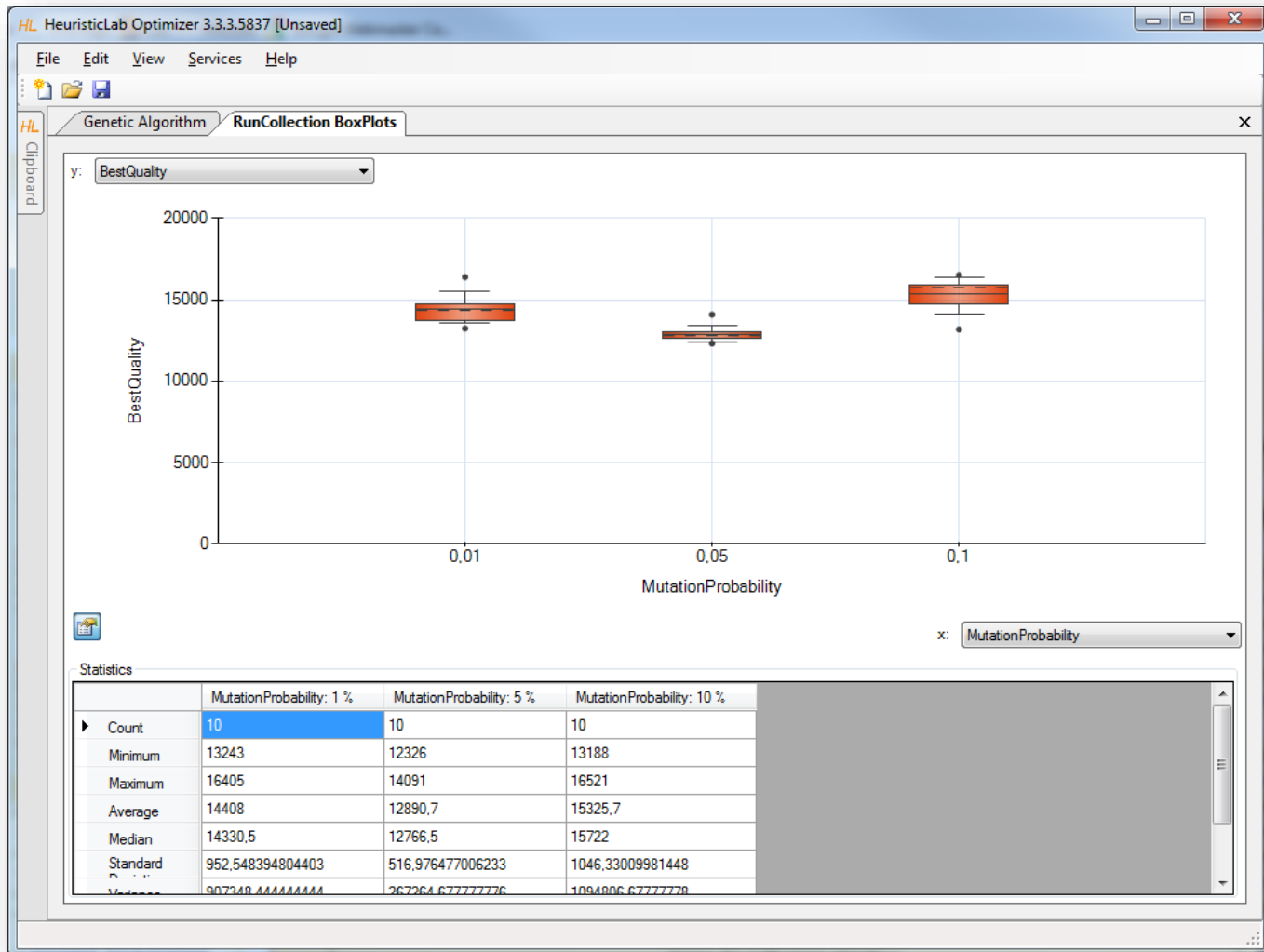
# Runs – BubbleChart



# 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

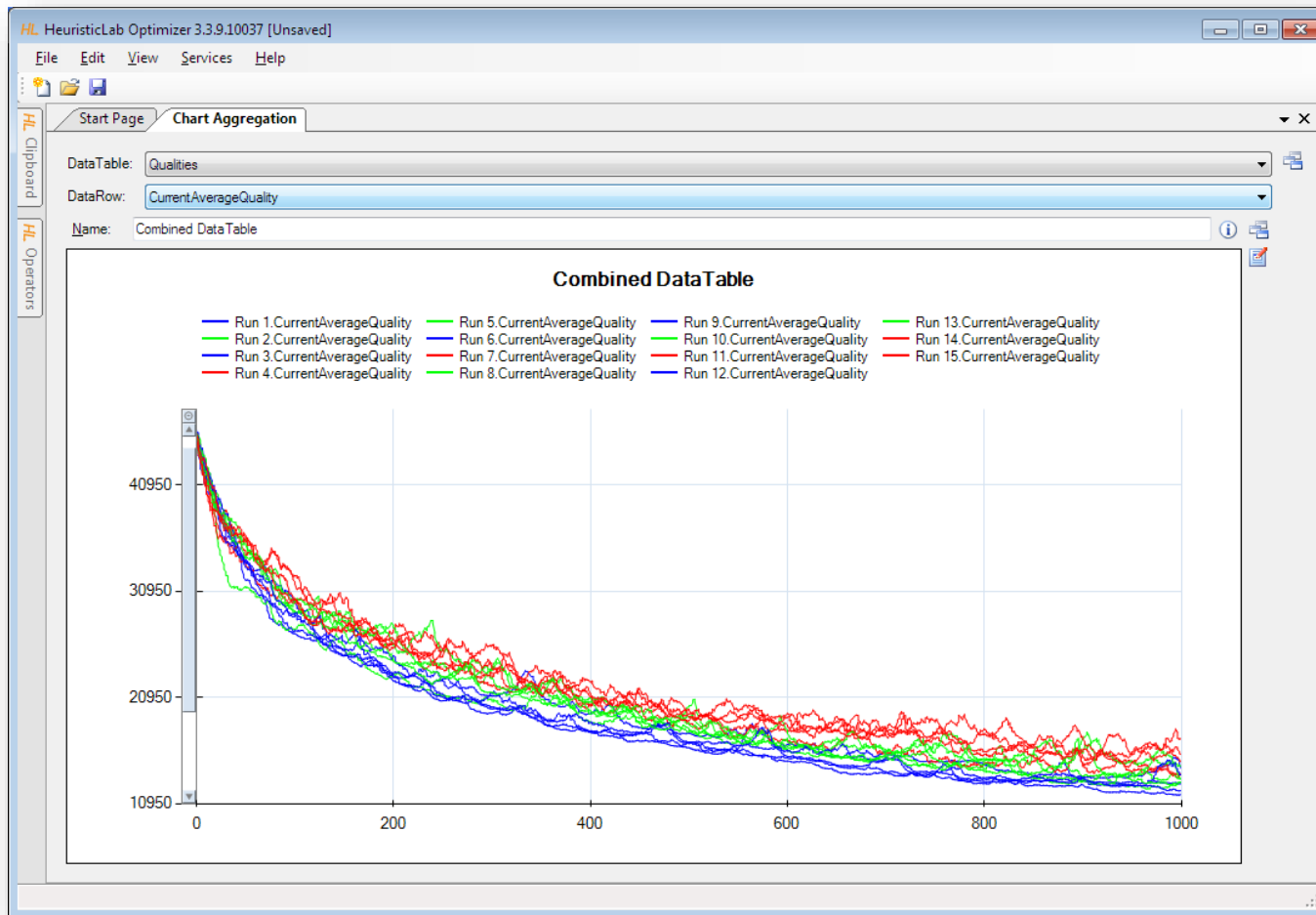
# Runs – BoxPlots



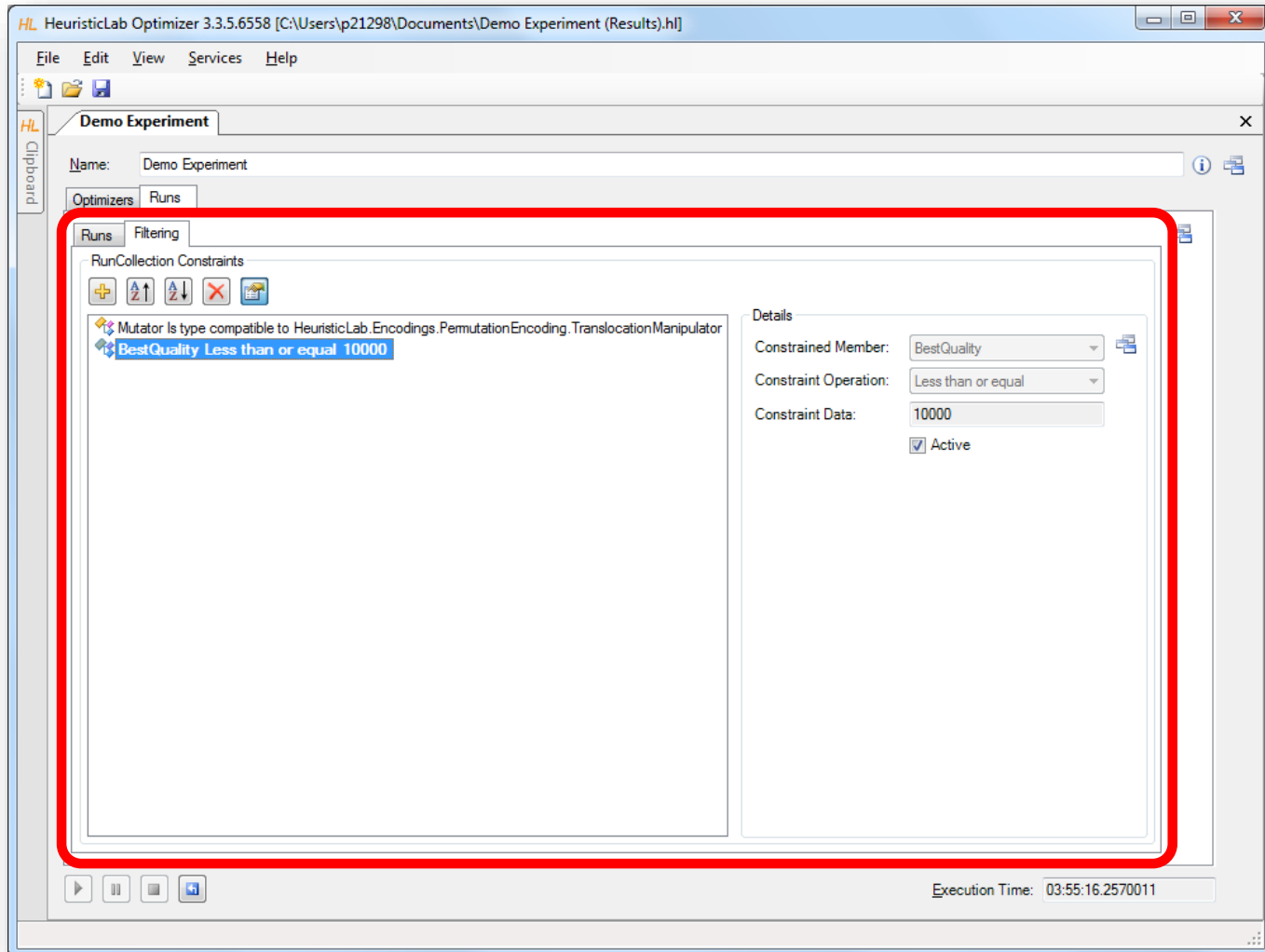
# Runs – BoxPlots

- 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



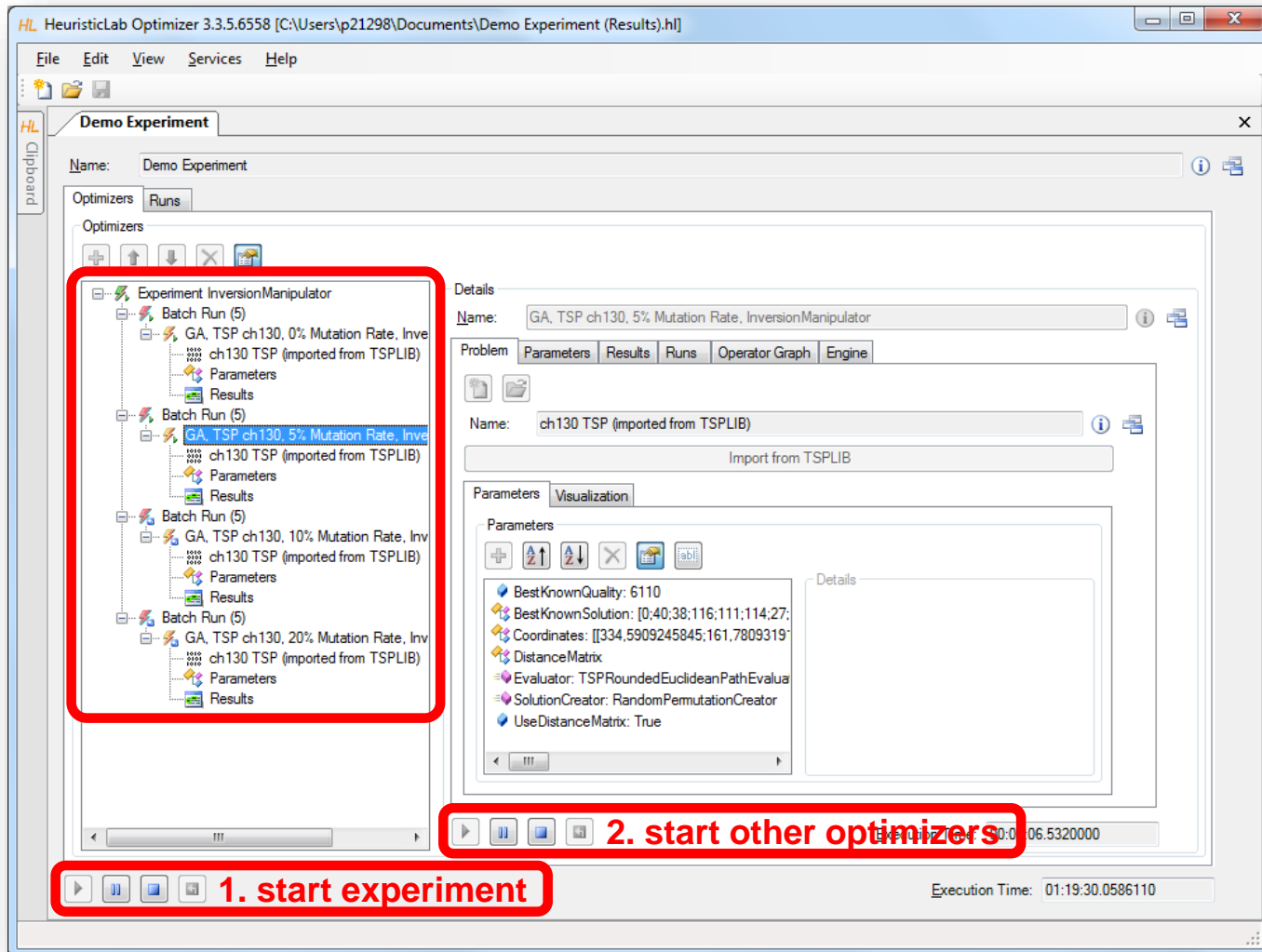
# Multi-core CPUs and Parallelization



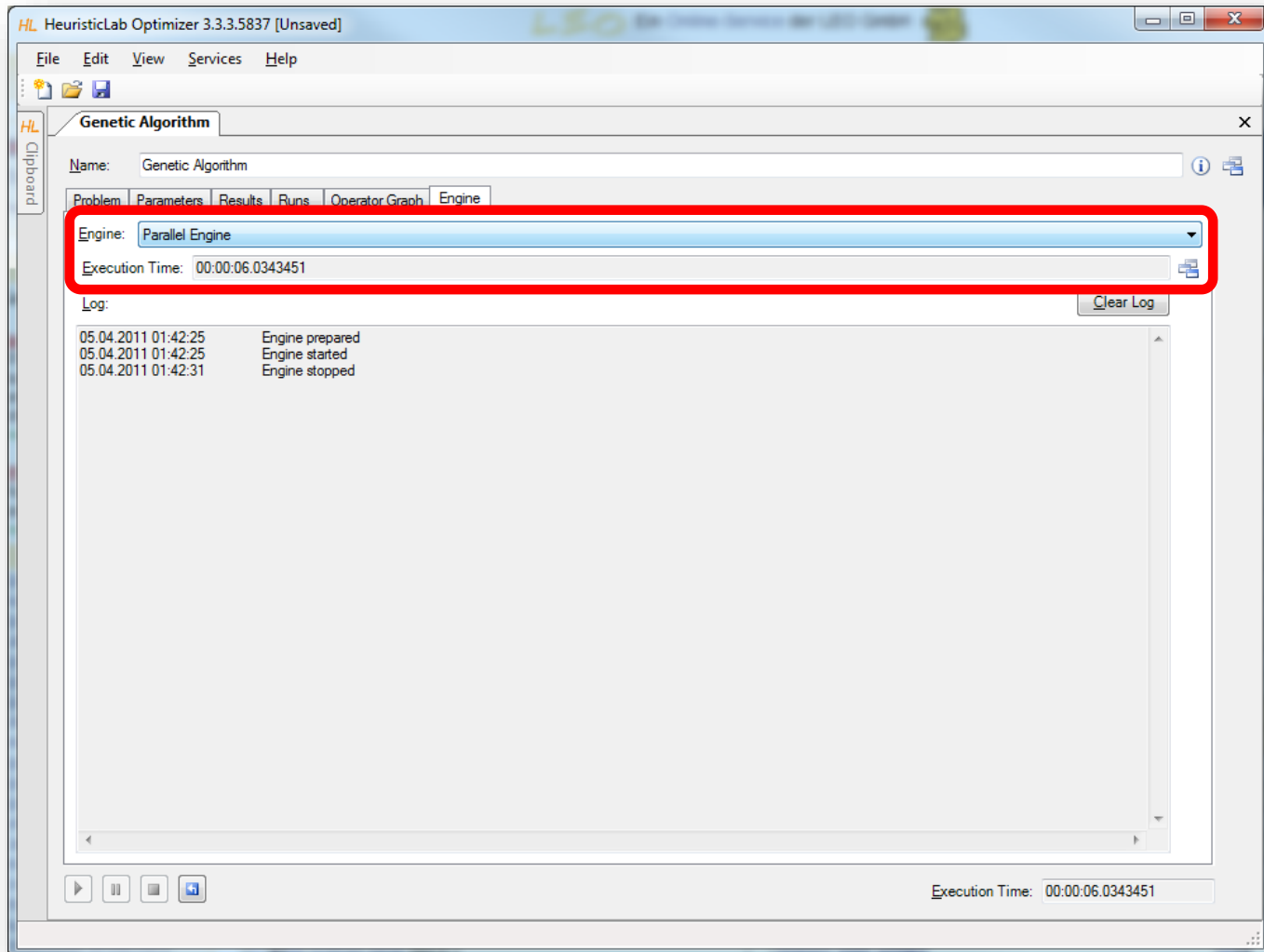
- Parallel execution of optimizers in experiments
  - optimizers in an experiment are executed sequentially from top to bottom per default
  - experiments support parallel execution of their optimizers
  - select a not yet executed optimizer and start it manually to utilize another core
  - execution 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



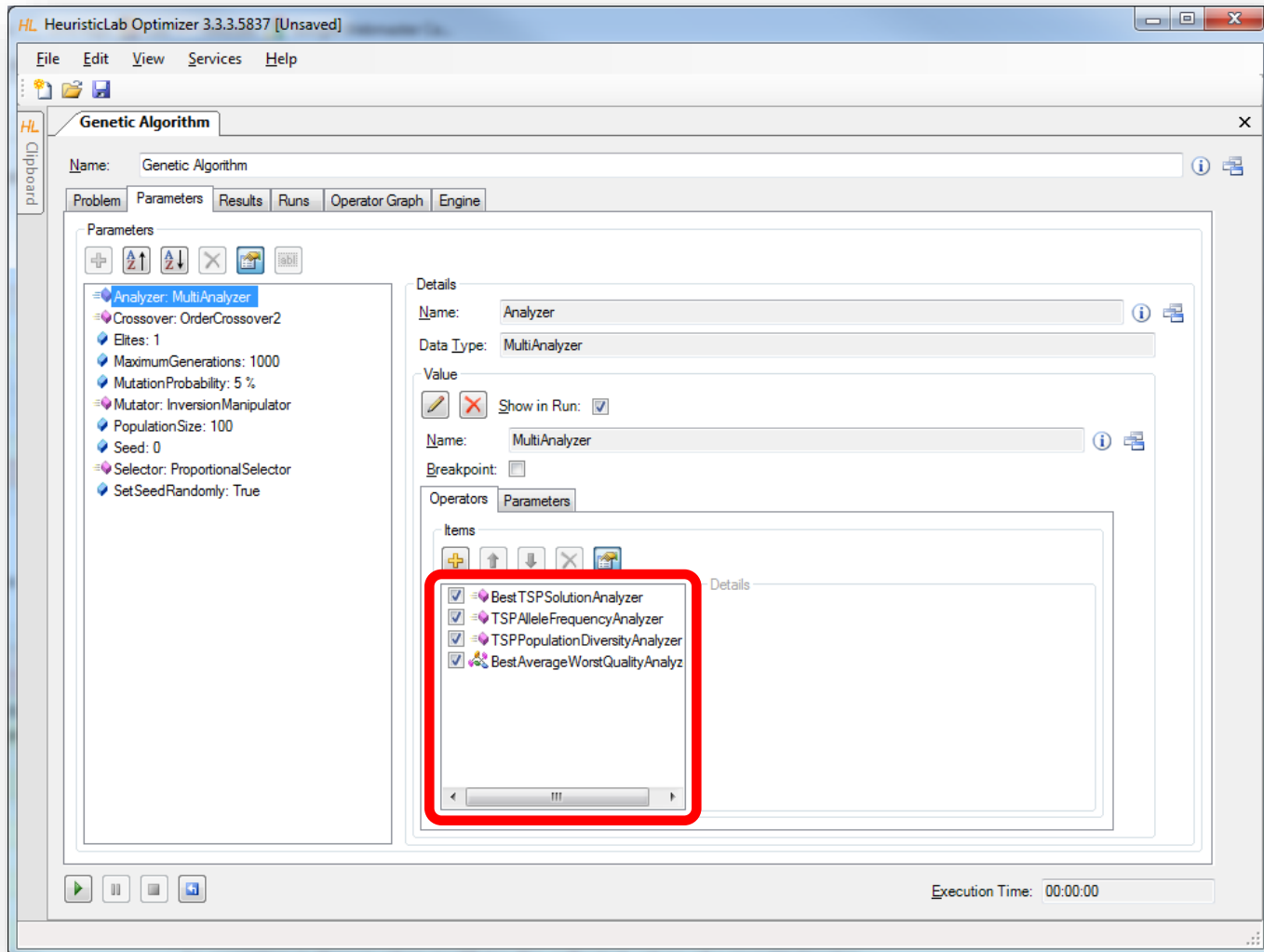
# Parallel Execution of Algorithms



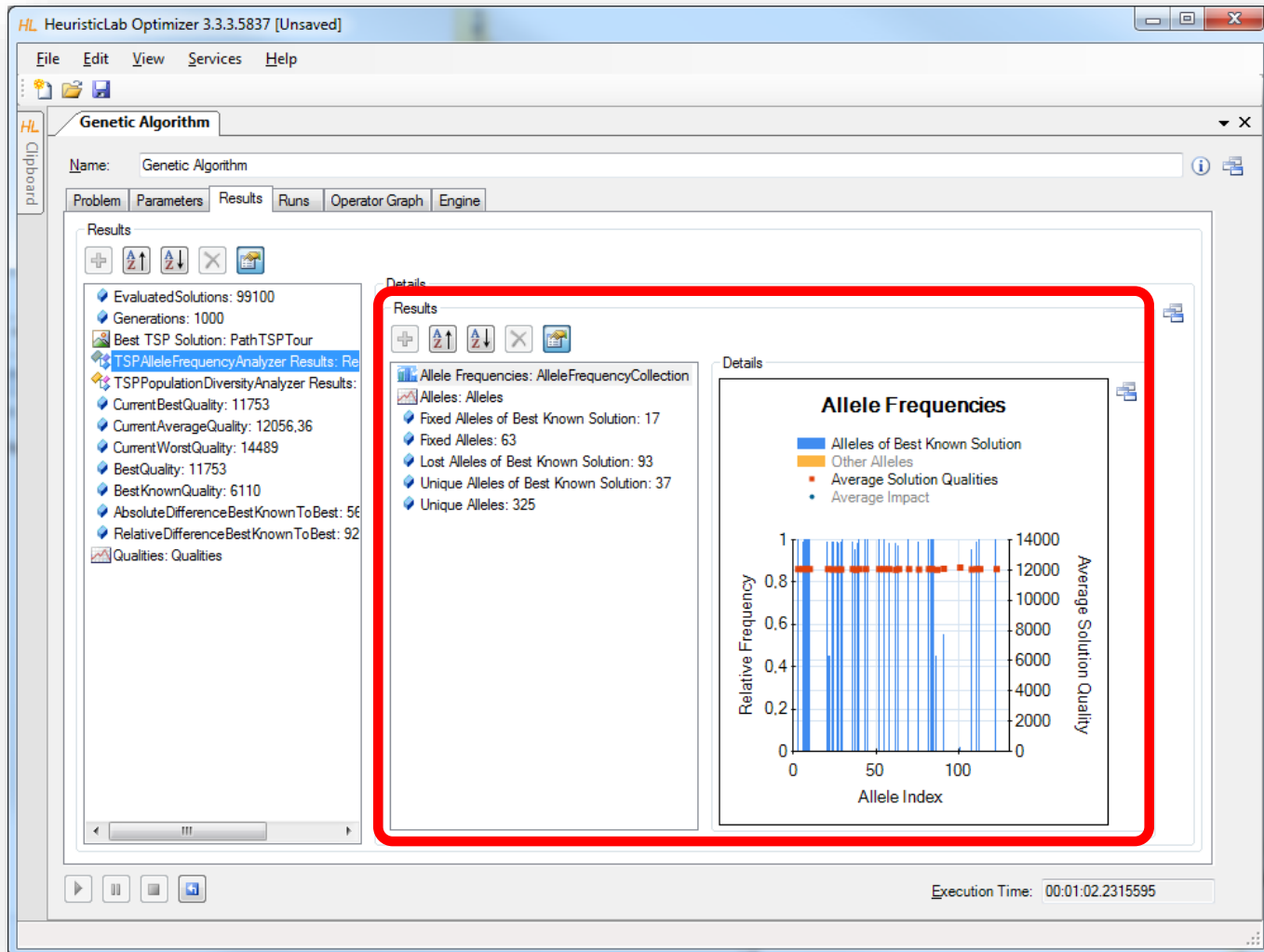
# Analyzers

- 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
  - ...

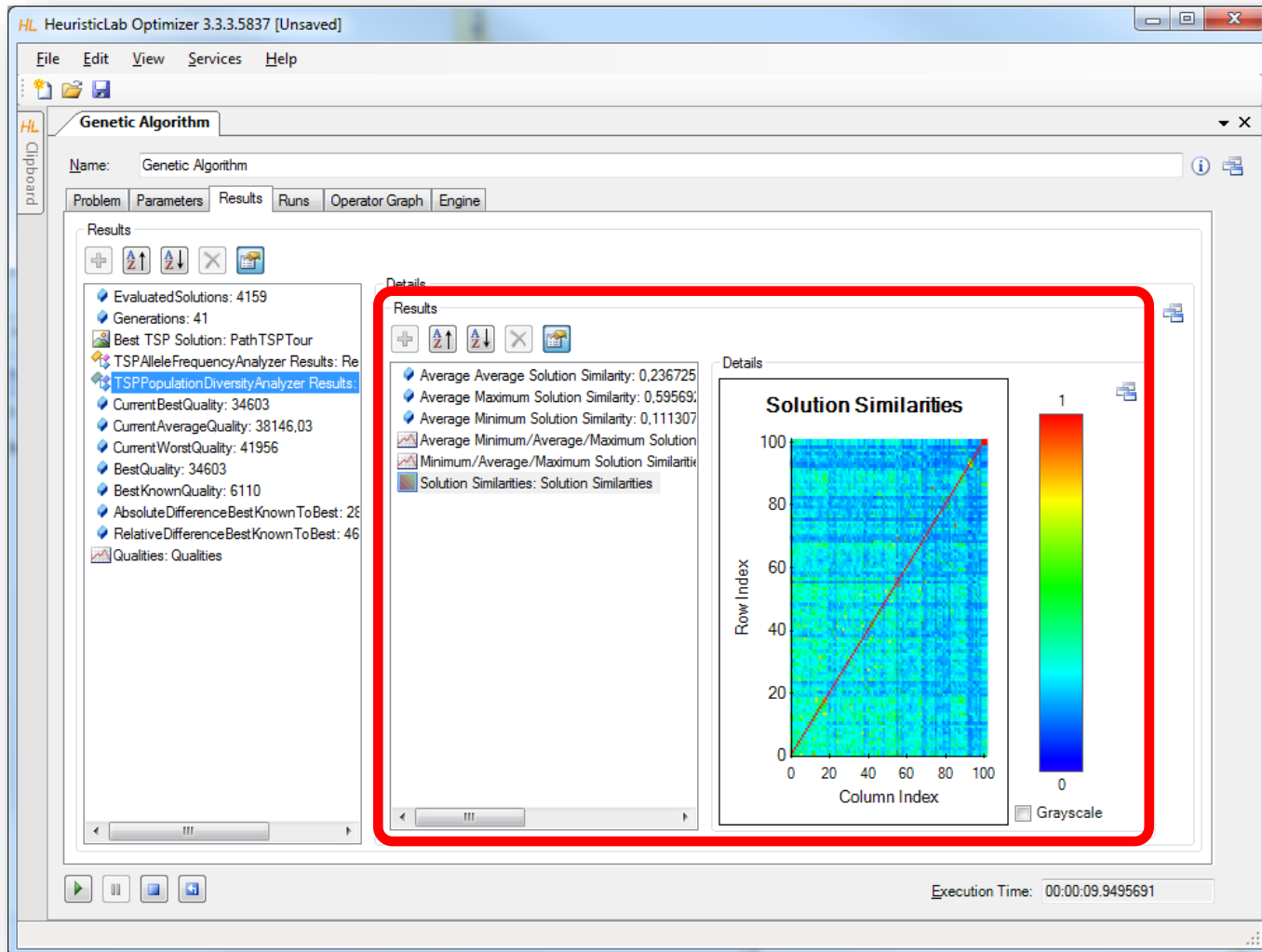
# Analyzers



# TSPAlleleFrequencyAnalyzer

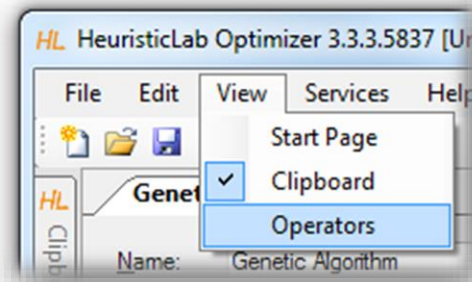
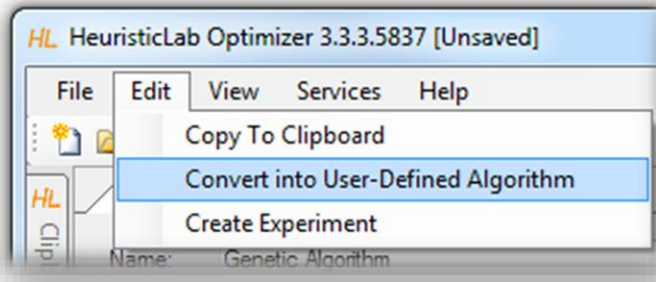


# TSP Population Diversity Analyzer



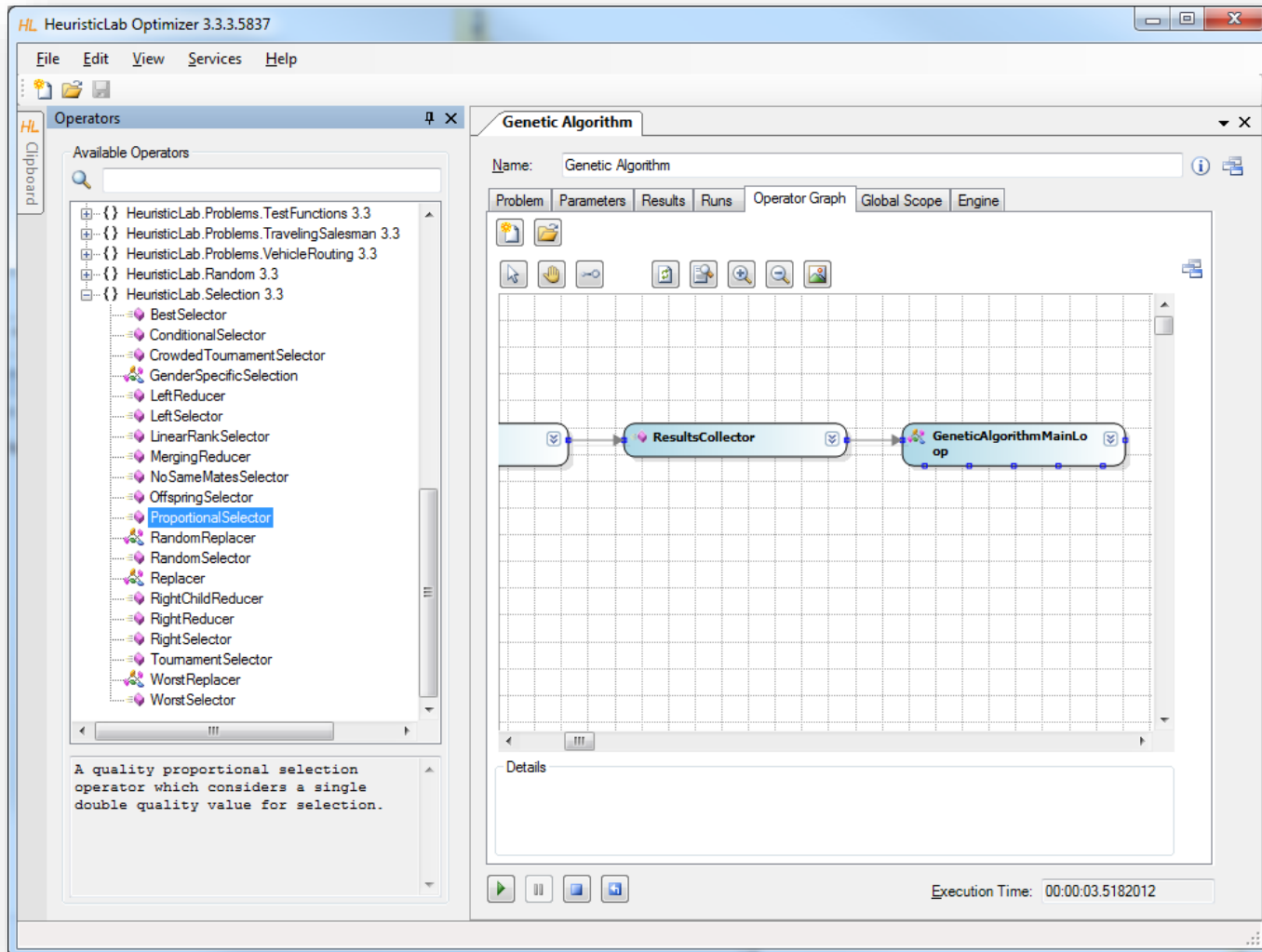
# Building User-Defined Algorithms

- 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



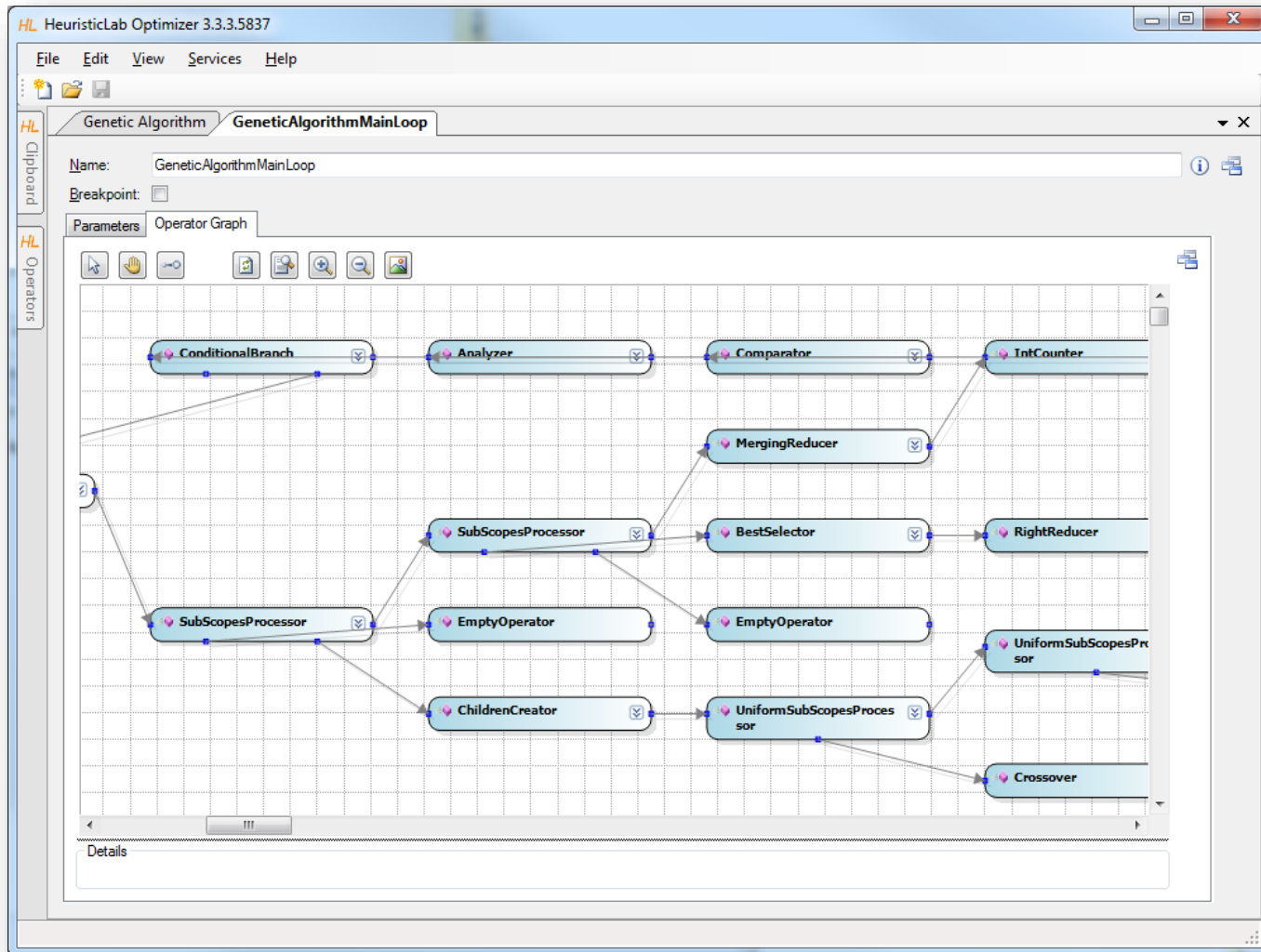
- Operators sidebar
  - drag & drop operators into an operator graph
- Programmable operators
  - add programmable operators in order to implement custom logic in an algorithm
  - no additional development environment needed
- Debug algorithms
  - use the debug engine to obtain detailed information during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

# Building User-Defined Algorithms

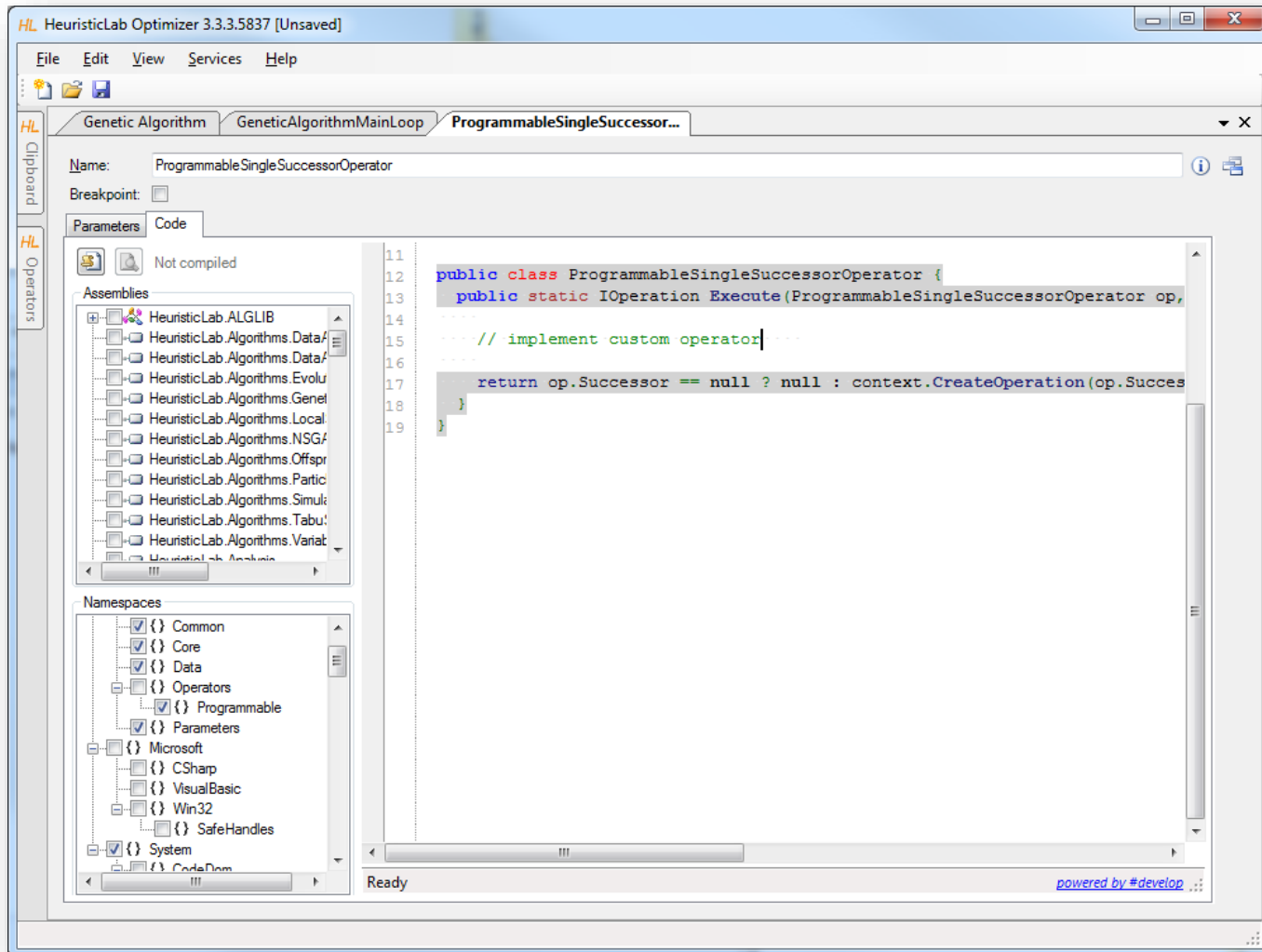




# Building User-Defined Algorithms

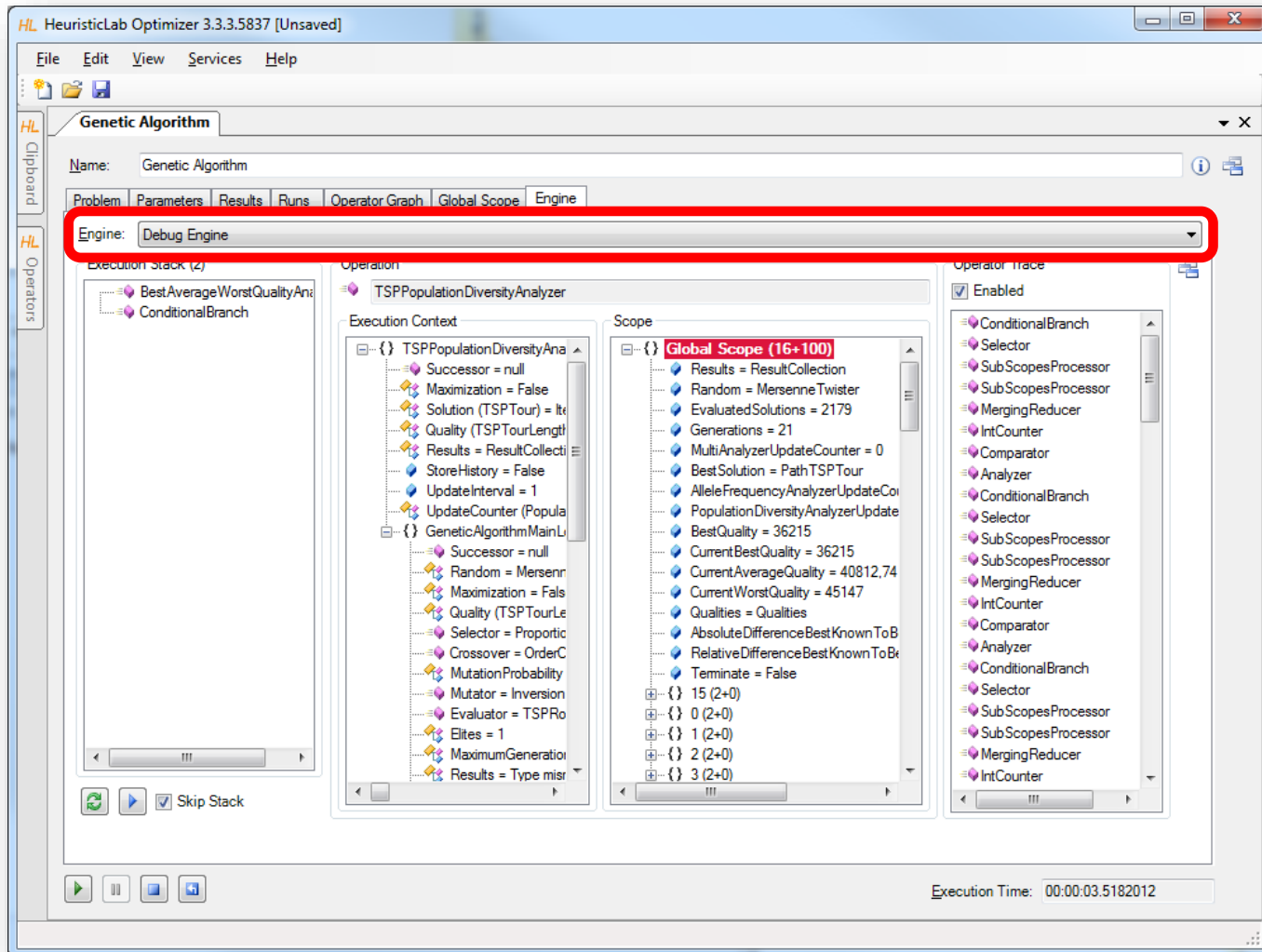


# Programmable Operators





# 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

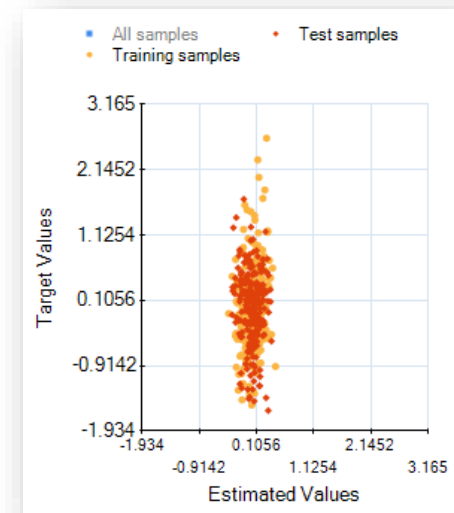
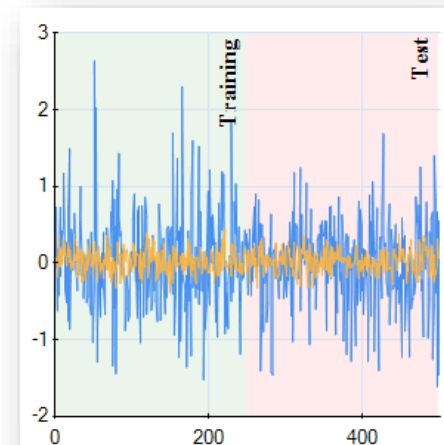


# Case Study: Regression

- 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

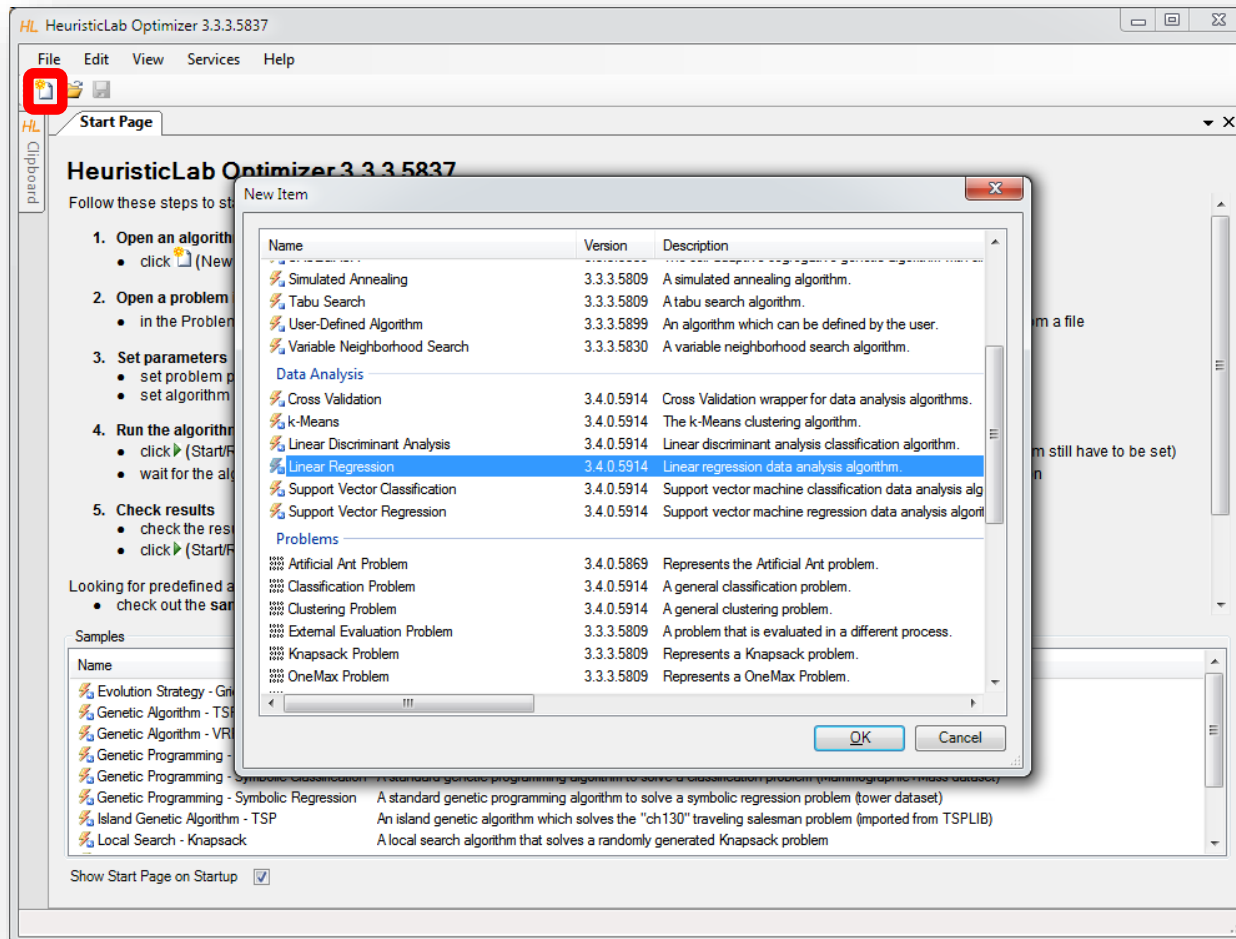
# Demonstration

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

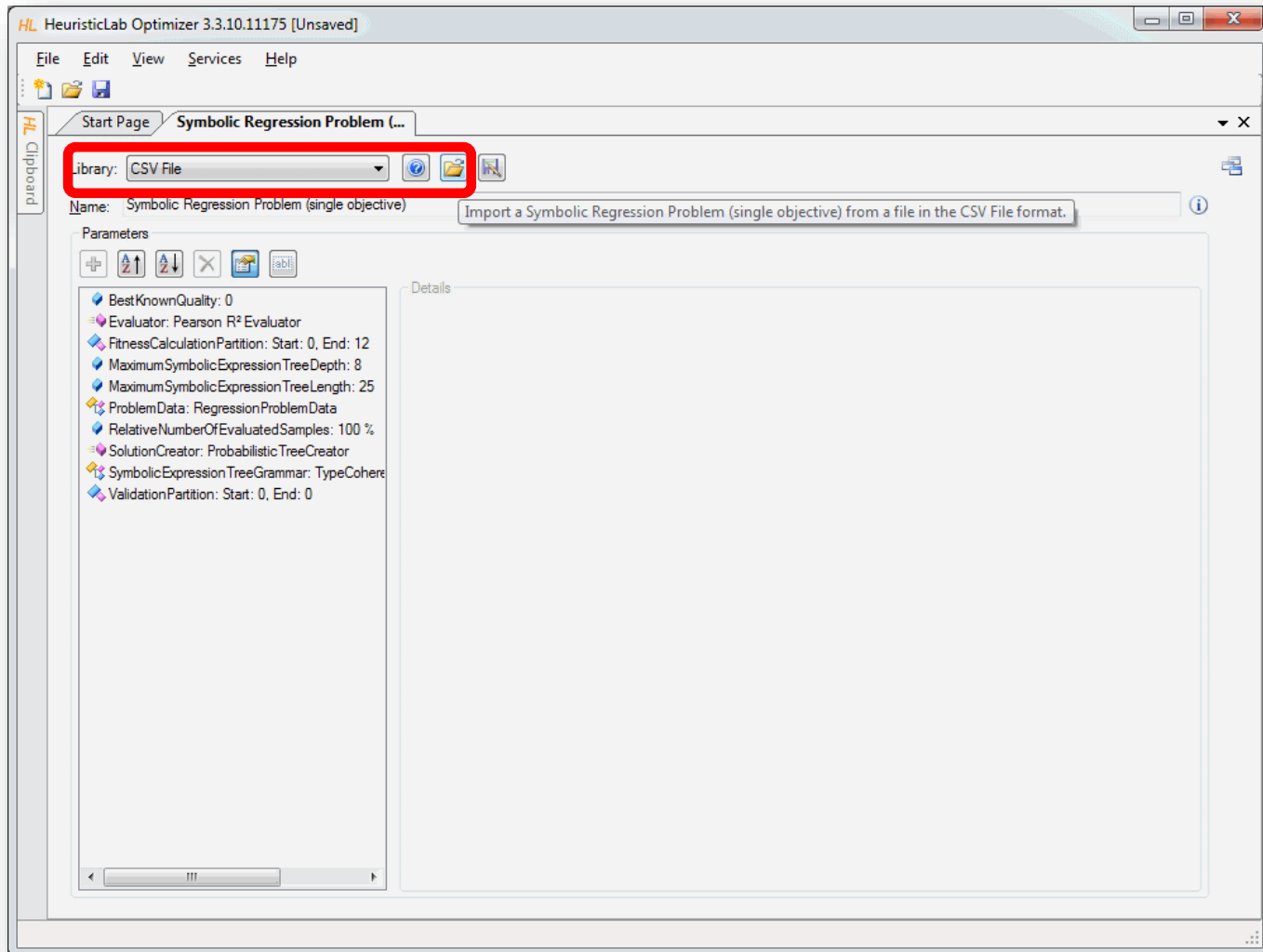


# Linear Regression

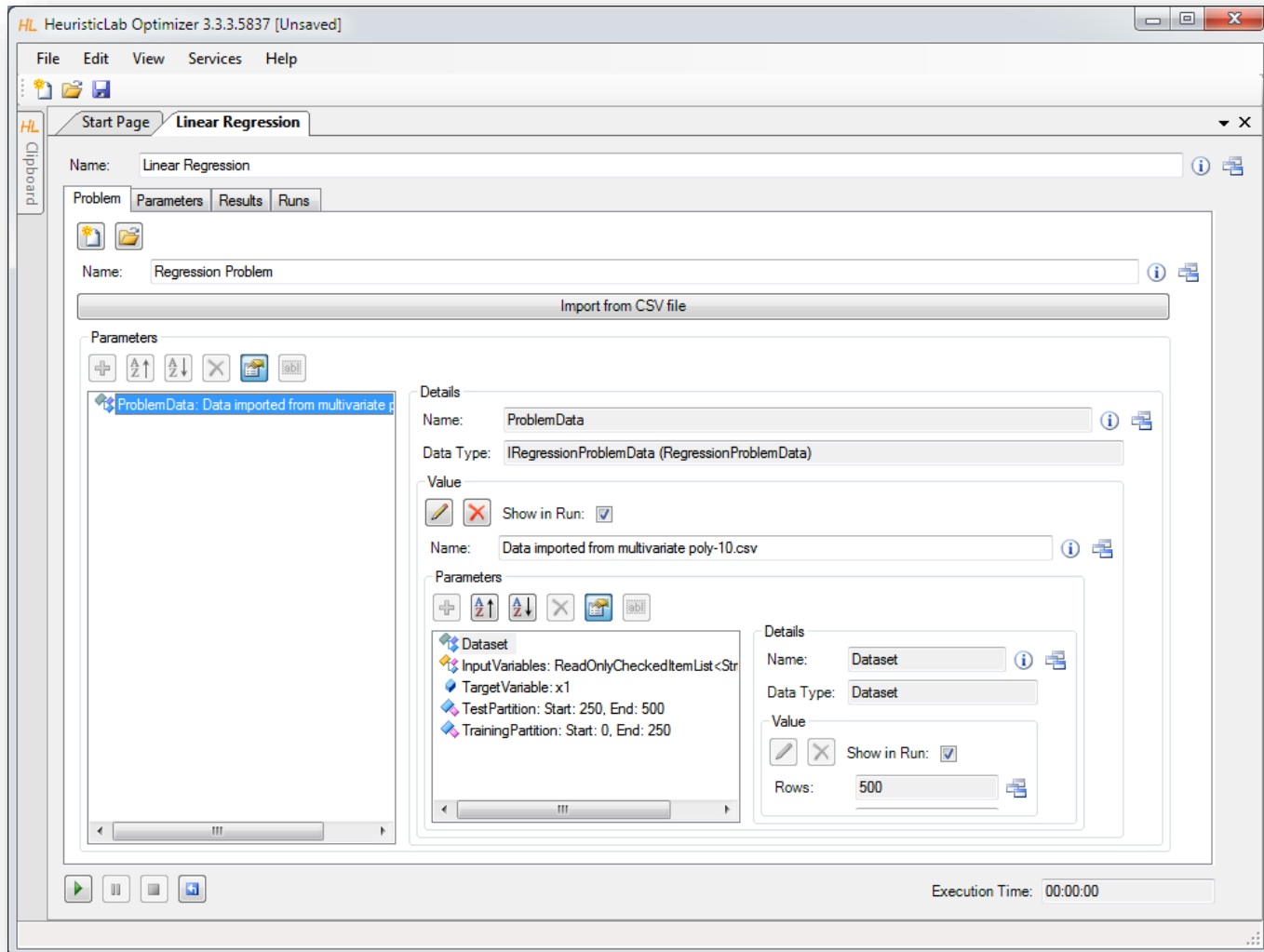
- Create new algorithm



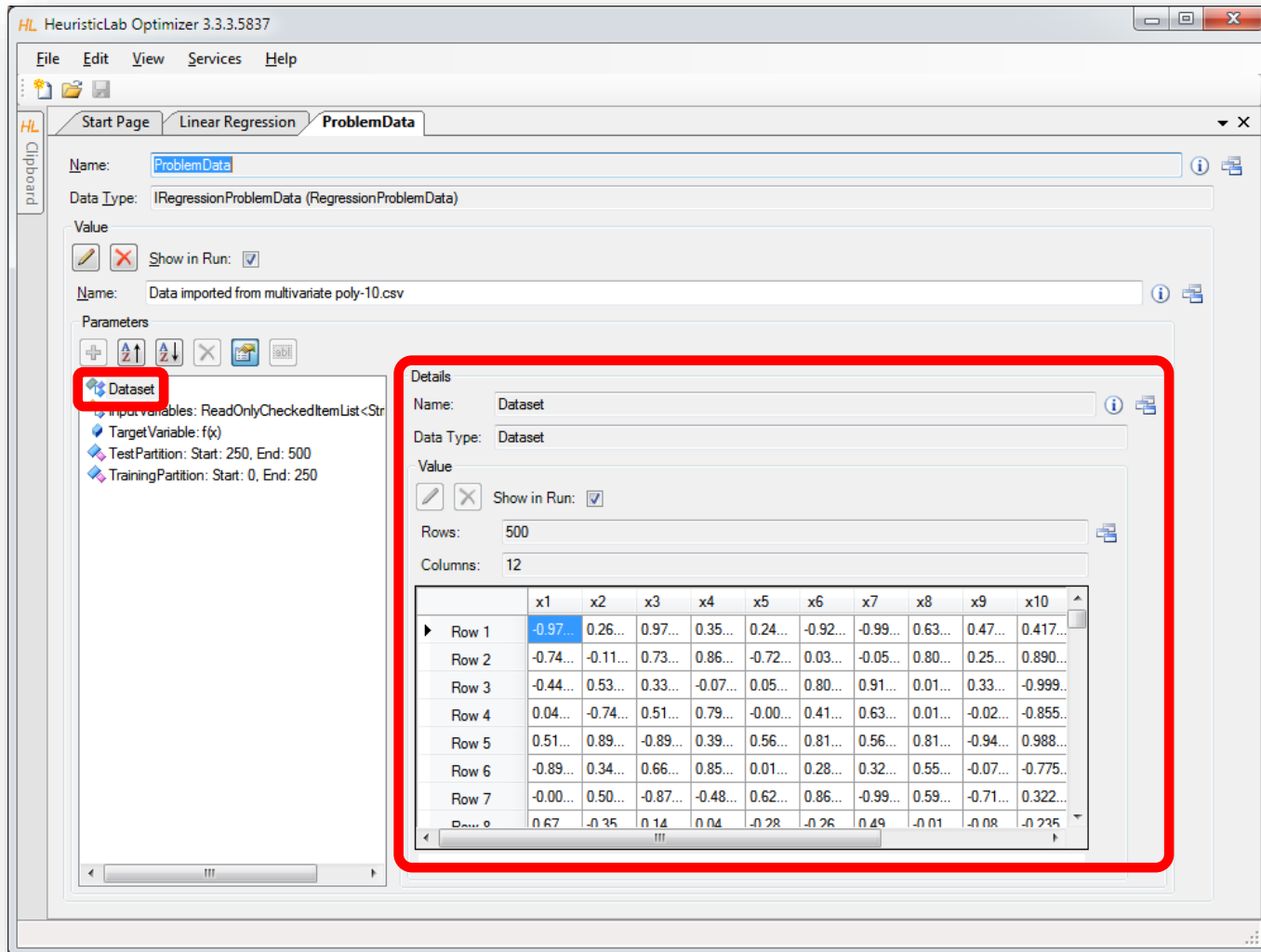
# Import Data from CSV-File



# 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

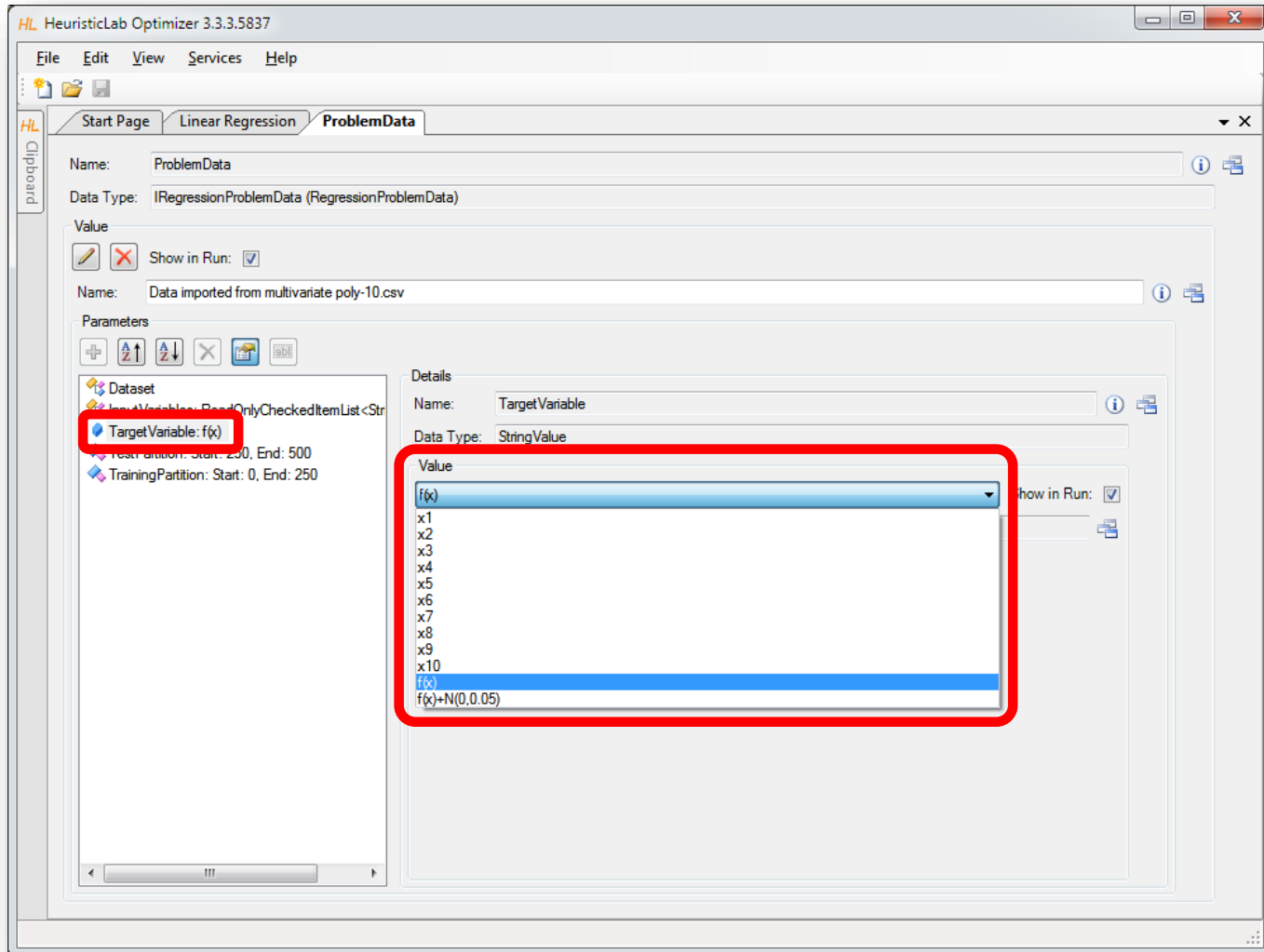
Show in Run:

Rows: 500

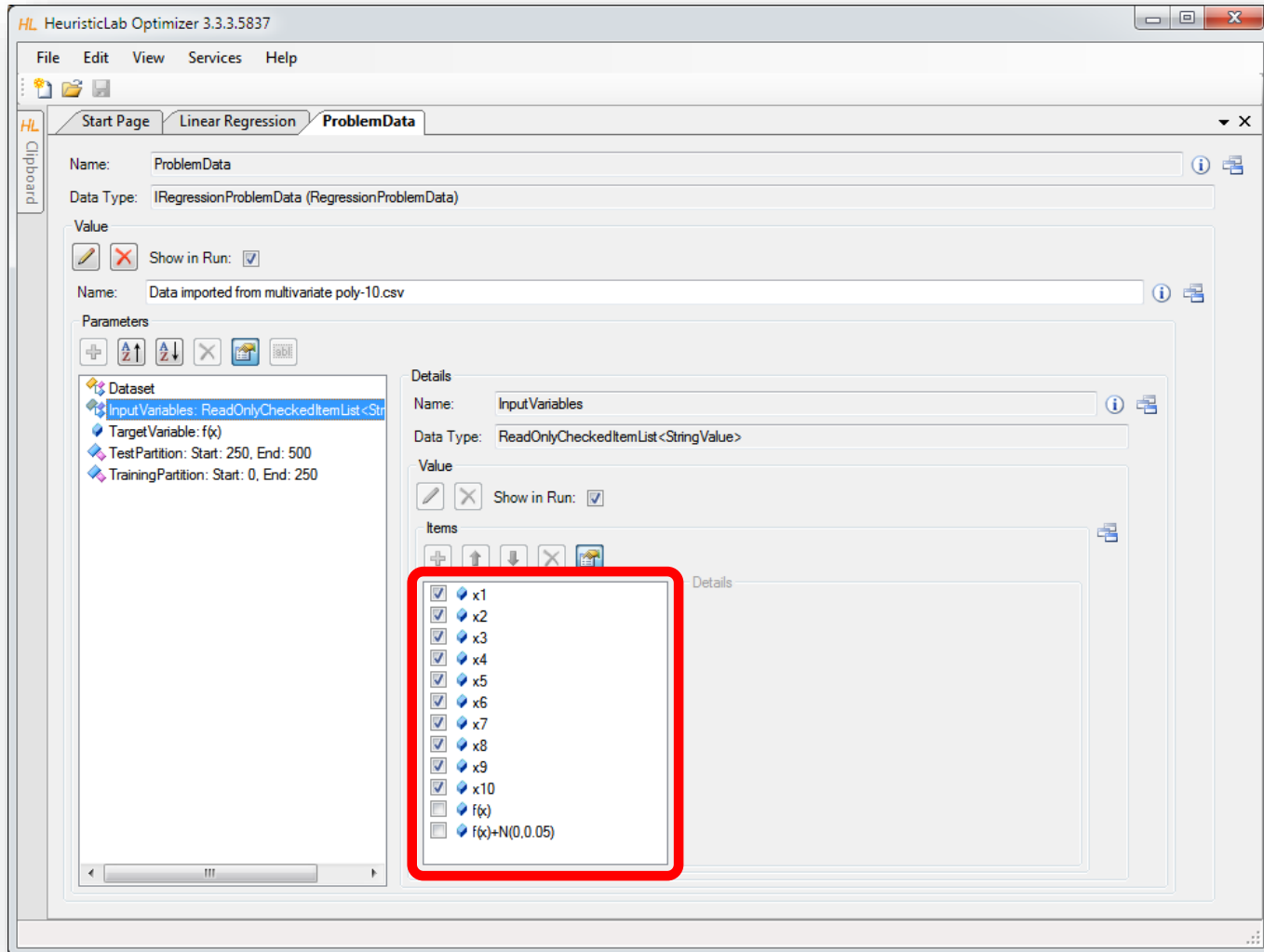
Columns: 12

	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

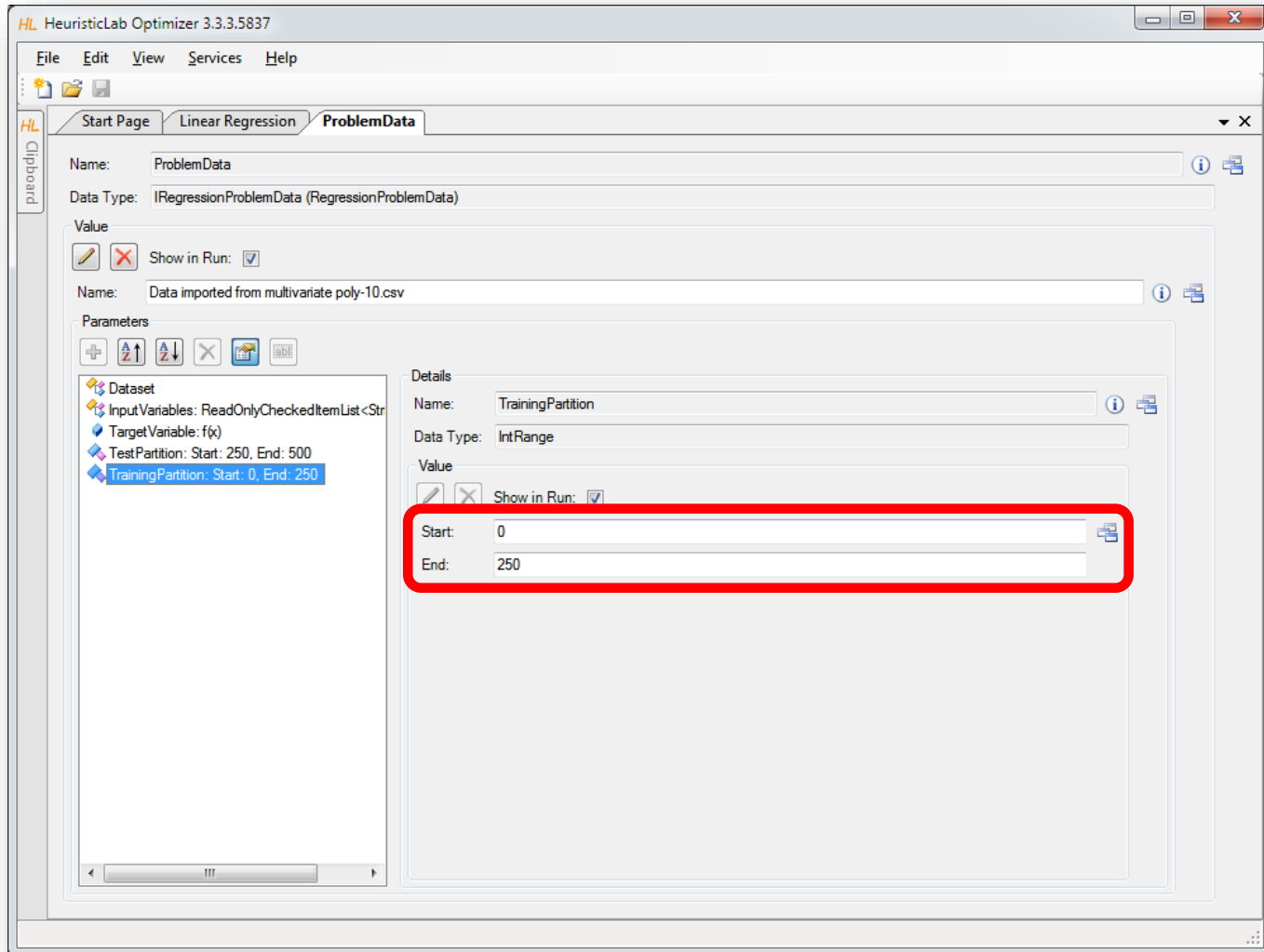


# Select Input Variables

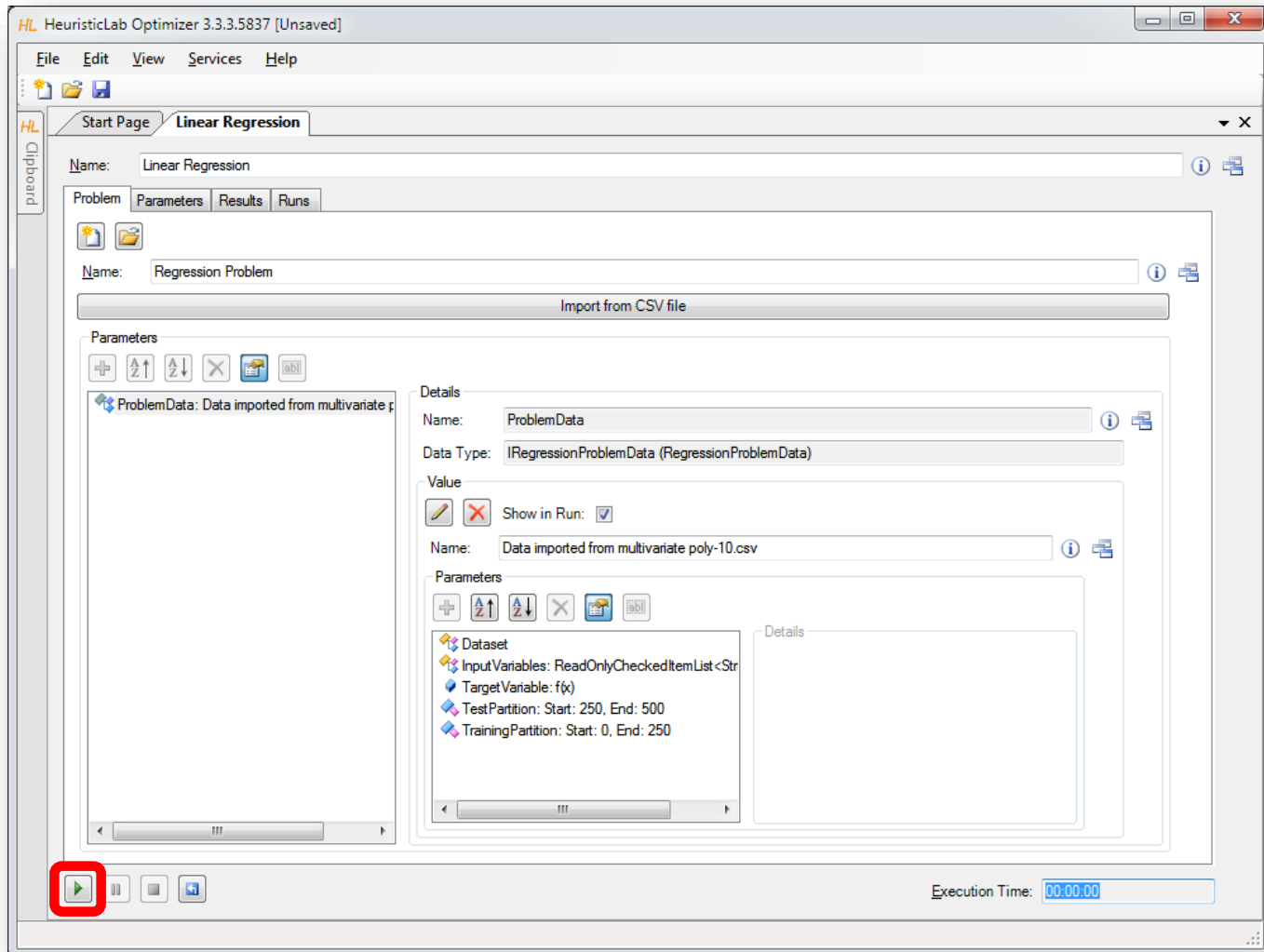




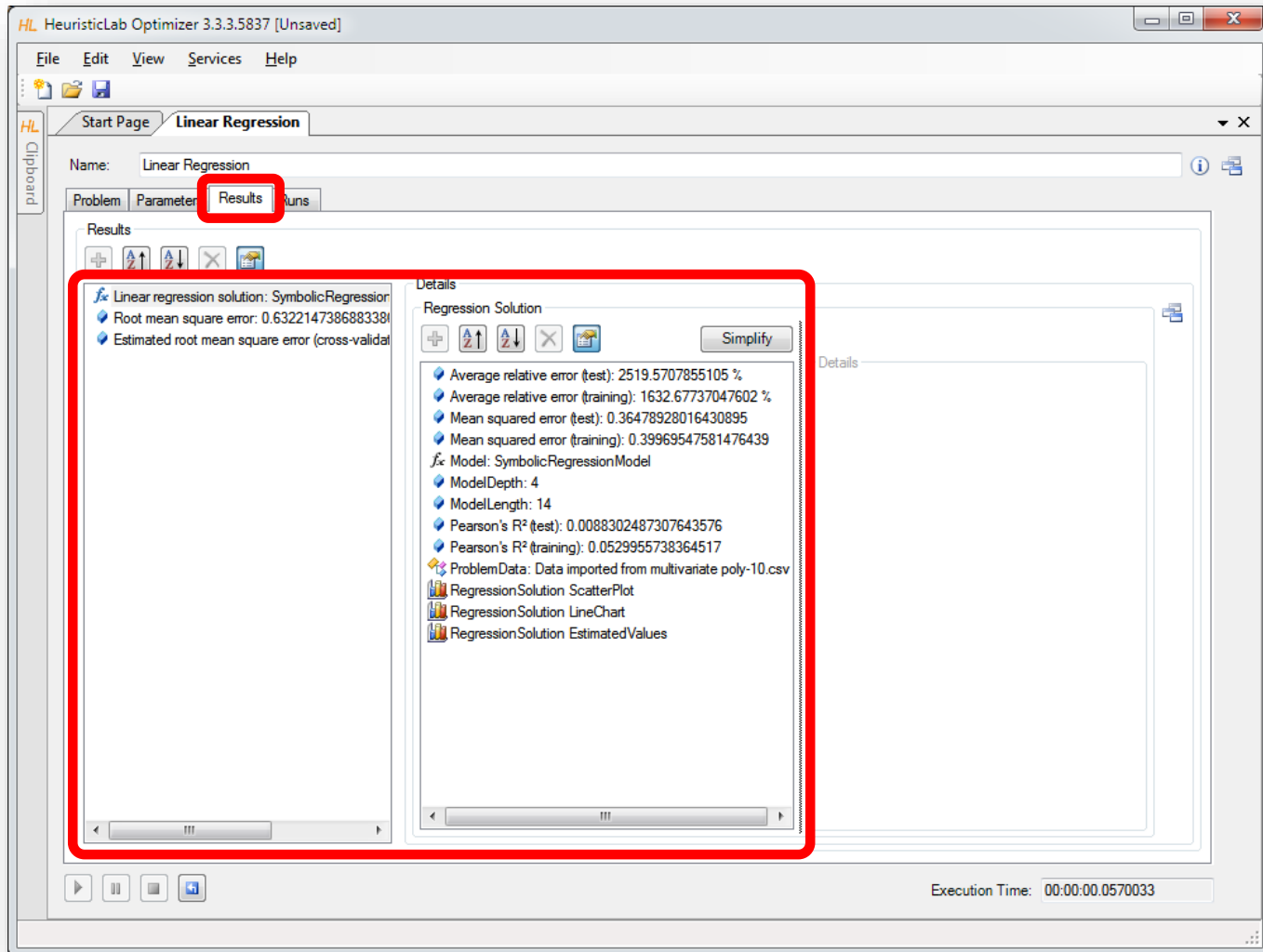
# Configure Training and Test Partitions



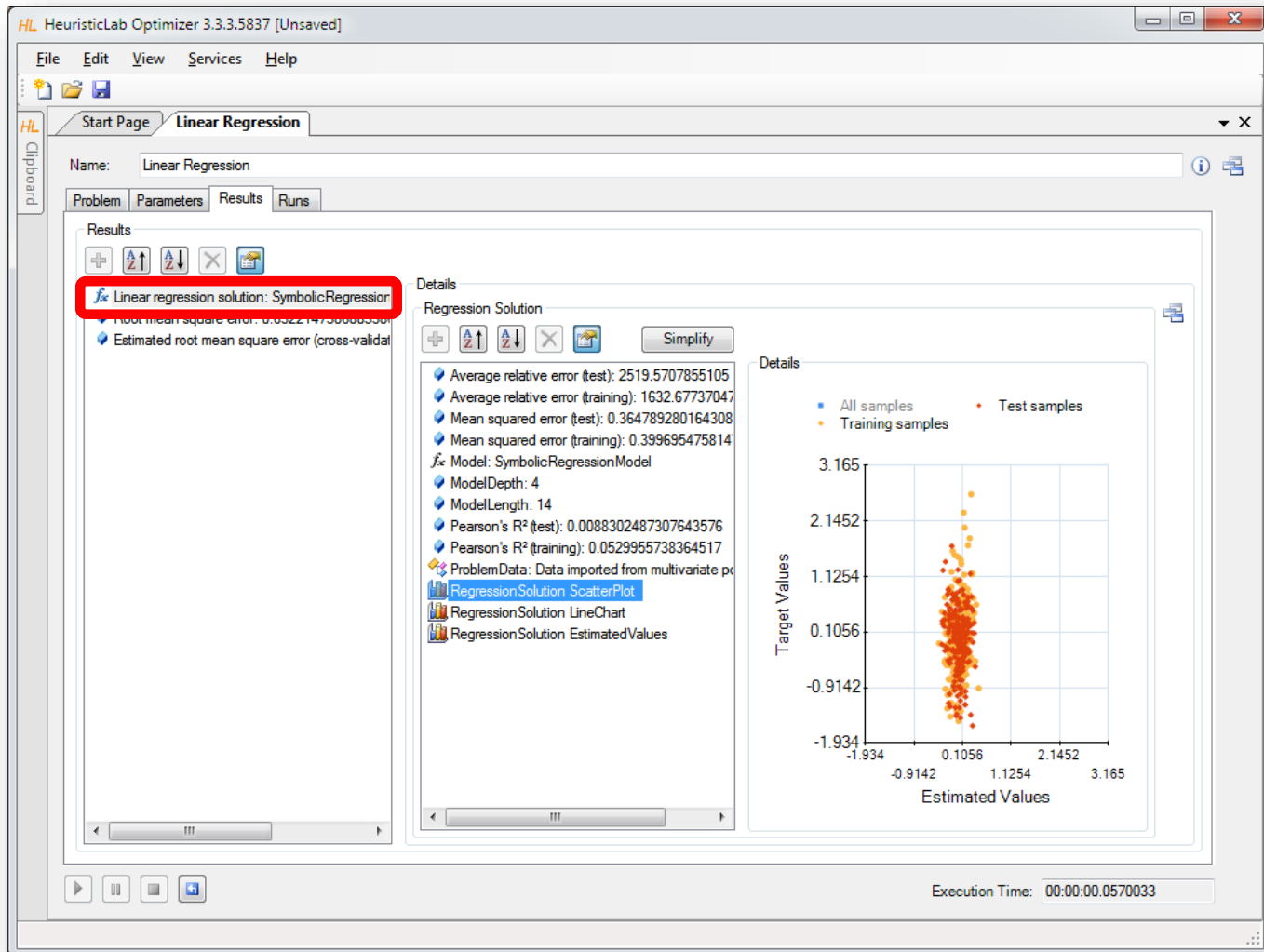
# Run Linear Regression



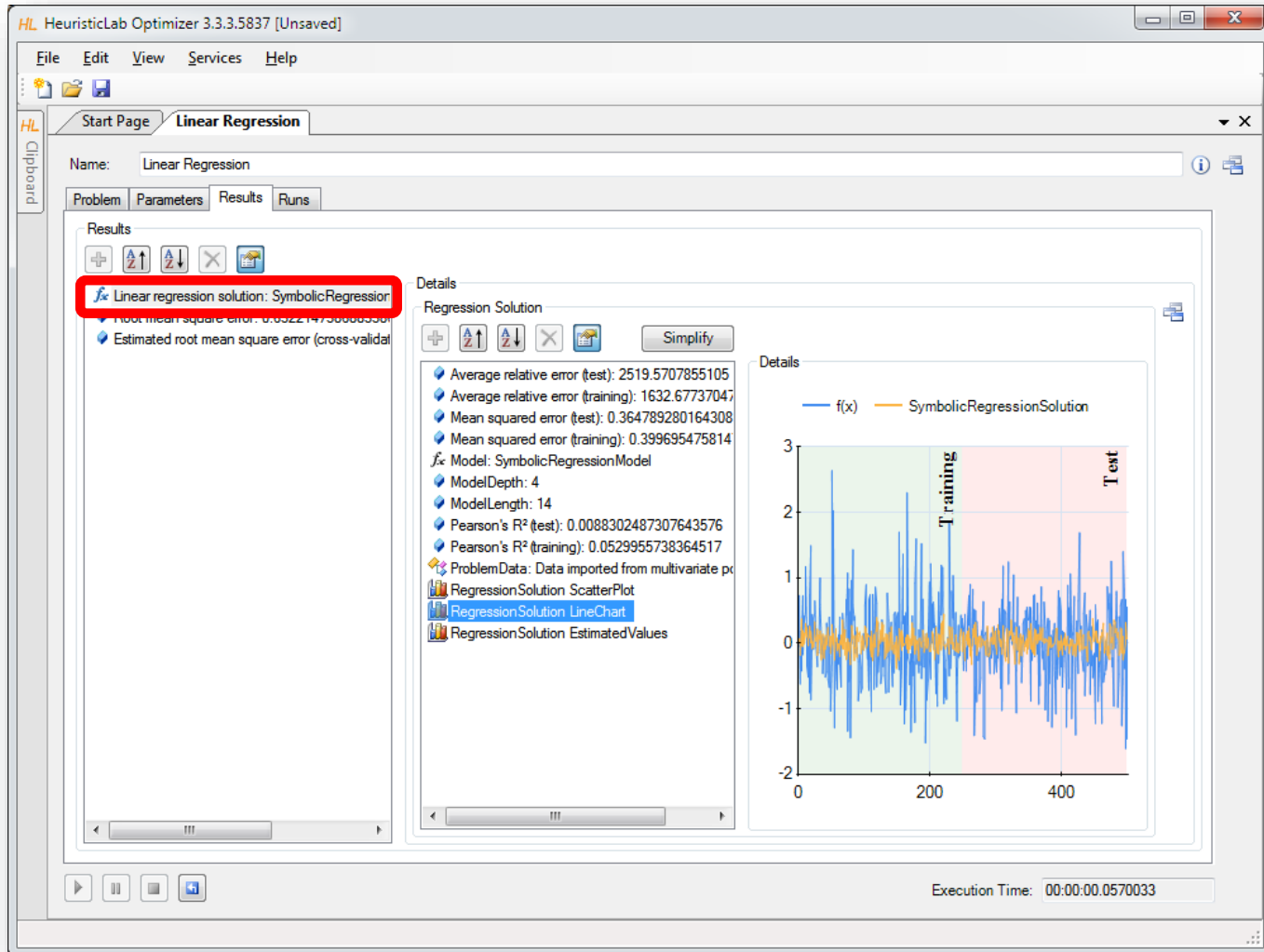
# Inspect Results



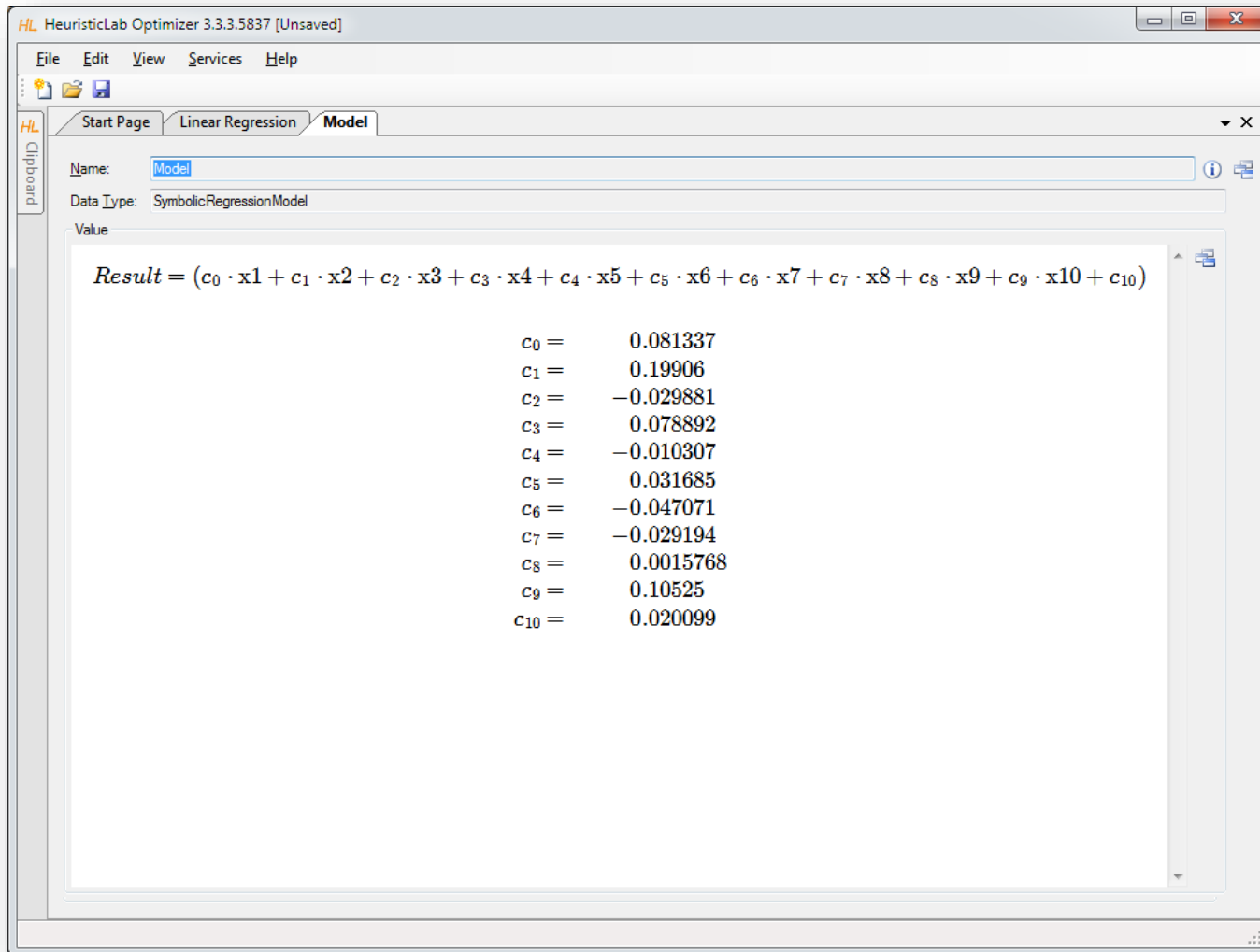
# Inspect Scatterplot of Predicted and Target Values



# 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

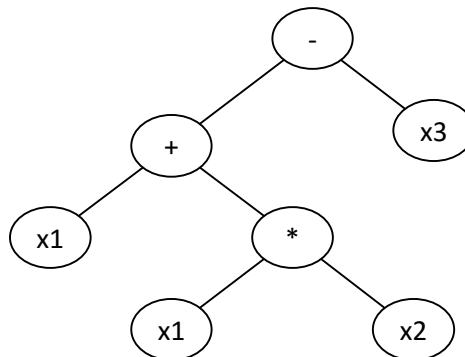
Value

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

$c_0$	=	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

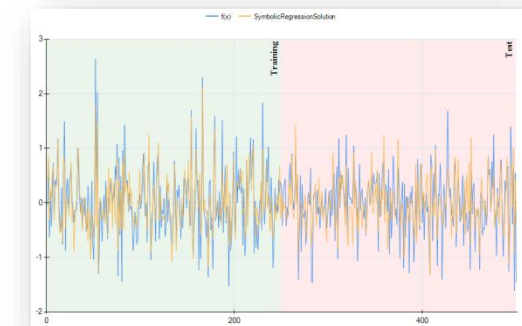
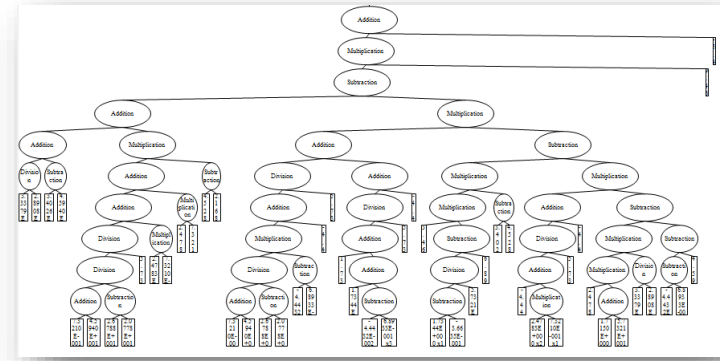
# Symbolic Regression with HeuristicLab

- 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



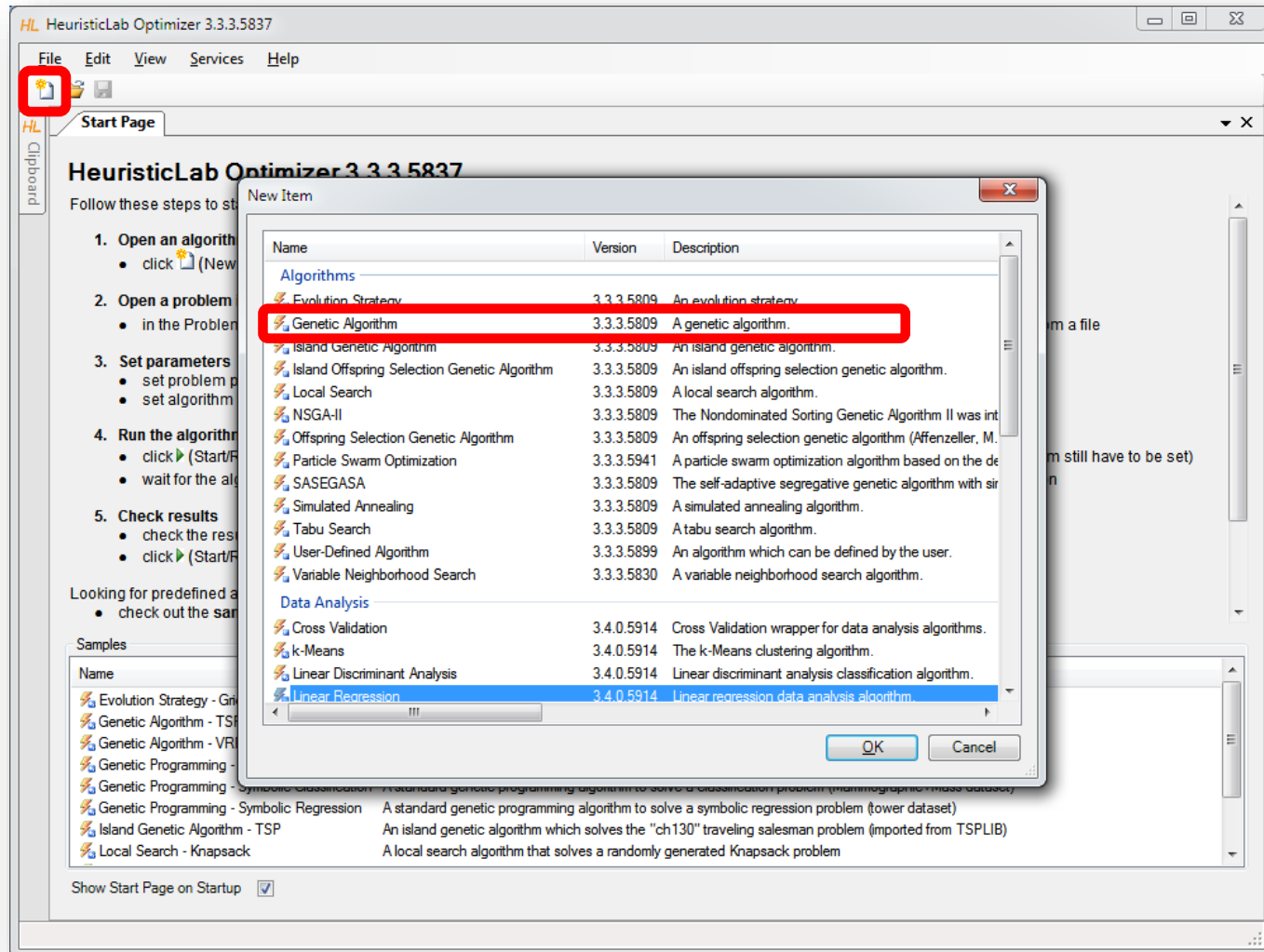
# Symbolic Regression with HeuristicLab

- 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

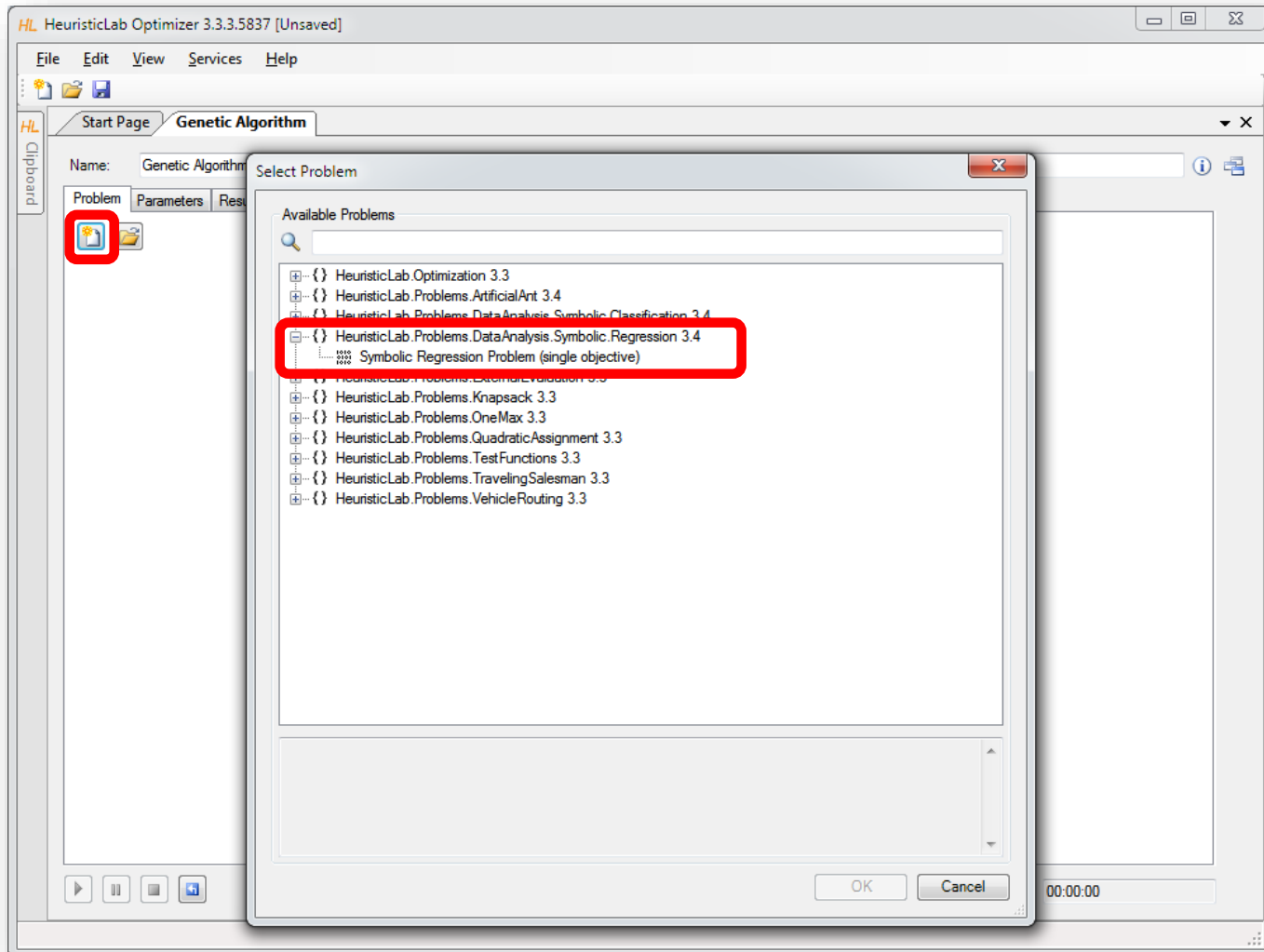




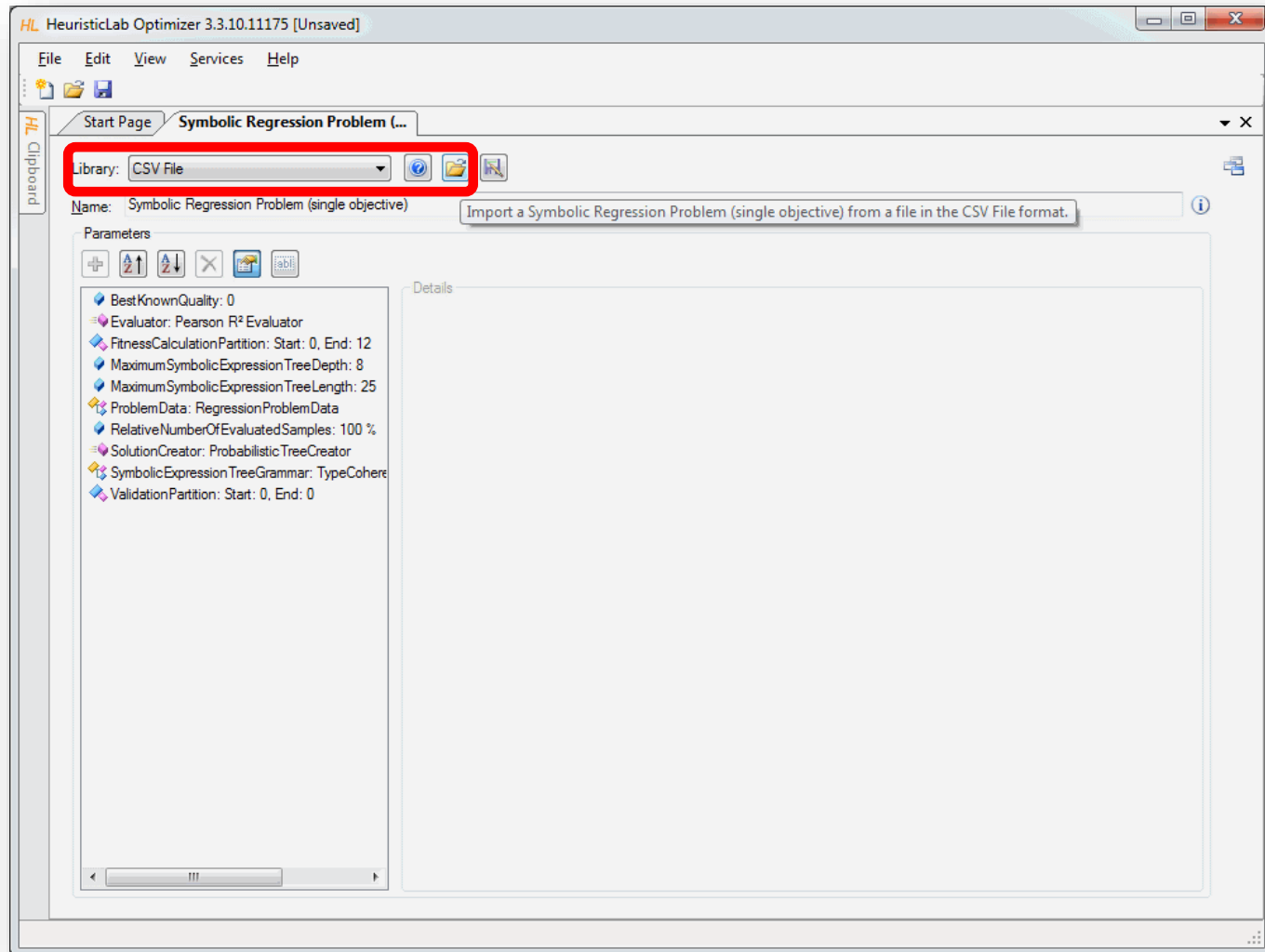
# Create New Genetic Algorithm



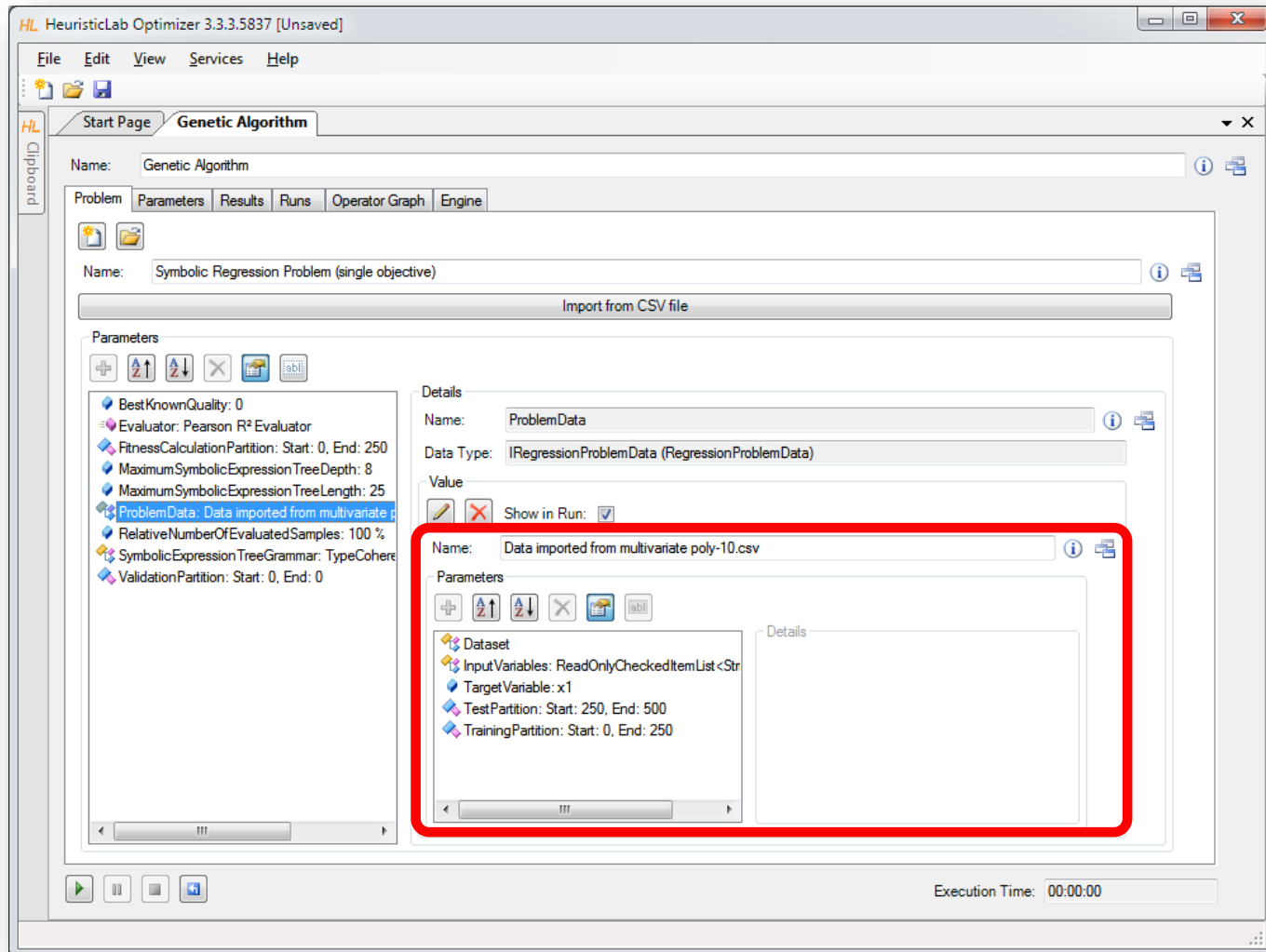
# Create New Symbolic Regression Problem



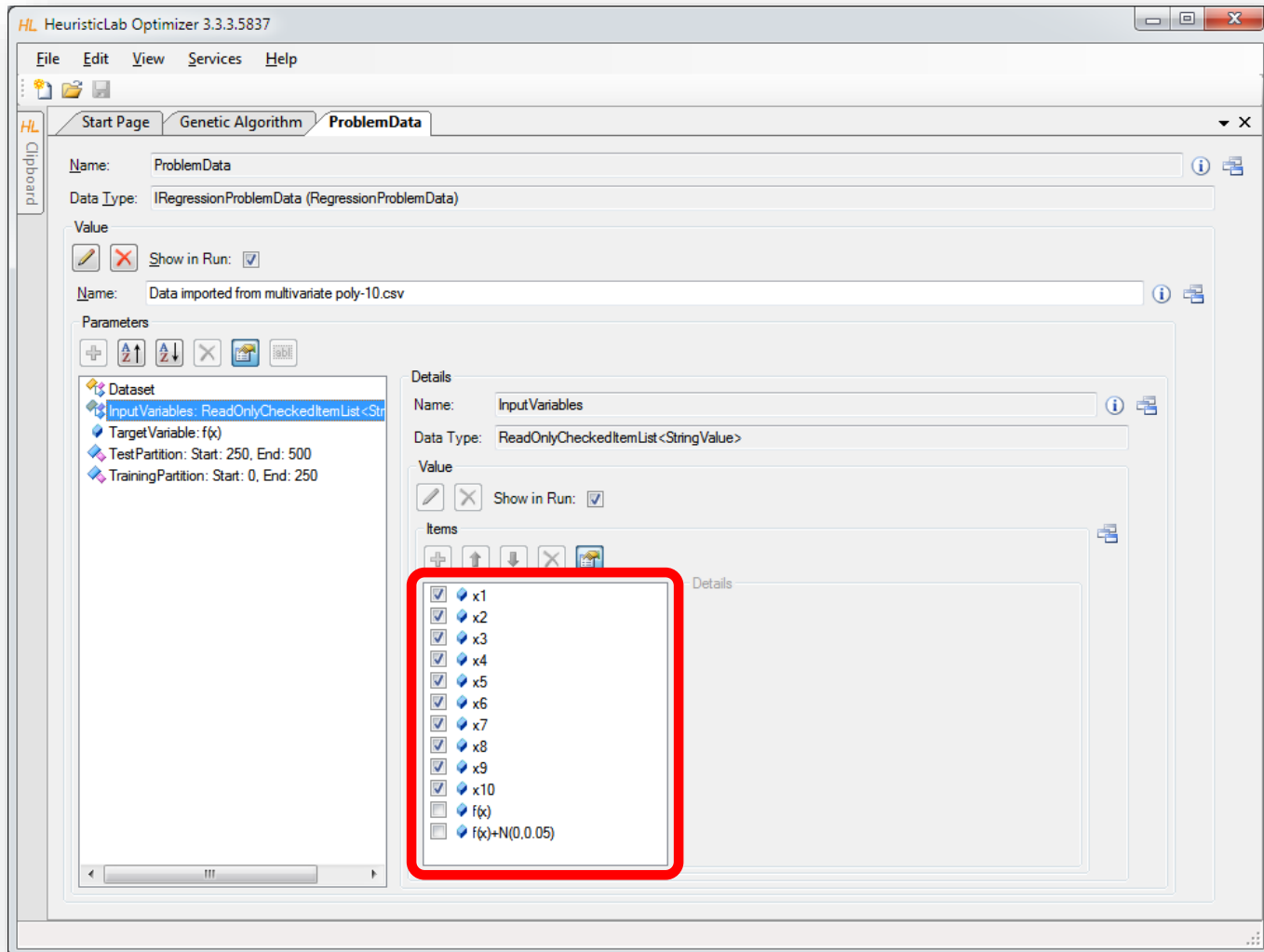
# Import Data



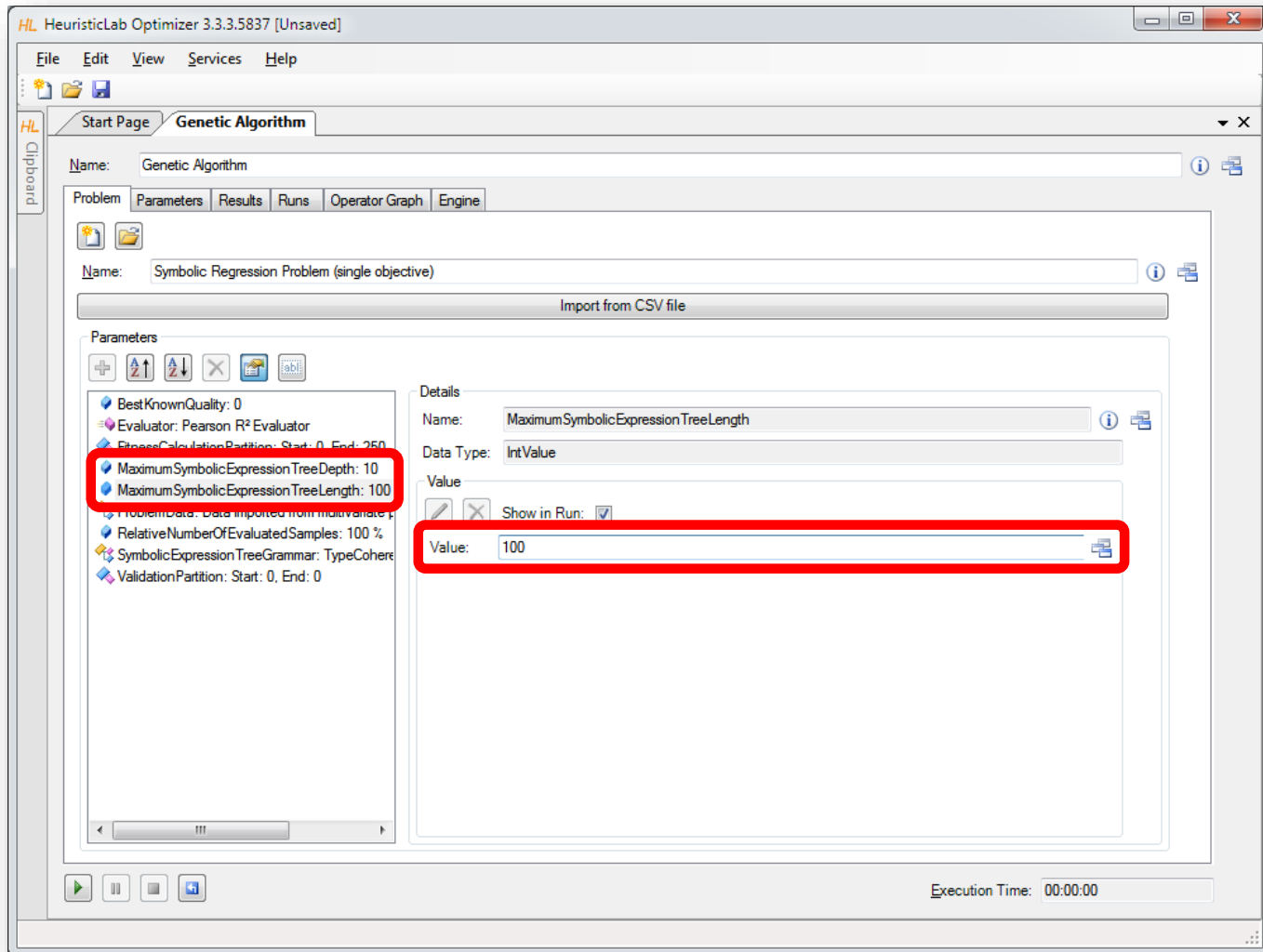
# Inspect Data and Configure Dataset



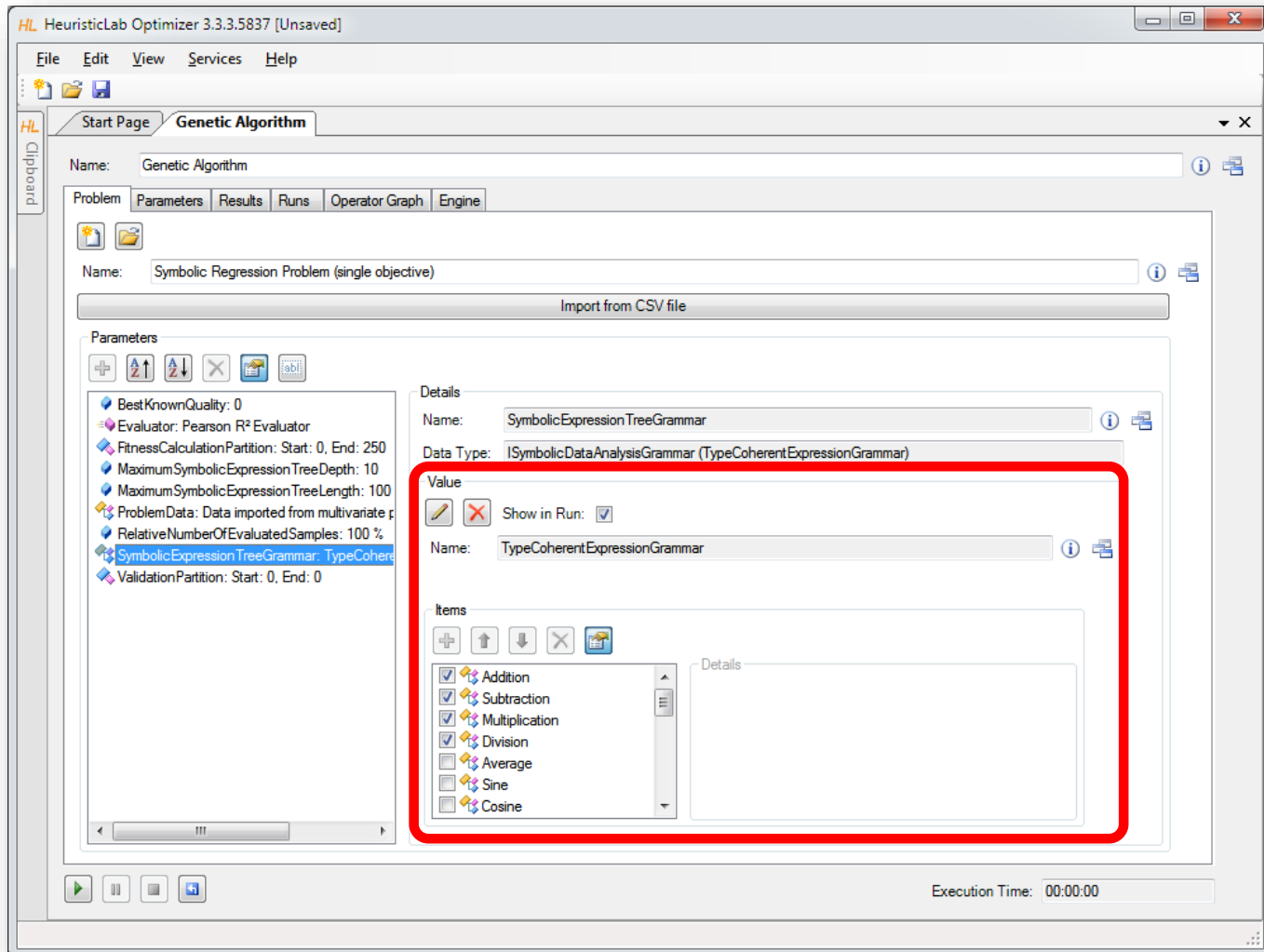
# Set Target and Input Variables



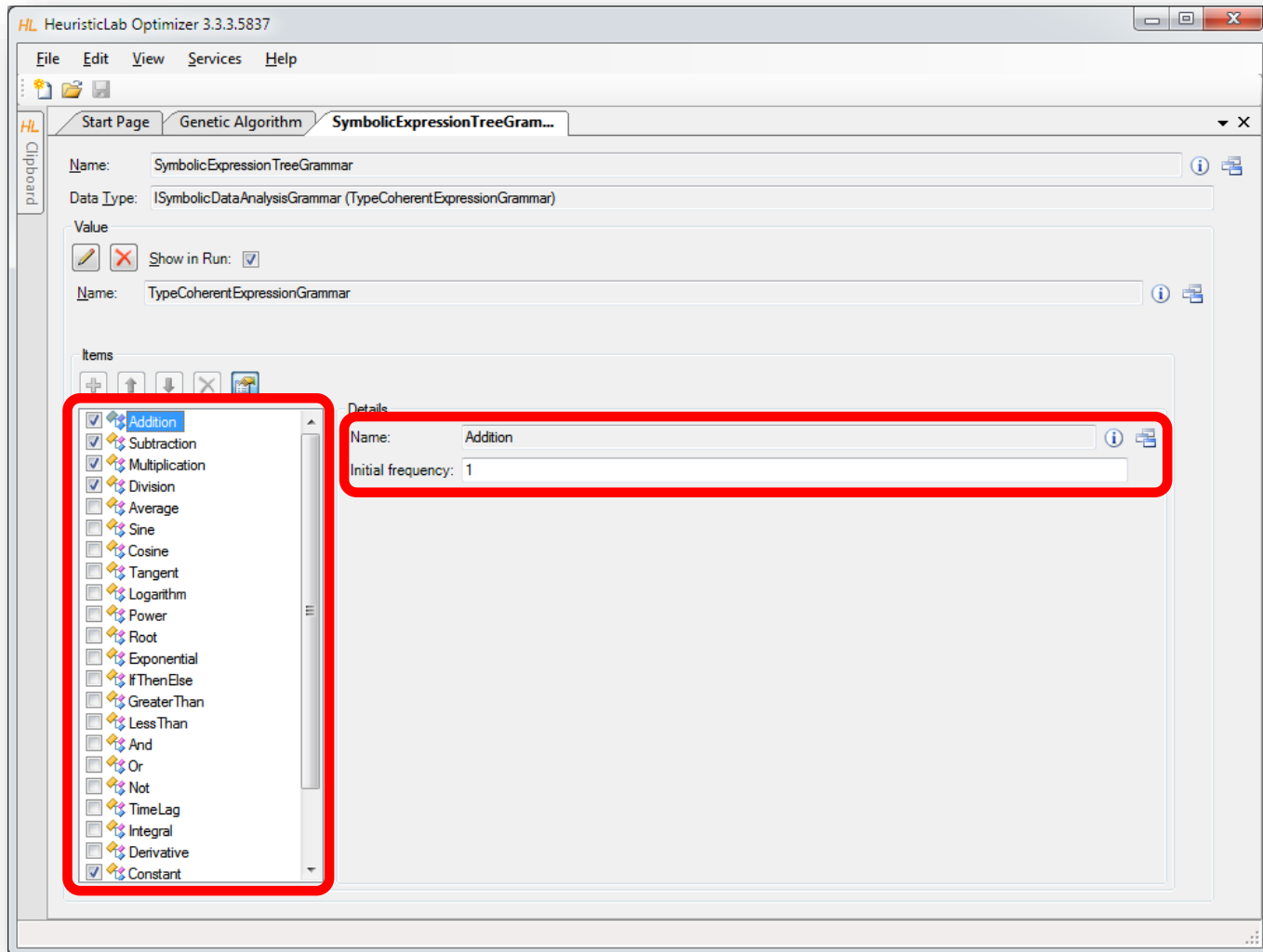
# Configure Maximal Model Depth and Length



# Configure Function Set (Grammar)

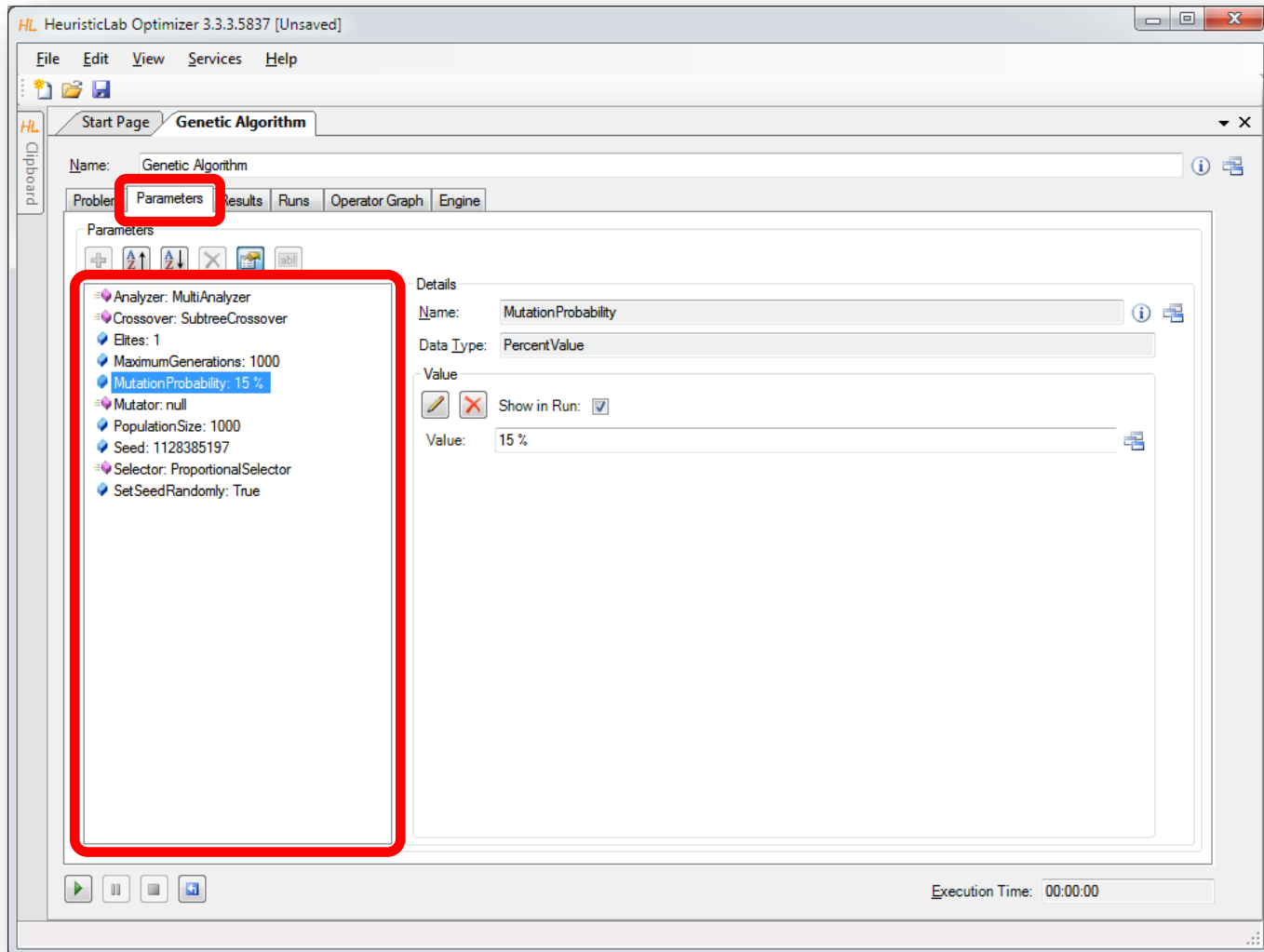


# Configure Function Set (Grammar)

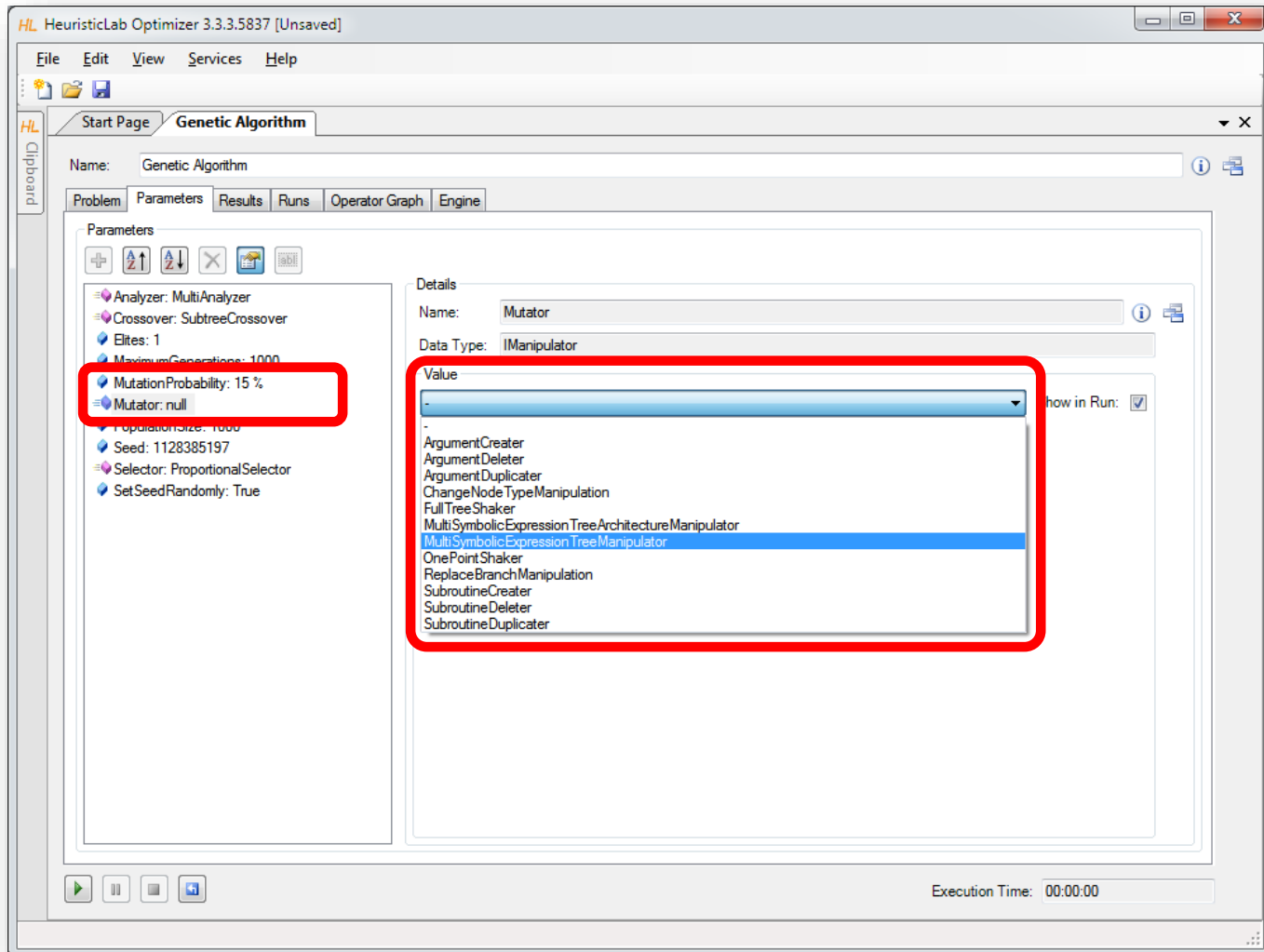




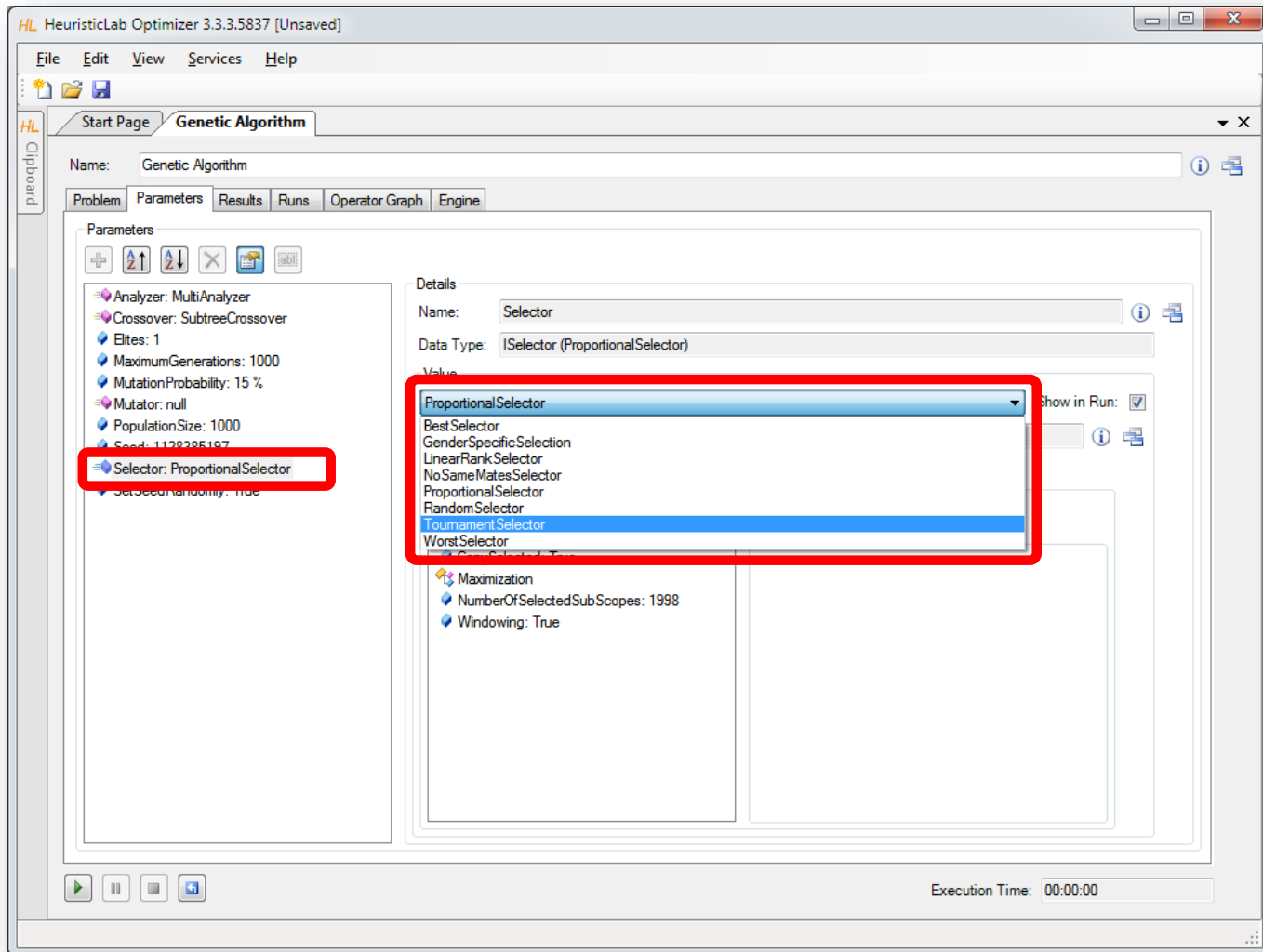
# Configure Algorithm Parameters



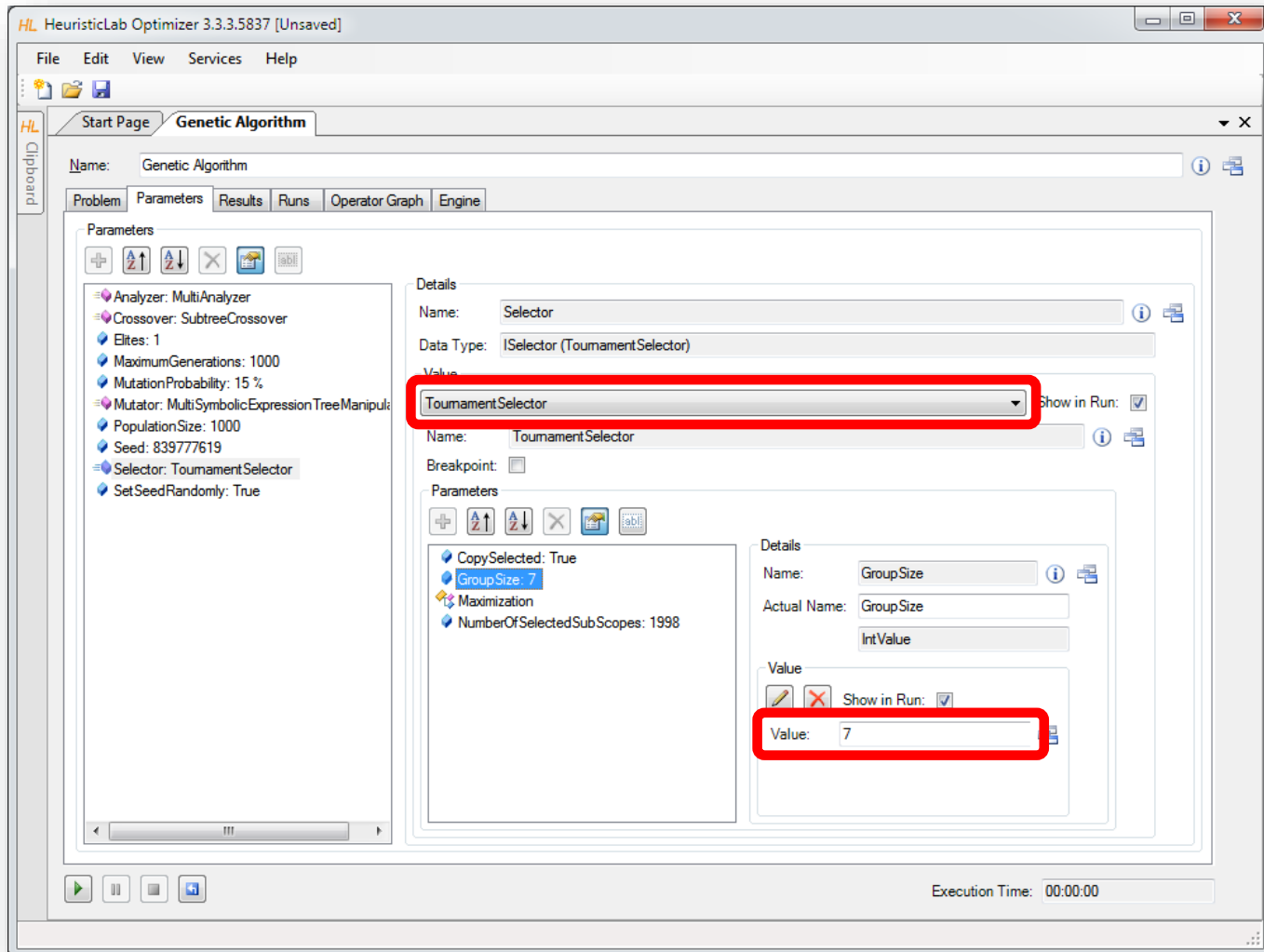
# Configure Mutation Operator



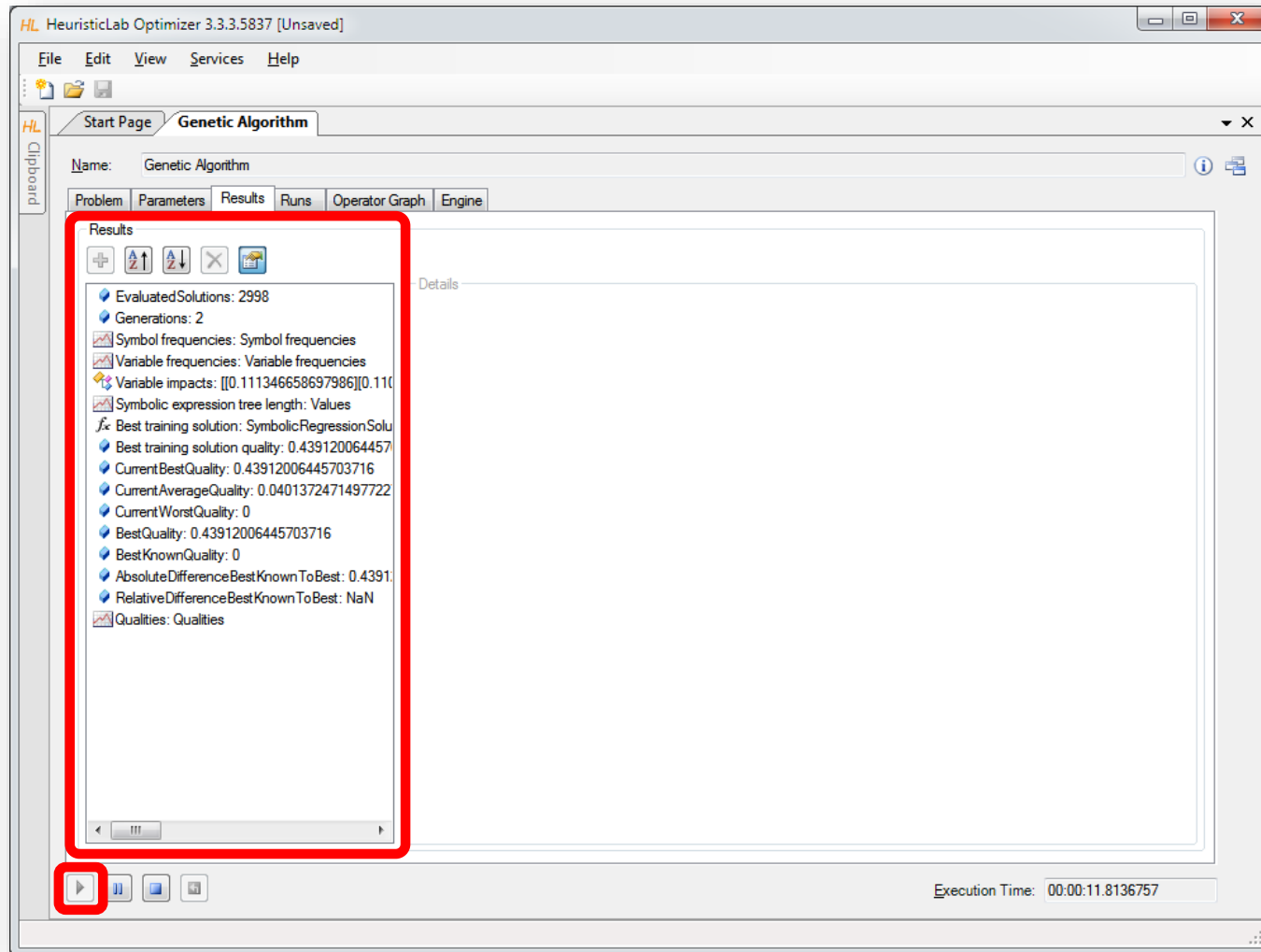
# Configure Selection Operator



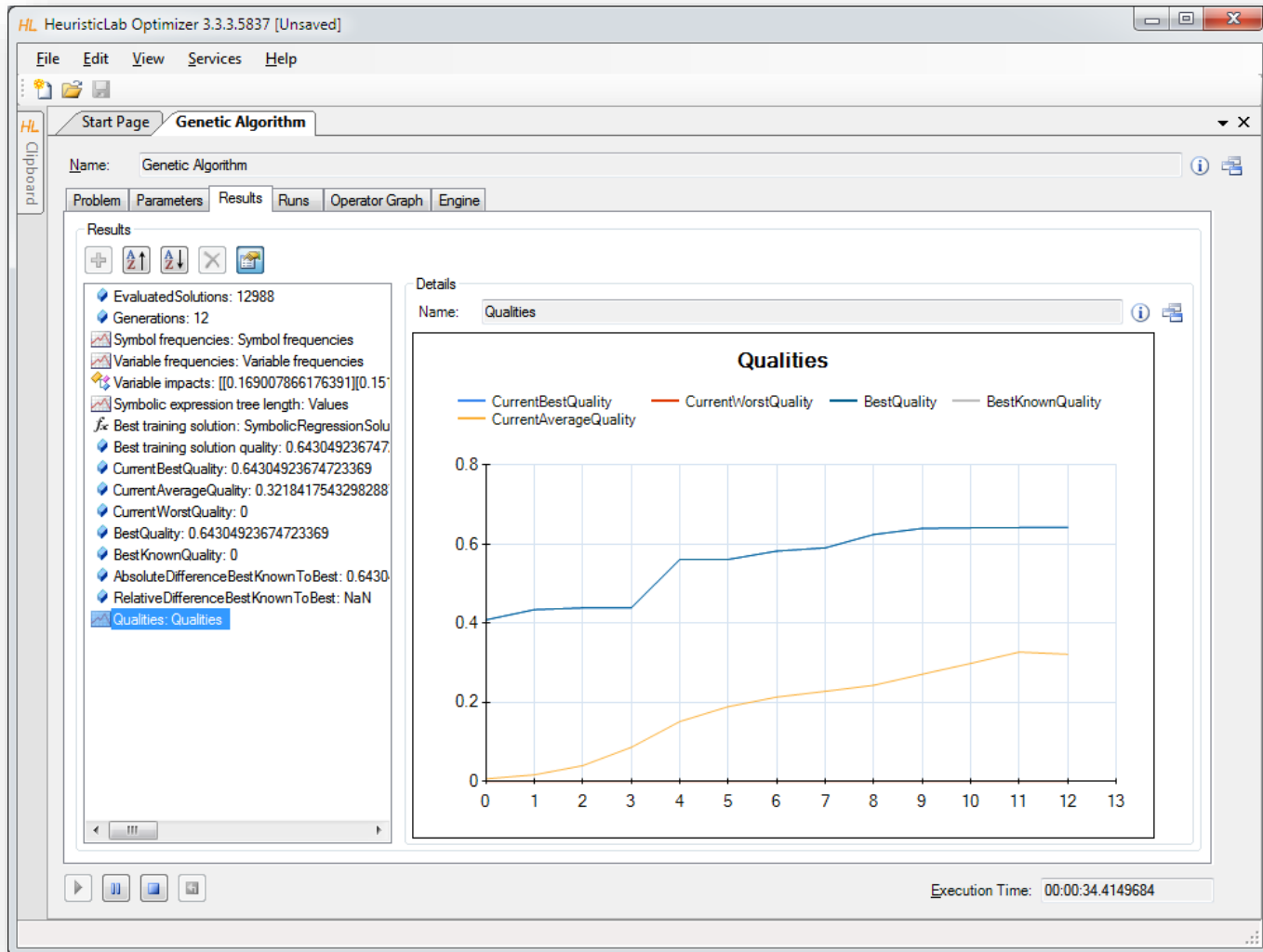
# Configure Tournament Group Size



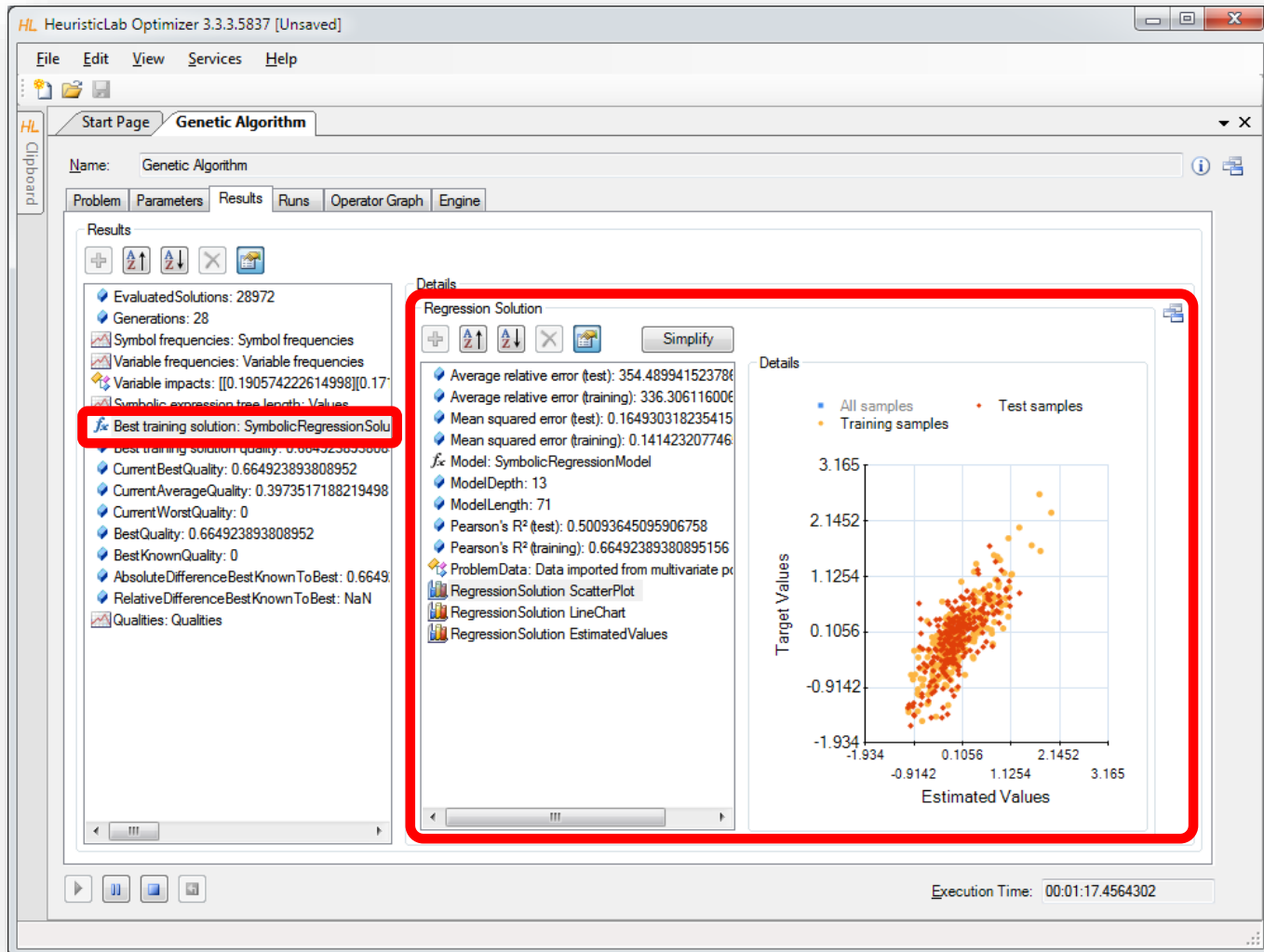
# Start Algorithm and Inspect Results



# Inspect Quality Chart



# Inspect Best Model on Training Partition



The screenshot shows the HeuristicLab Optimizer interface. The main window is titled "HL HeuristicLab Optimizer 3.3.3.5837 [Unsaved]". The "Genetic Algorithm" is selected in the "Start Page" tab. The "Results" tab is active, displaying a list of results. The "Best training solution: SymbolicRegressionSolu" is highlighted with a red box. The "Details" panel shows the "Regression Solution" details, including the average relative error (test and training), mean squared error (test and training), and model statistics (depth, length, Pearson's R<sup>2</sup> for test and training). A scatter plot titled "Regression Solution ScatterPlot" is also visible, showing Target Values vs. Estimated Values. The plot includes data for "All samples" (blue squares) and "Training samples" (orange circles). The x-axis is labeled "Estimated Values" and the y-axis is labeled "Target Values". The plot shows a strong positive correlation between the estimated and target values.

HL HeuristicLab Optimizer 3.3.3.5837 [Unsaved]

File Edit View Services Help

Start Page Genetic Algorithm

Name: Genetic Algorithm

Problem Parameters Results Runs Operator Graph Engine

Clipboard

Results

- Evaluated Solutions: 28972
- Generations: 28
- Symbol frequencies: Symbol frequencies
- Variable frequencies: Variable frequencies
- Variable impacts: [[0.190574222614998][0.17...
- Symbolic expression tree length: Values
- Best training solution: SymbolicRegressionSolu**
- Best training solution quality: 0.664923893808952
- Current Best Quality: 0.664923893808952
- Current Average Quality: 0.3973517188219498
- Current Worst Quality: 0
- Best Quality: 0.664923893808952
- Best Known Quality: 0
- Absolute Difference Best Known To Best: 0.6649...
- Relative Difference Best Known To Best: NaN
- Qualities: Qualities

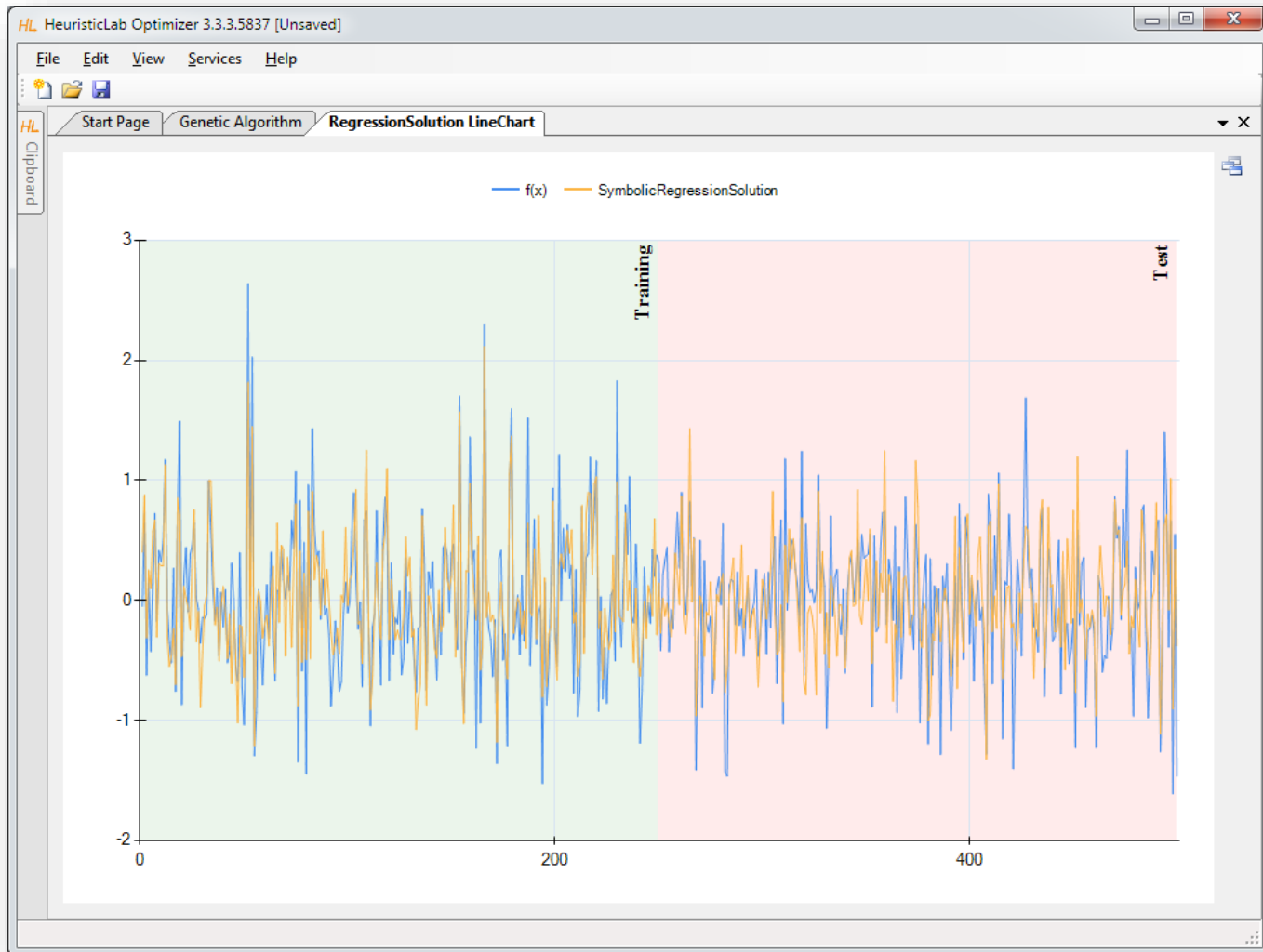
Details

Regression Solution

- Average relative error (test): 354.489941523788
- Average relative error (training): 336.306116006
- Mean squared error (test): 0.164930318235415
- Mean squared error (training): 0.141423207746
- Model: SymbolicRegressionModel
- Model Depth: 13
- Model Length: 71
- Pearson's R<sup>2</sup> (test): 0.50093645095906758
- Pearson's R<sup>2</sup> (training): 0.66492389380895156
- Problem Data: Data imported from multivariate p...
- Regression Solution ScatterPlot
- Regression Solution LineChart
- Regression Solution Estimated Values

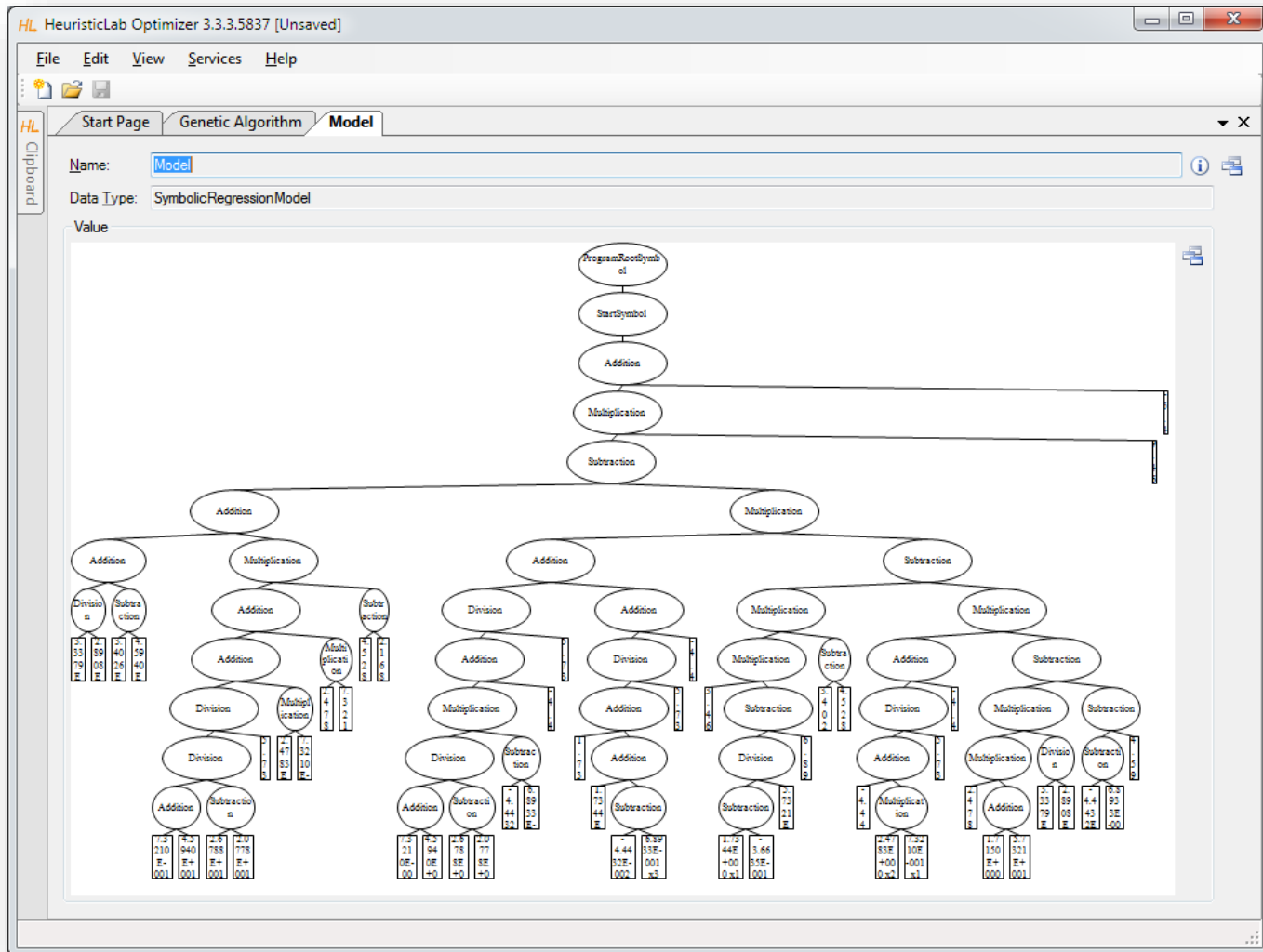
Execution Time: 00:01:17.4564302

# Inspect Linechart of Best Model on Training Partition



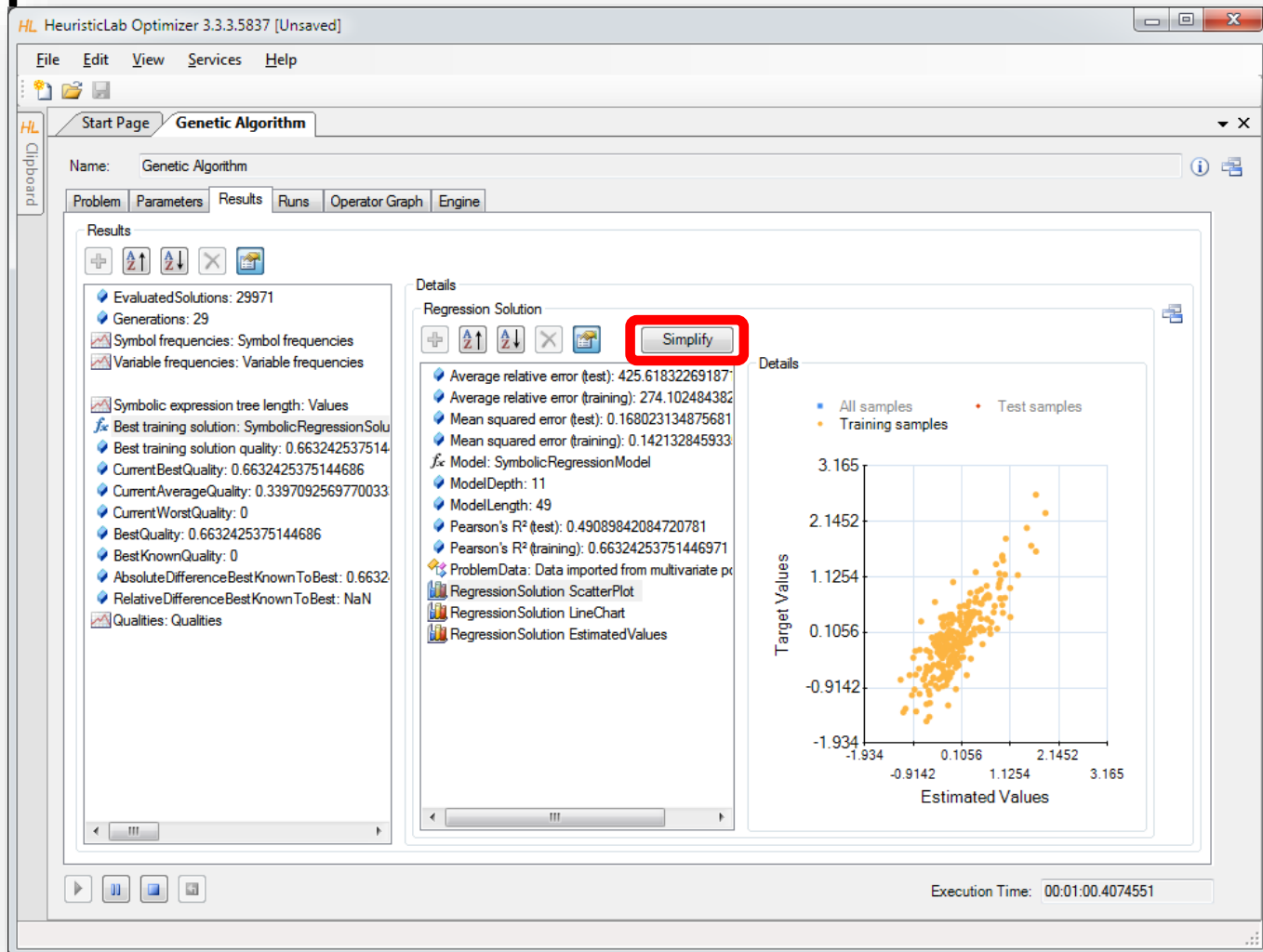


# Inspect Structure of Best Model on Training Partition

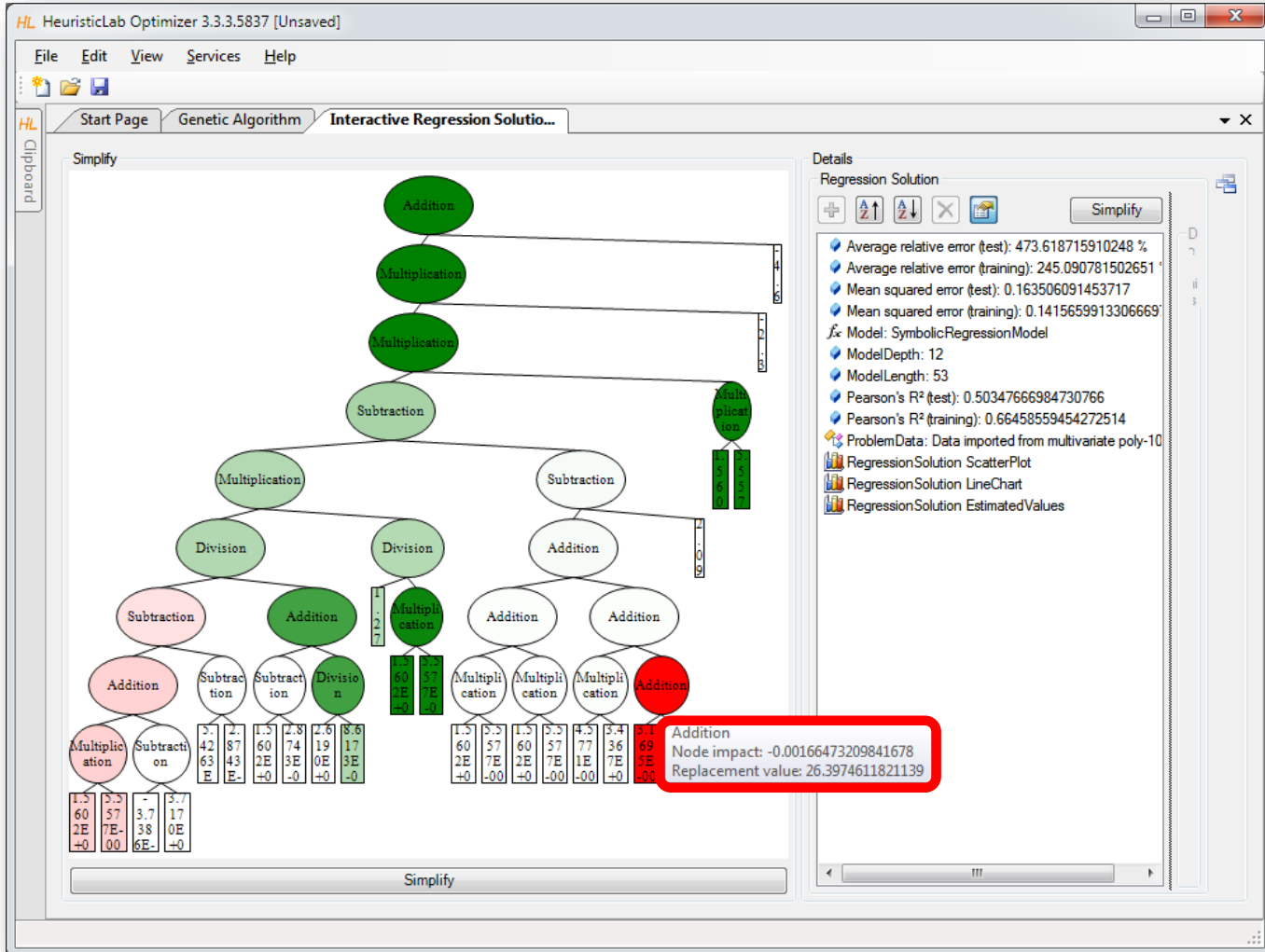




# Detailed Model Analysis and Simplification



# Symbolic Simplification and Node Impacts



The screenshot shows the HeuristicLab Optimizer interface. The main window displays a symbolic regression tree with nodes labeled with mathematical operations: Addition, Multiplication, Subtraction, and Division. The tree is rooted at an Addition node. A red box highlights a specific node in the tree, which is an Addition node. A tooltip for this node shows the following information:

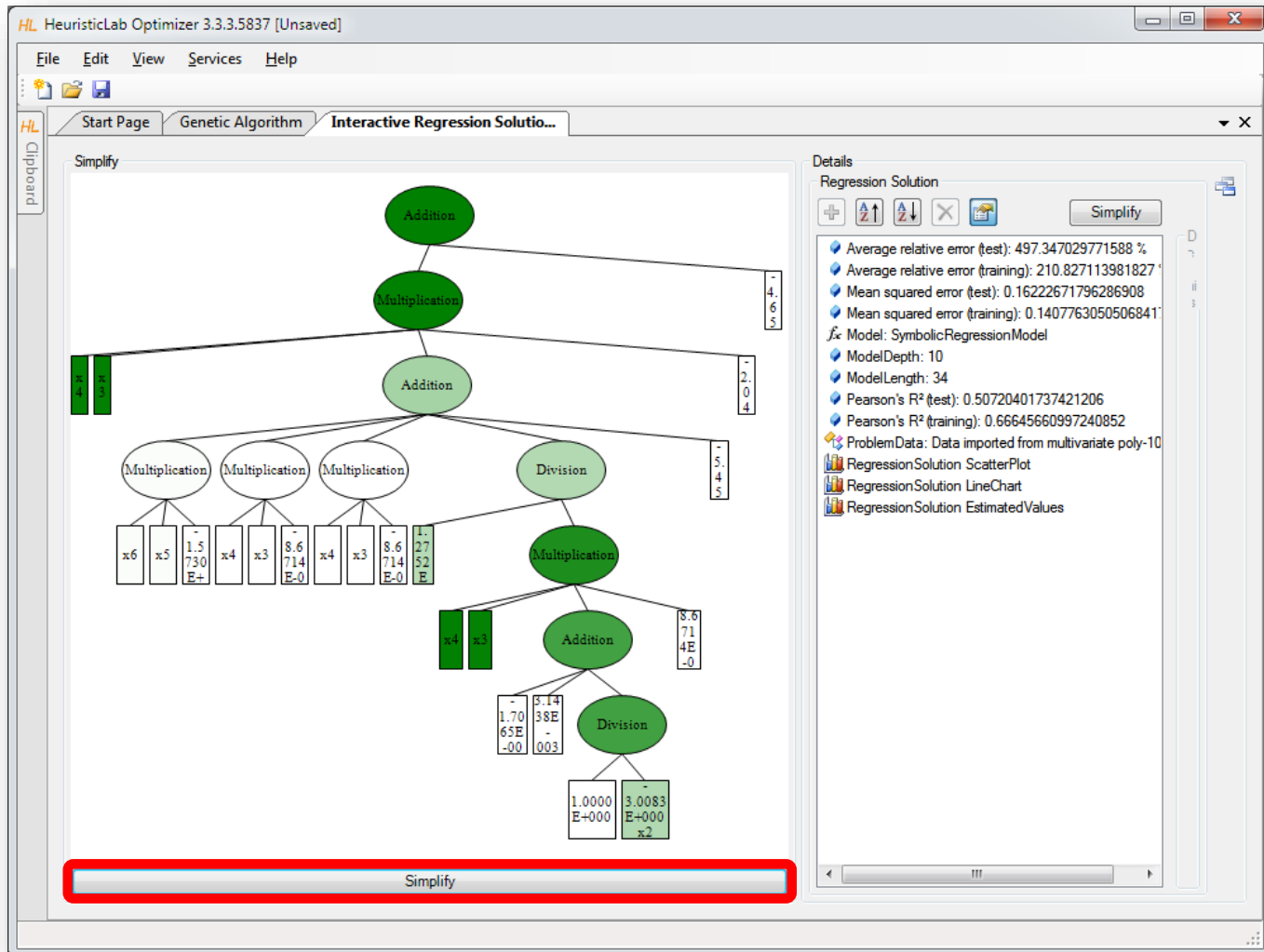
**Addition**  
Node impact: -0.00166473209841678  
Replacement value: 26.3974611821139

The right-hand side of the window shows the 'Details' panel for the 'Regression Solution'. It includes a 'Simplify' button and the following statistics:

- 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 R<sup>2</sup> (test): 0.50347666984730766
- Pearson's R<sup>2</sup> (training): 0.66458559454272514
- ProblemData: Data imported from multivariate poly-10
- RegressionSolution ScatterPlot
- RegressionSolution LineChart
- RegressionSolution EstimatedValues



# Automatic Symbolic Simplification



The screenshot displays the HeuristicLab Optimizer interface. The main window shows an "Interactive Regression Solution" with a symbolic regression tree. 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: -1.7065E-00)
- Level 6: Under the Addition node: Division (Value: 3.0083E+00)
- Level 7: Under the Division node: 1.0000E+000, 3.0083E+000, x2.

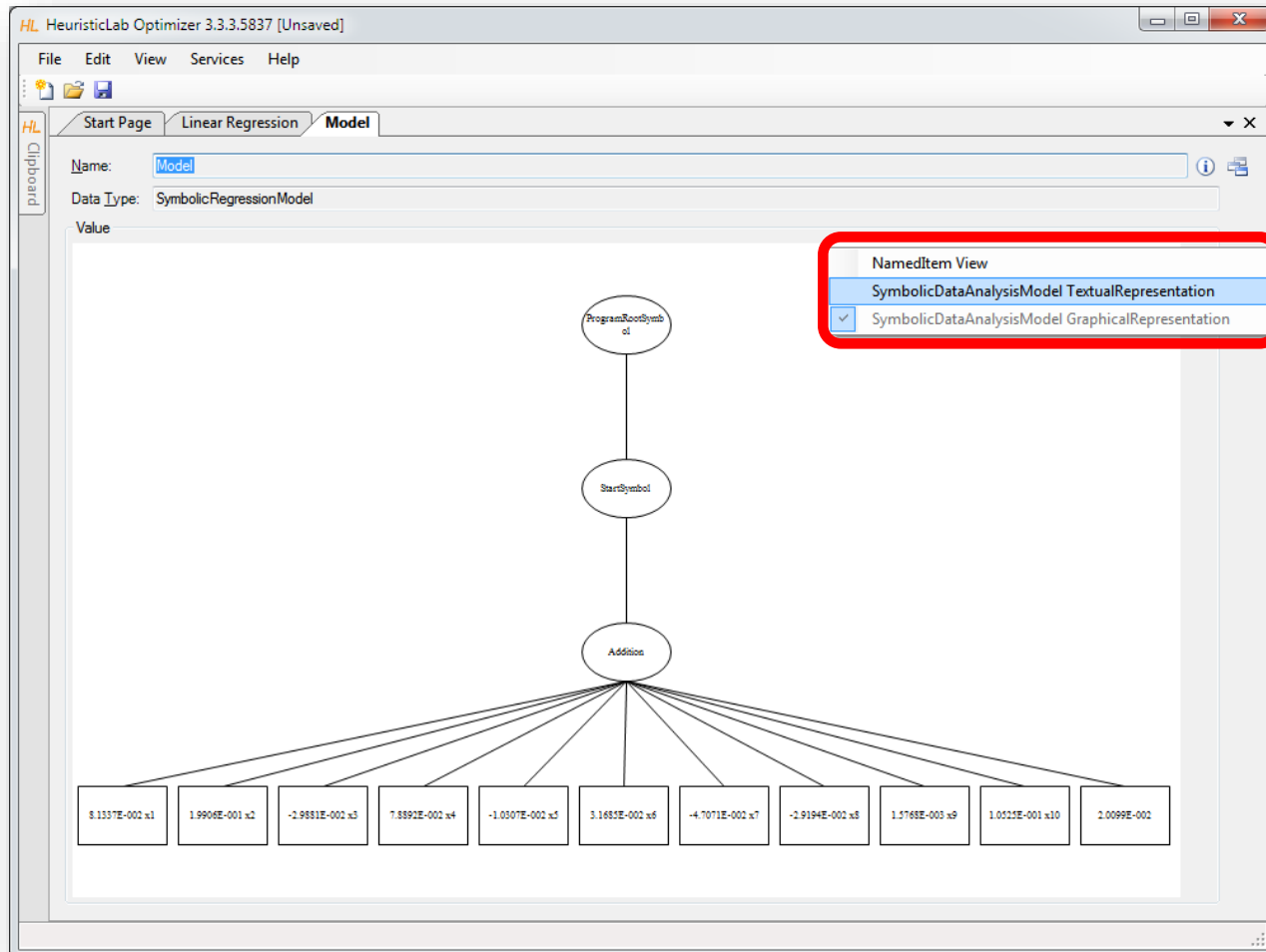
The "Details" panel on the right provides the following information:

- 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 R<sup>2</sup> (test): 0.50720401737421206
- Pearson's R<sup>2</sup> (training): 0.66645660997240852
- ProblemData: Data imported from multivariate poly-10
- RegressionSolution ScatterPlot
- RegressionSolution LineChart
- RegressionSolution EstimatedValues

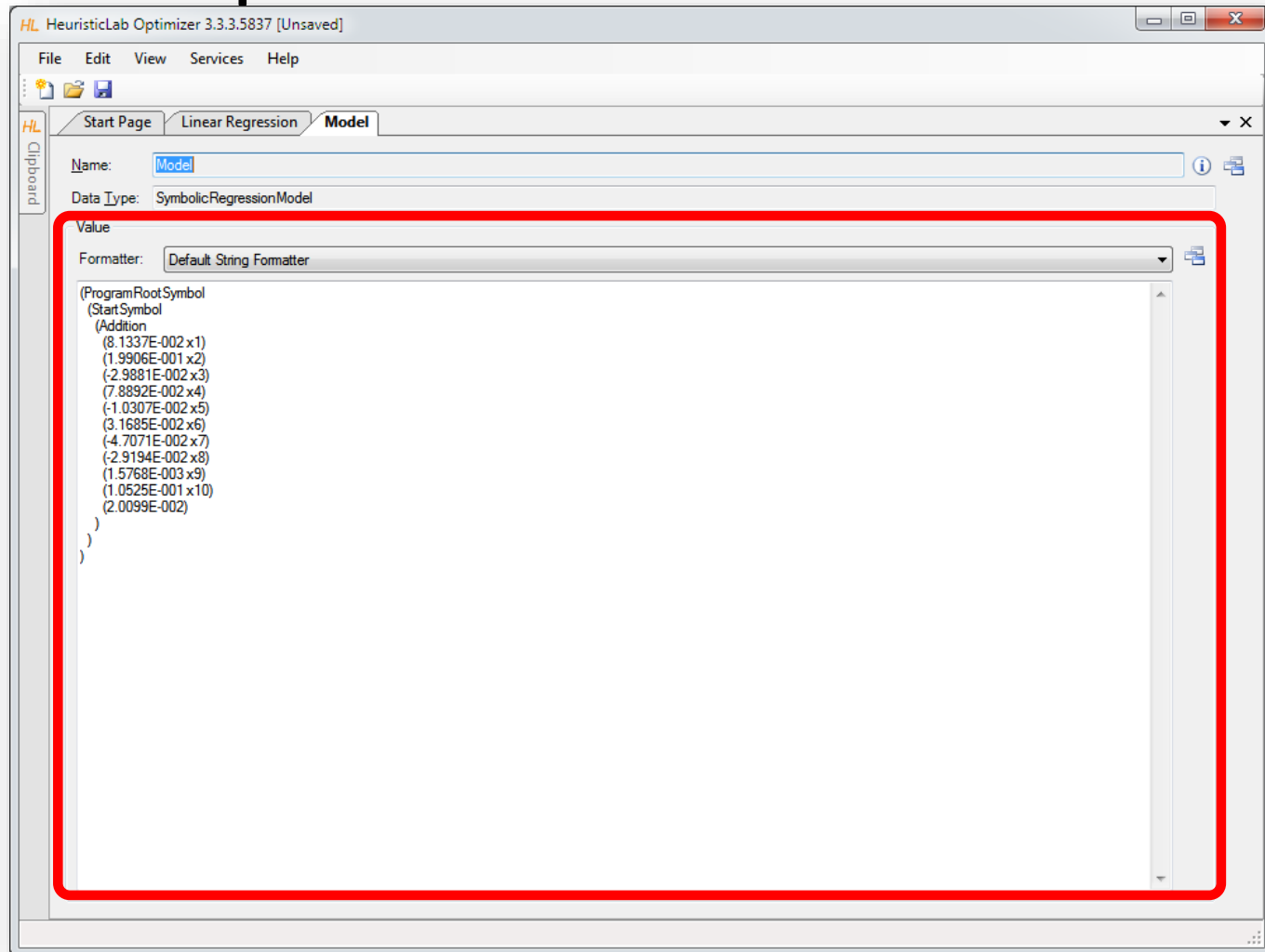
A red box highlights the "Simplify" button at the bottom of the tree view.

# Textual Representations Are Also Available

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

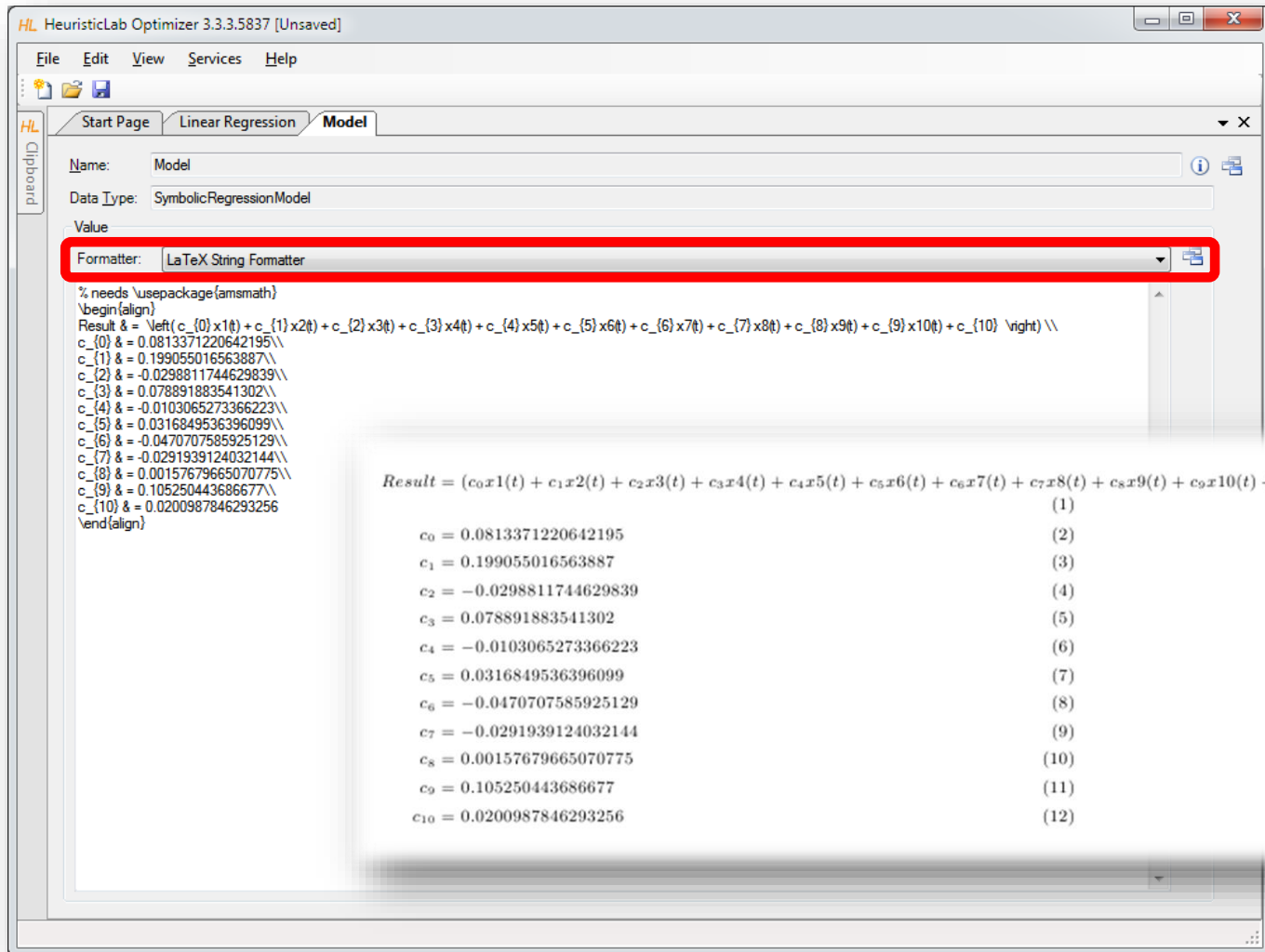


# Default Textual Representation for Model Export





# Textual Representation for Export to LaTeX



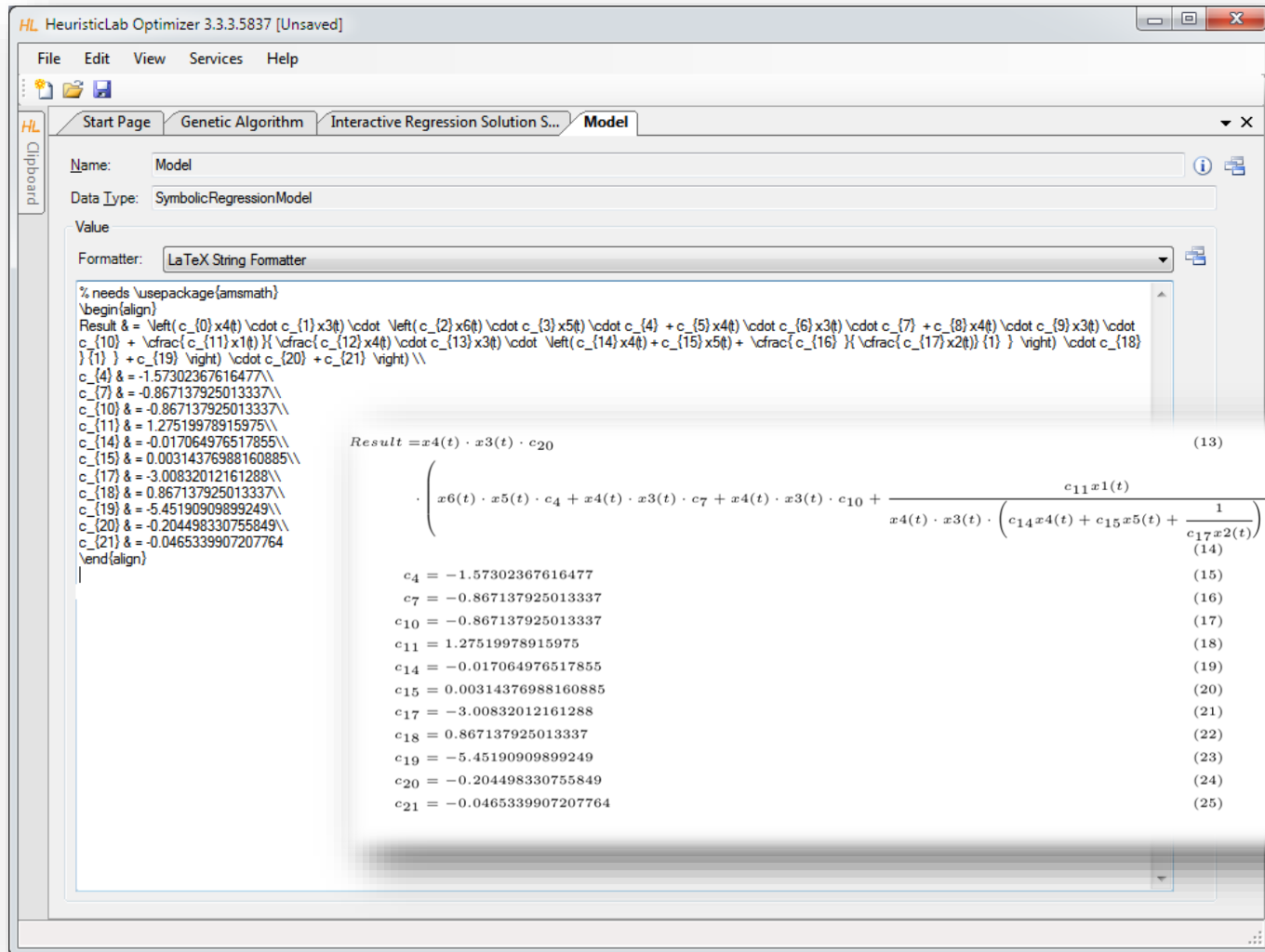
The screenshot shows the HeuristicLab Optimizer interface. The 'Model' tab is active, and the 'Formatter' dropdown is set to 'LaTeX String Formatter'. The main text area contains LaTeX code for a symbolic regression model. A red box highlights the 'Formatter' dropdown. A preview window shows the rendered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



The screenshot shows the HeuristicLab Optimizer interface with a model named 'Model' of type 'SymbolicRegressionModel'. The 'Value' field is set to 'LaTeX String Formatter'. The main window displays the LaTeX code for the model's result, which is a complex symbolic expression involving multiple variables and coefficients. Below the code, the result is rendered as a mathematical equation with numbered labels (13) through (24) for each coefficient.

```

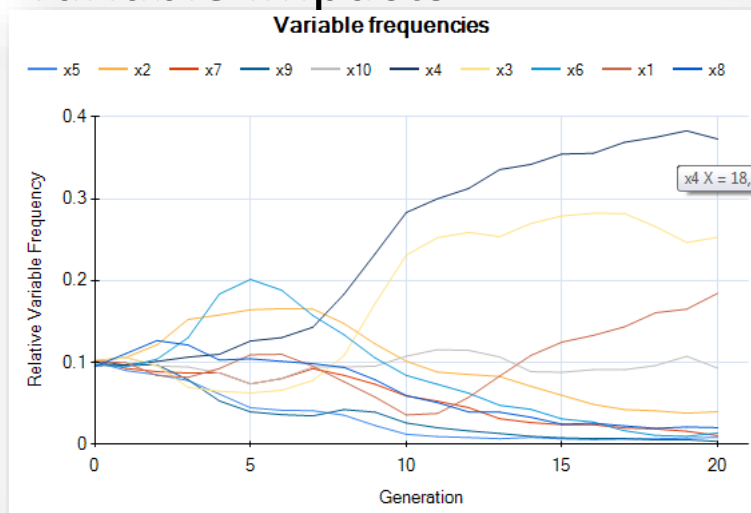
% needs \usepackage{amsmath}
\begin{align}
Result &= \left( c_4 x_4(t) + c_7 x_7(t) + c_{10} x_{10}(t) + c_{11} x_{11}(t) + c_{14} x_{14}(t) + c_{15} x_{15}(t) + c_{17} x_{17}(t) + c_{18} x_{18}(t) + c_{19} x_{19}(t) + c_{20} x_{20}(t) + c_{21} x_{21}(t) \right) \\
&+ \frac{c_{12} x_2(t) + c_{13} x_3(t) + c_{16} x_6(t)}{c_{17} x_7(t)} + \frac{c_{14} x_4(t) + c_{15} x_5(t)}{c_{17} x_7(t)} + \frac{c_{18} x_8(t)}{c_{17} x_7(t)} + \frac{c_{19} x_9(t)}{c_{17} x_7(t)} + \frac{c_{20} x_{10}(t) + c_{21} x_{11}(t)}{c_{17} x_7(t)} \\
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}

```

$$\begin{aligned}
 Result &= x_4(t) \cdot x_3(t) \cdot c_{20} & (13) \\
 &\cdot \left( x_6(t) \cdot x_5(t) \cdot c_4 + x_4(t) \cdot x_3(t) \cdot c_7 + x_4(t) \cdot x_3(t) \cdot c_{10} + \frac{c_{11} x_1(t)}{x_4(t) \cdot x_3(t) \cdot \left( c_{14} x_4(t) + c_{15} x_5(t) + \frac{1}{c_{17} x_2(t)} \right) \cdot c_{18}} + c_{19} \right) + c_{21} \\
 c_4 &= -1.57302367616477 & (15) \\
 c_7 &= -0.867137925013337 & (16) \\
 c_{10} &= -0.867137925013337 & (17) \\
 c_{11} &= 1.27519978915975 & (18) \\
 c_{14} &= -0.017064976517855 & (19) \\
 c_{15} &= 0.00314376988160885 & (20) \\
 c_{17} &= -3.00832012161288 & (21) \\
 c_{18} &= 0.867137925013337 & (22) \\
 c_{19} &= -5.45190909899249 & (23) \\
 c_{20} &= -0.204498330755849 & (24) \\
 c_{21} &= -0.0465339907207764 & (25)
 \end{aligned}$$

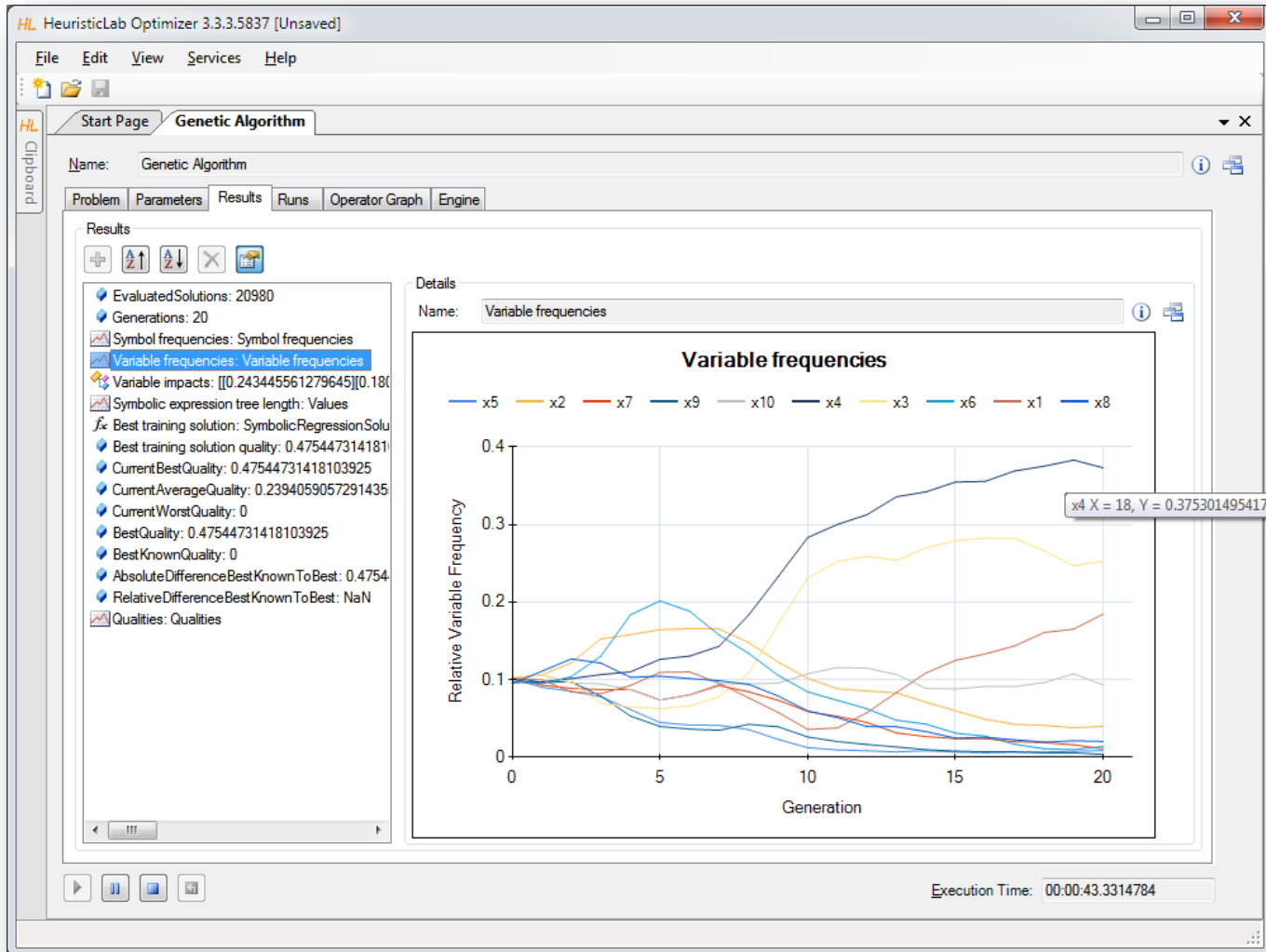
# Variable Relevance Analysis

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

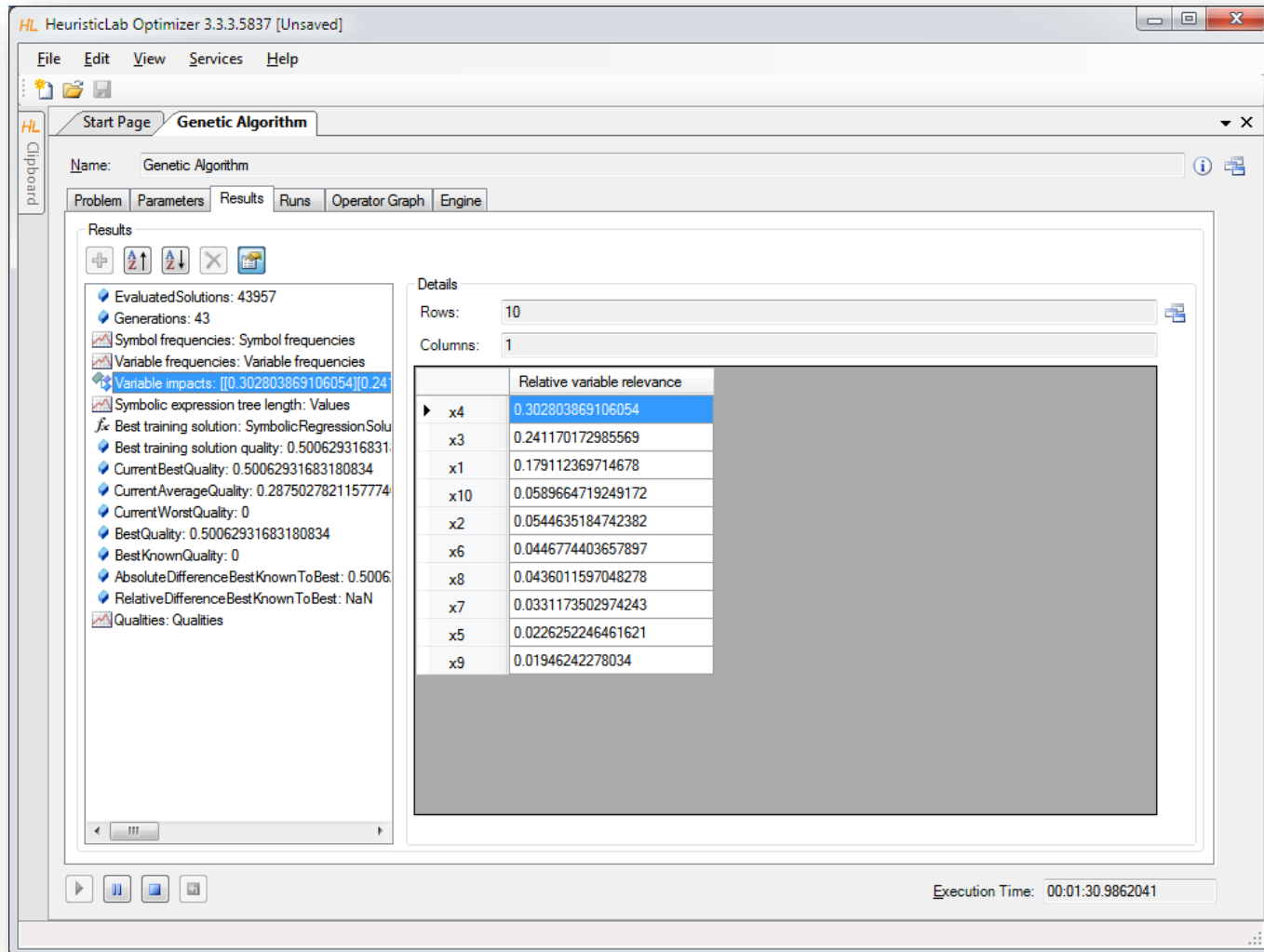


	Relative variable relevance
x4	0.302803869106054
x3	0.241170172985569
x1	0.179112369714678
x10	0.0589664719249172
x2	0.0544635184742382
x6	0.0446774403657897
x8	0.0436011597048278
x7	0.0331173502974243
x5	0.0226252246461621
x9	0.01946242278034

# Inspect Variable Frequency Chart



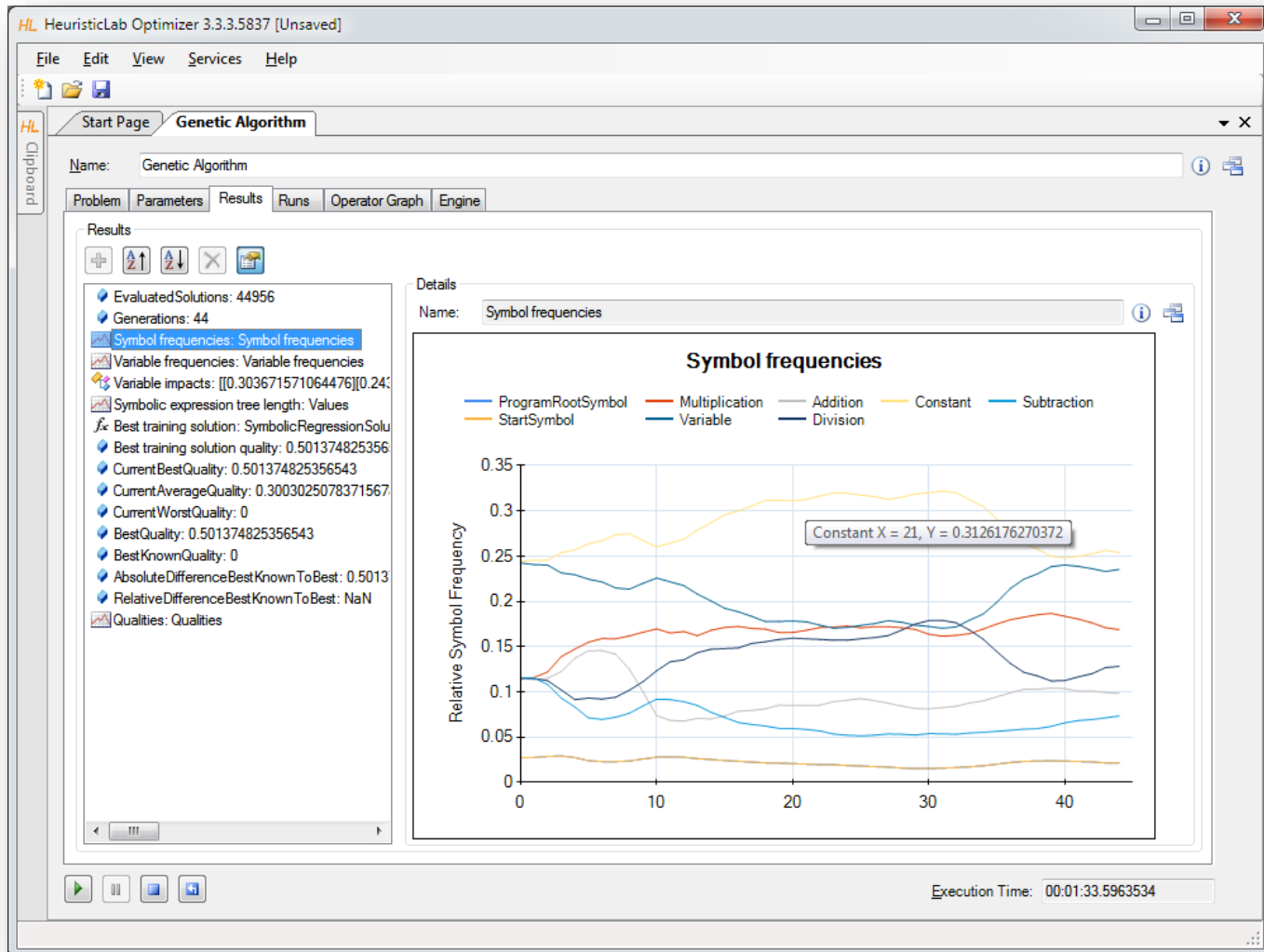
# Inspect Variable Impacts



The screenshot shows the HeuristicLab Optimizer interface. The main window is titled "HL HeuristicLab Optimizer 3.3.3.5837 [Unsaved]". The "Results" tab is active, displaying a list of results on the left and a table of "Relative variable relevance" on the right. The table lists variables x1 through x10 with their respective relevance values. The variable x4 has the highest relevance, highlighted in blue.

	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

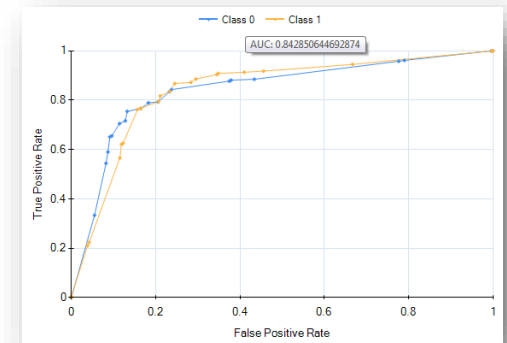
# Inspect Symbol Frequencies



# 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



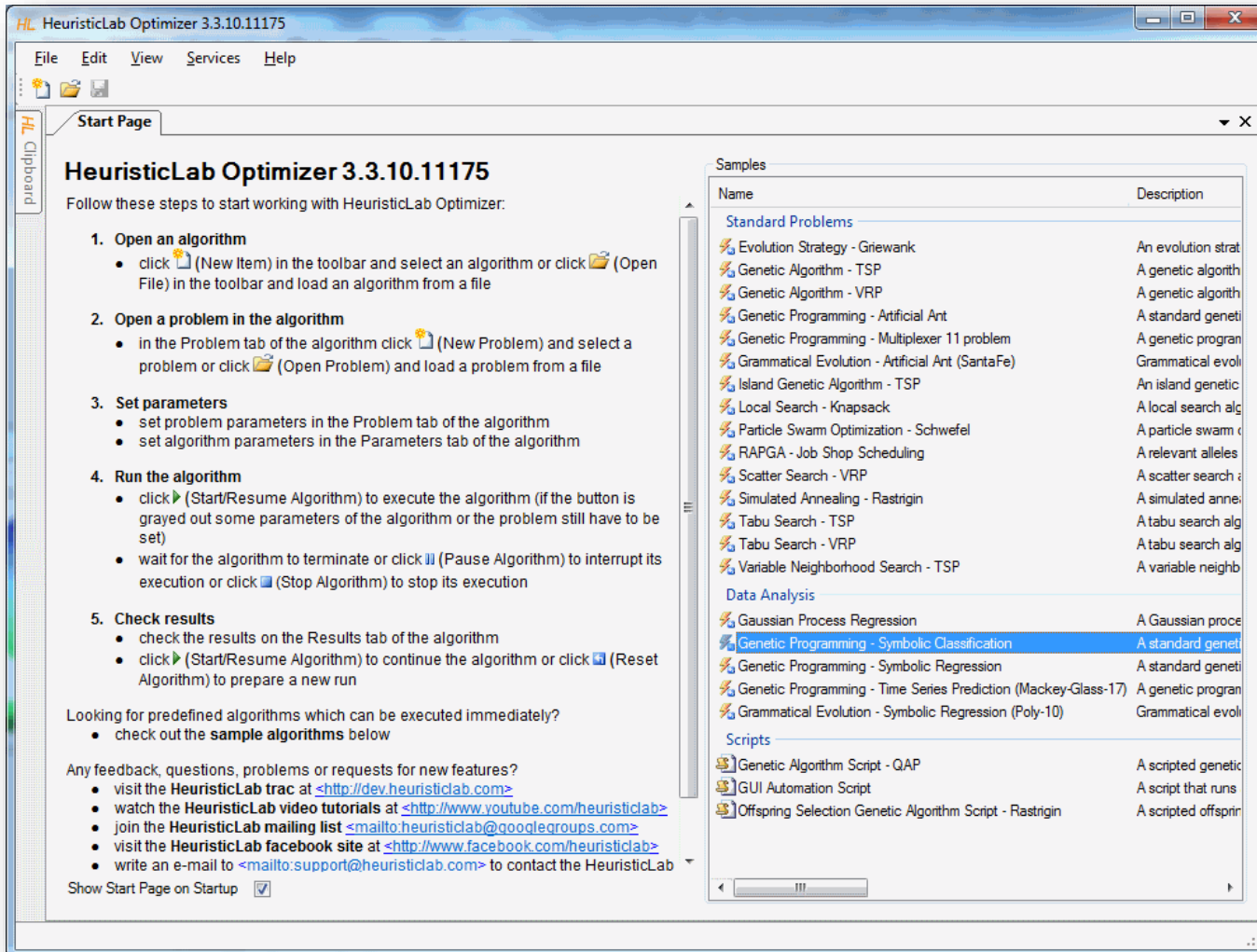
	Actual Class 0	Actual Class 1
Predicted Class 0	197	29
Predicted Class 1	64	190

# 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 list of instructions for starting a new optimization run. On the right, a 'Samples' panel lists various optimization problems and scripts, with 'Genetic Programming - Symbolic Classification' selected.

**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

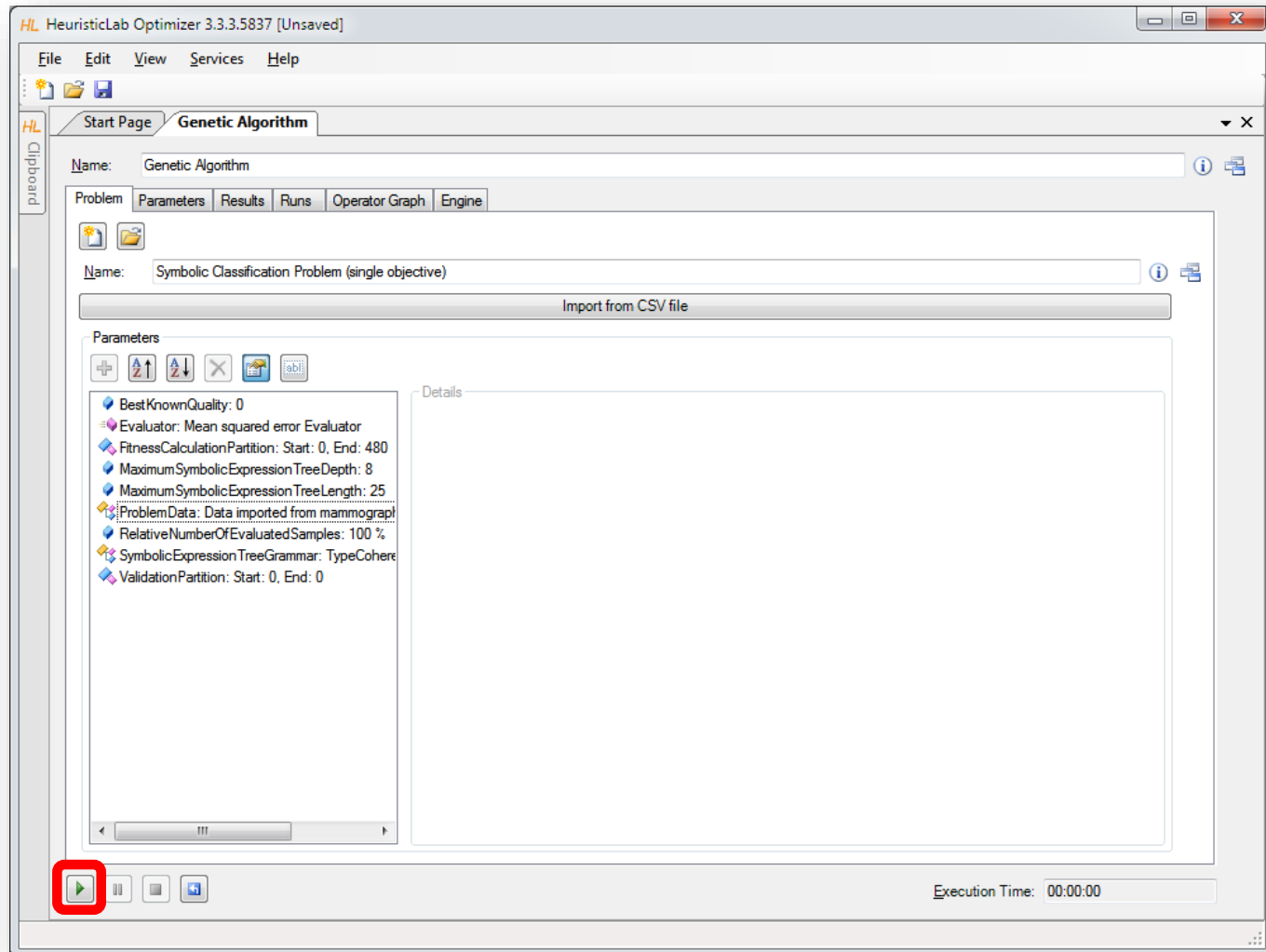
Any feedback, questions, problems or requests for new features?

- 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

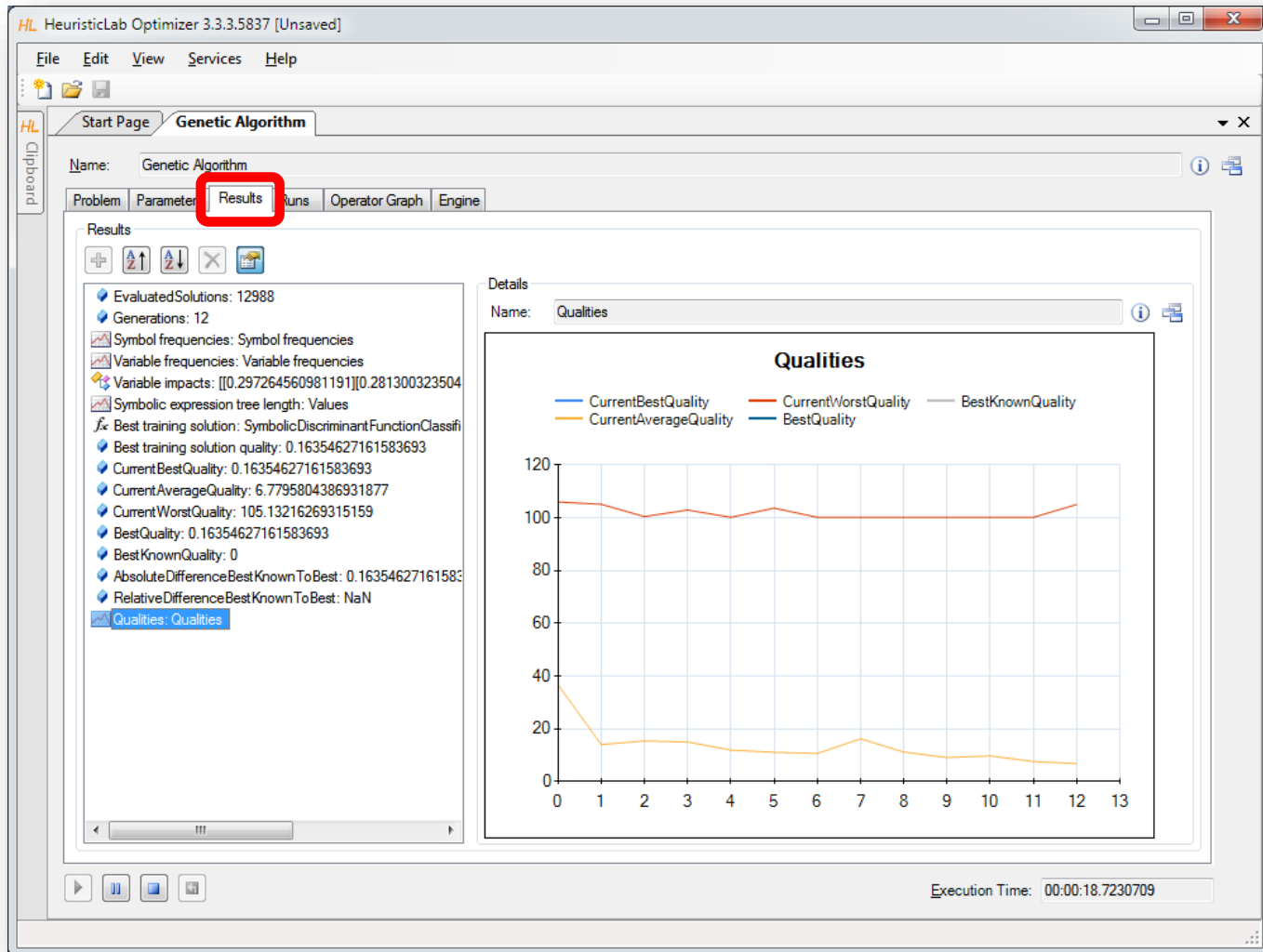
Show Start Page on Startup

Name	Description
<b>Standard Problems</b>	
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 e
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
<b>Data Analysis</b>	
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
<b>Scripts</b>	
Genetic Algorithm Script - QAP	A scripted genetic
GUI Automation Script	A script that runs
Offspring Selection Genetic Algorithm Script - Rastrigin	A scripted offsprin

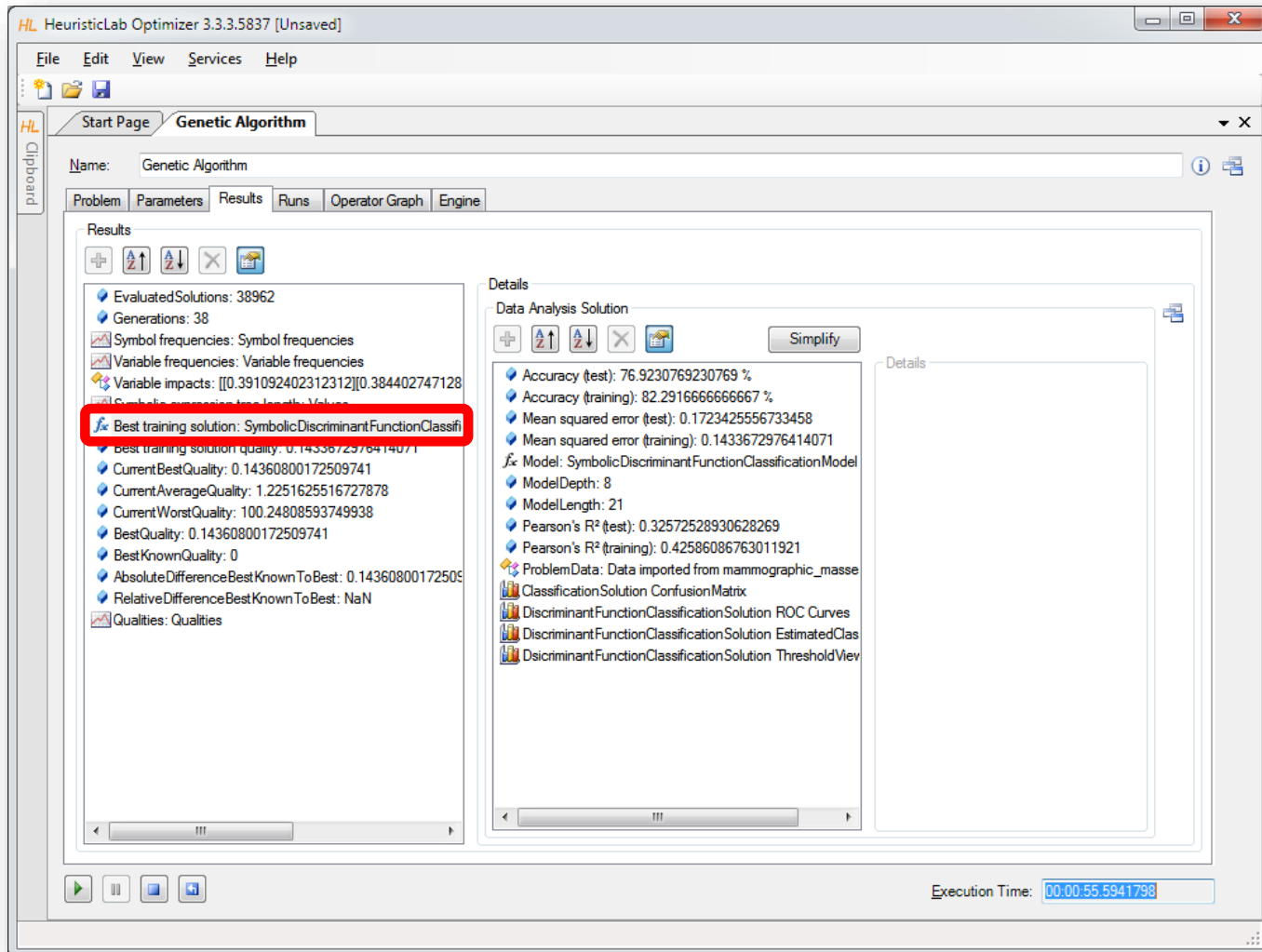
# Configure and Run Algorithm



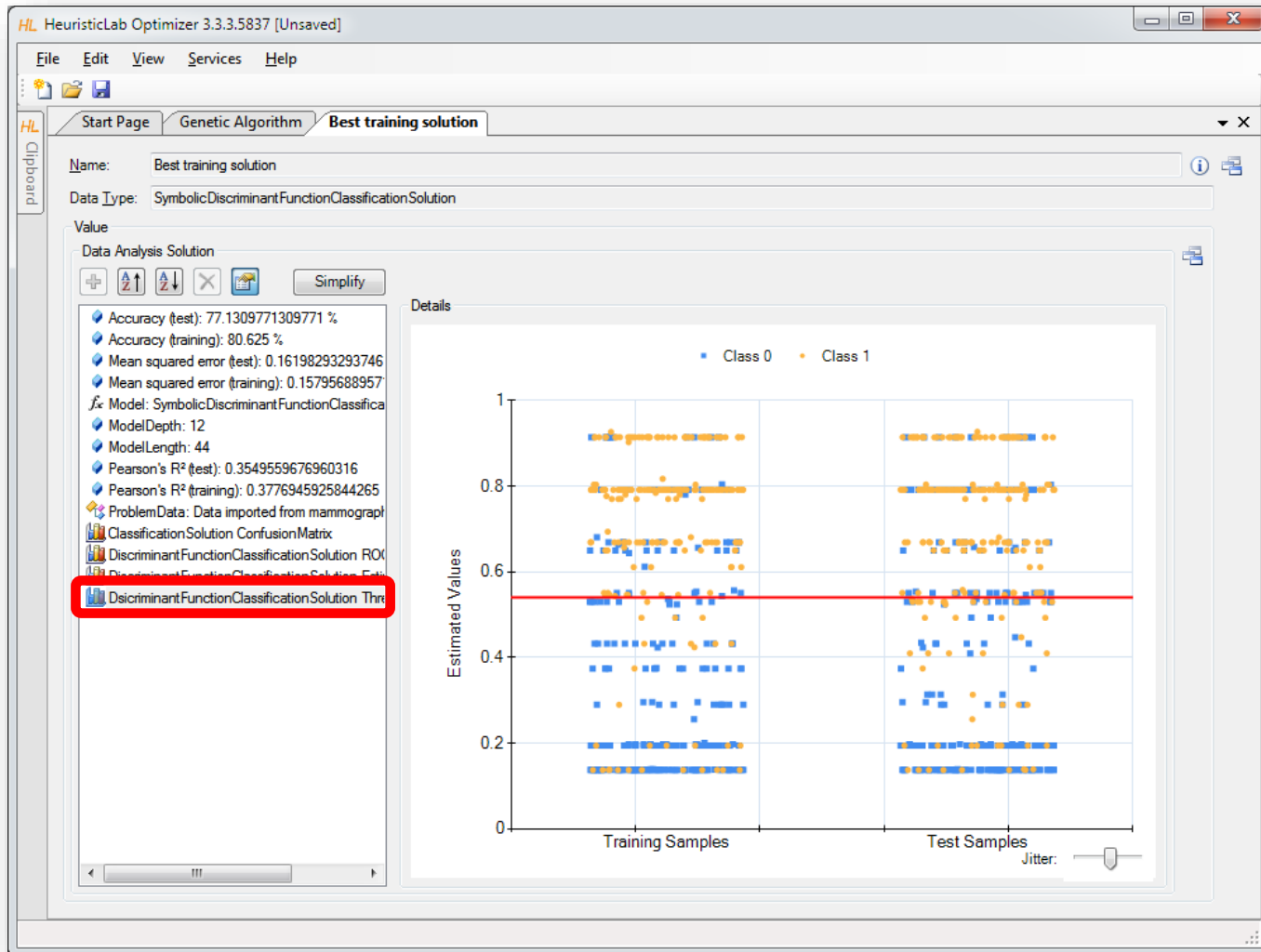
# Inspect Quality Linechart



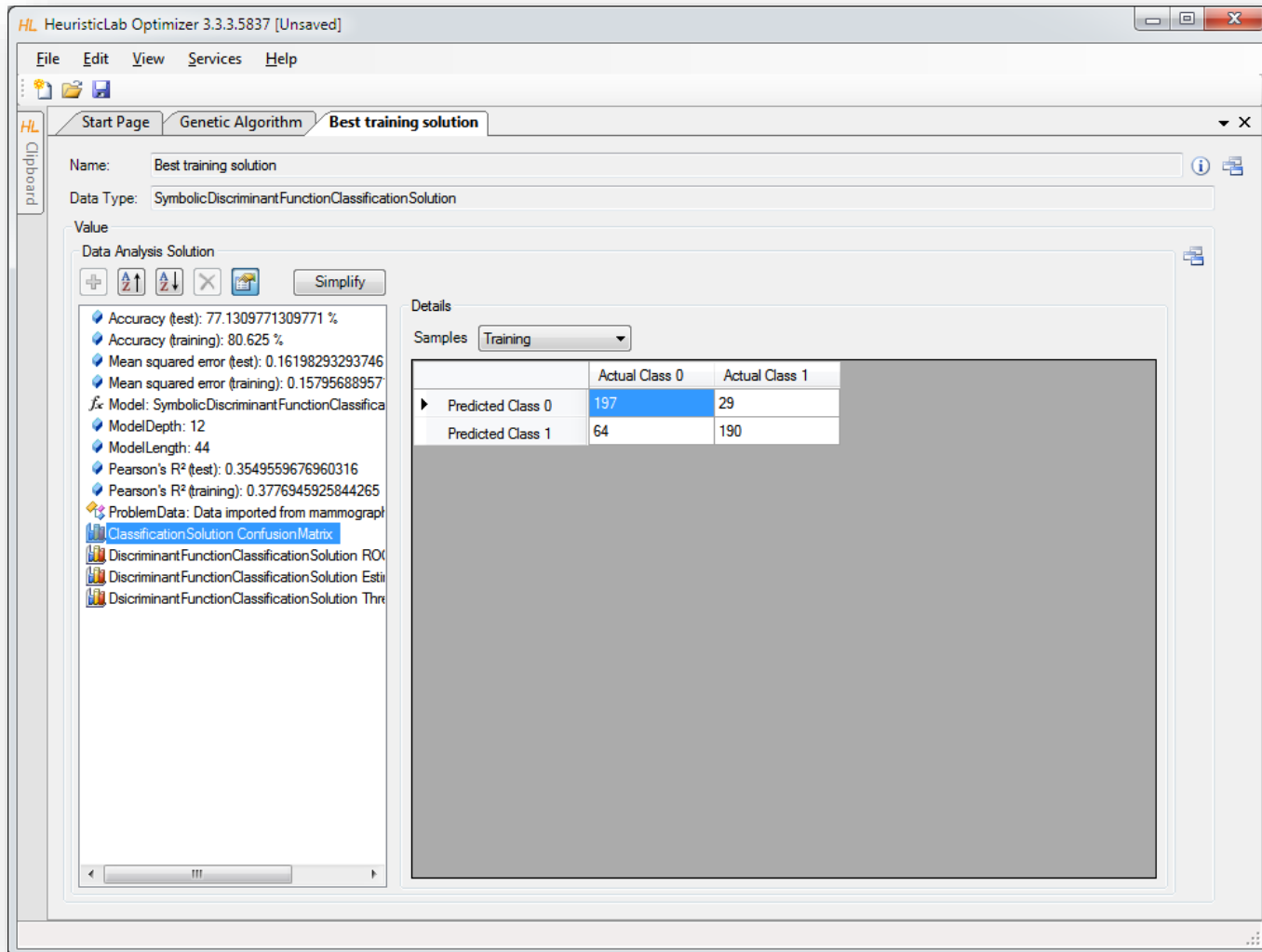
# Inspect Best Training Solution



# Inspect Model Output and Thresholds



# Inspect Confusion Matrix



HL HeuristicLab Optimizer 3.3.3.5837 [Unsaved]

File Edit View Services Help

Start Page Genetic Algorithm **Best training solution**

Name: Best training solution

Data Type: SymbolicDiscriminantFunctionClassificationSolution

Value

Data Analysis Solution

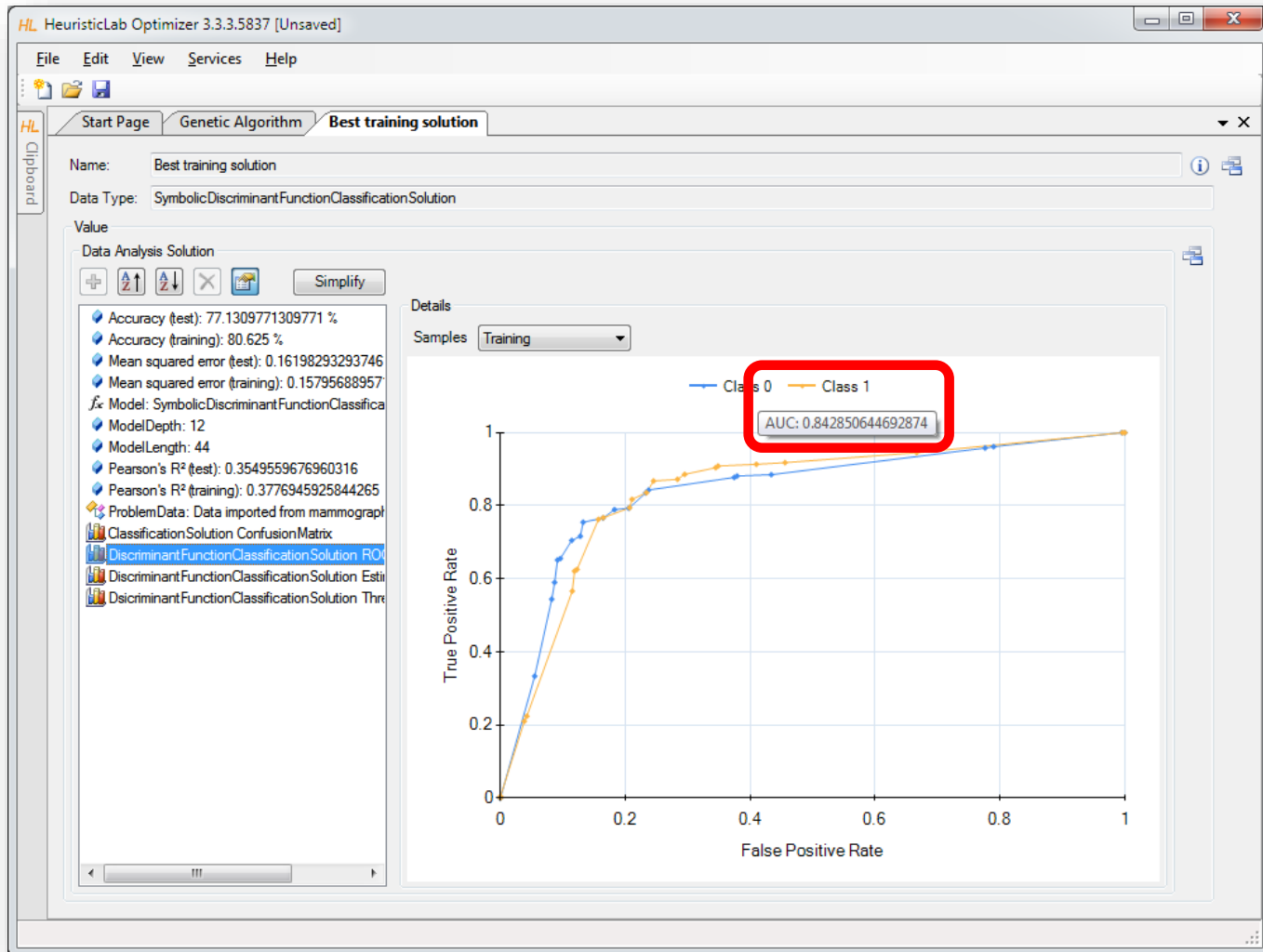
Accuracy (test): 77.1309771309771 %  
Accuracy (training): 80.625 %  
Mean squared error (test): 0.16198293293746  
Mean squared error (training): 0.15795688957  
Model: SymbolicDiscriminantFunctionClassificationSolution  
ModelDepth: 12  
ModelLength: 44  
Pearson's R<sup>2</sup> (test): 0.3549559676960316  
Pearson's R<sup>2</sup> (training): 0.3776945925844265  
ProblemData: Data imported from mammograph  
ClassificationSolution ConfusionMatrix  
DiscriminantFunctionClassificationSolution RO  
DiscriminantFunctionClassificationSolution Esti  
DiscriminantFunctionClassificationSolution Thre

Details

Samples Training

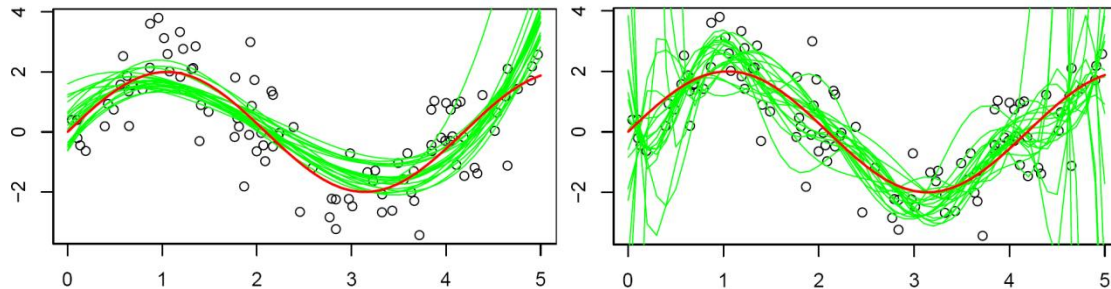
	Actual Class 0	Actual Class 1
Predicted Class 0	197	29
Predicted Class 1	64	190

# Inspect ROC Curve



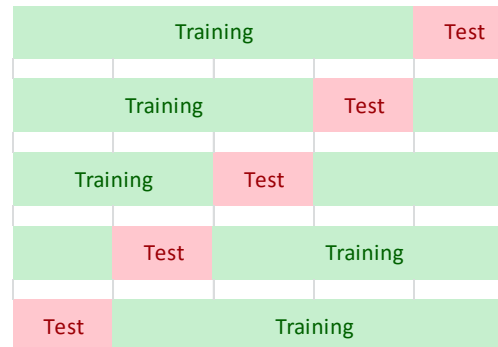
# Validation of Results

- Overfitting = memorizing data



- Strategies to reduce overfitting

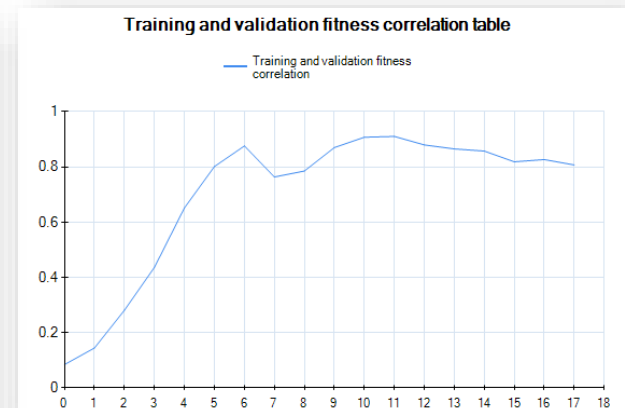
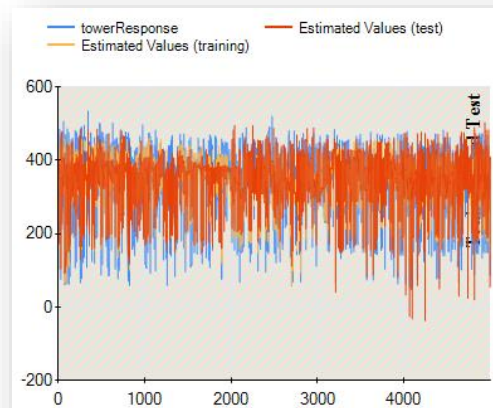
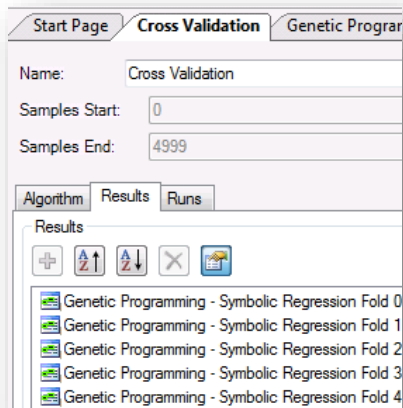
- validation partition
- cross-validation



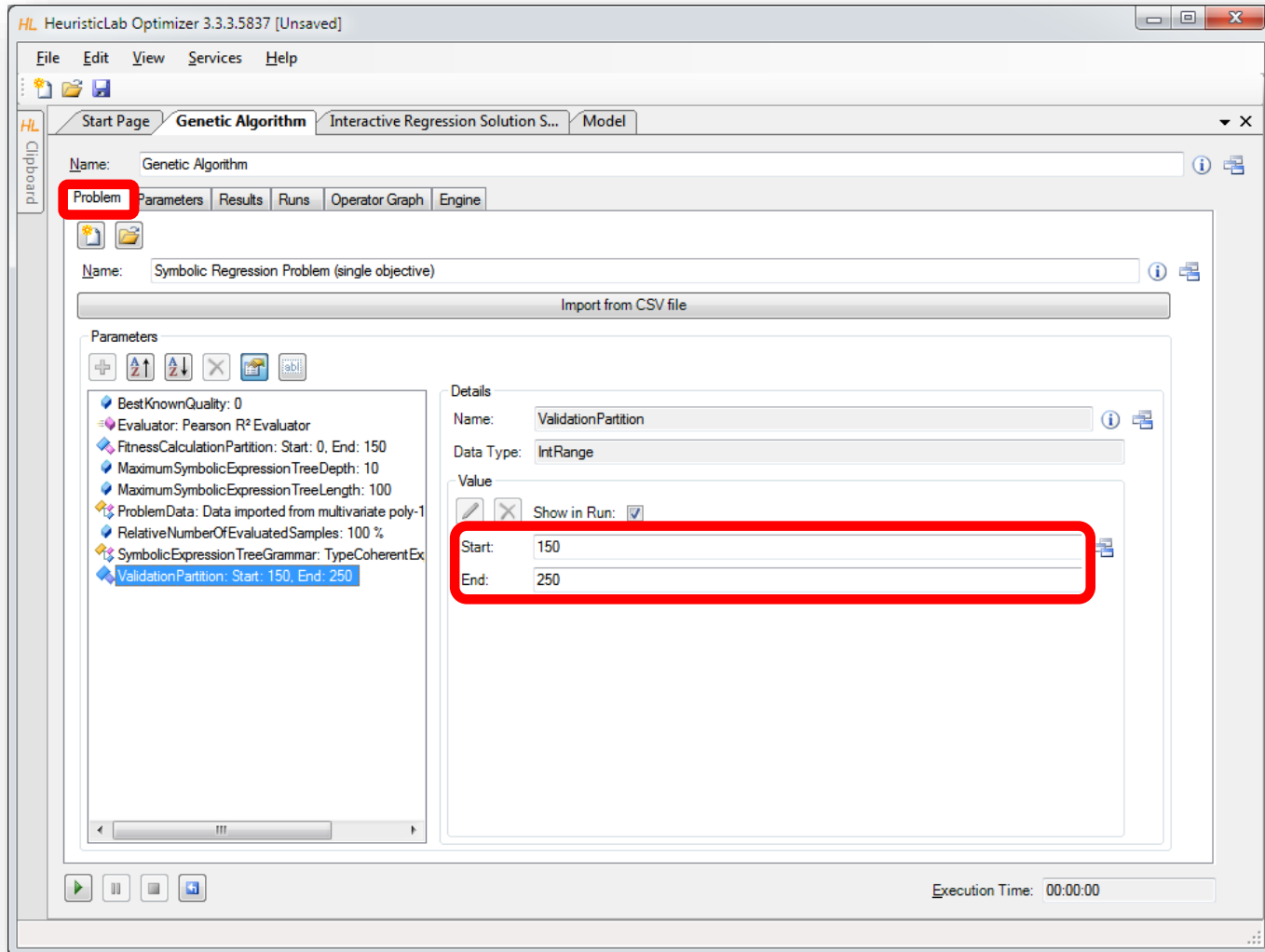


# Validation of Results

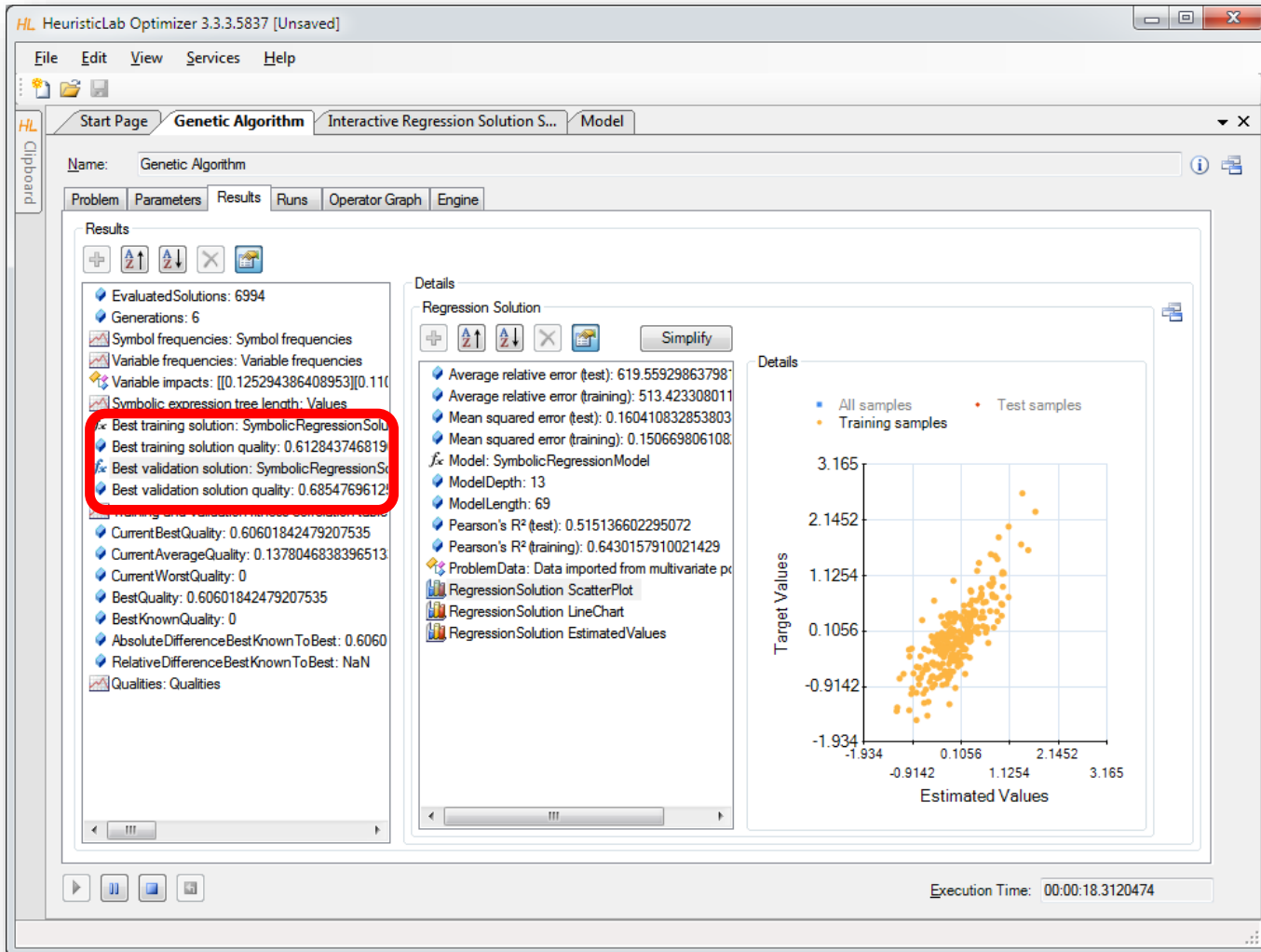
- Demonstration
  - Configuration of a validation set
  - Inspection of best solution on validation set
  - Analysis of training- and validation fitness correlation
  - Cross-validation
    - Configuration
    - Analysis of results



# 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 details:

- 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

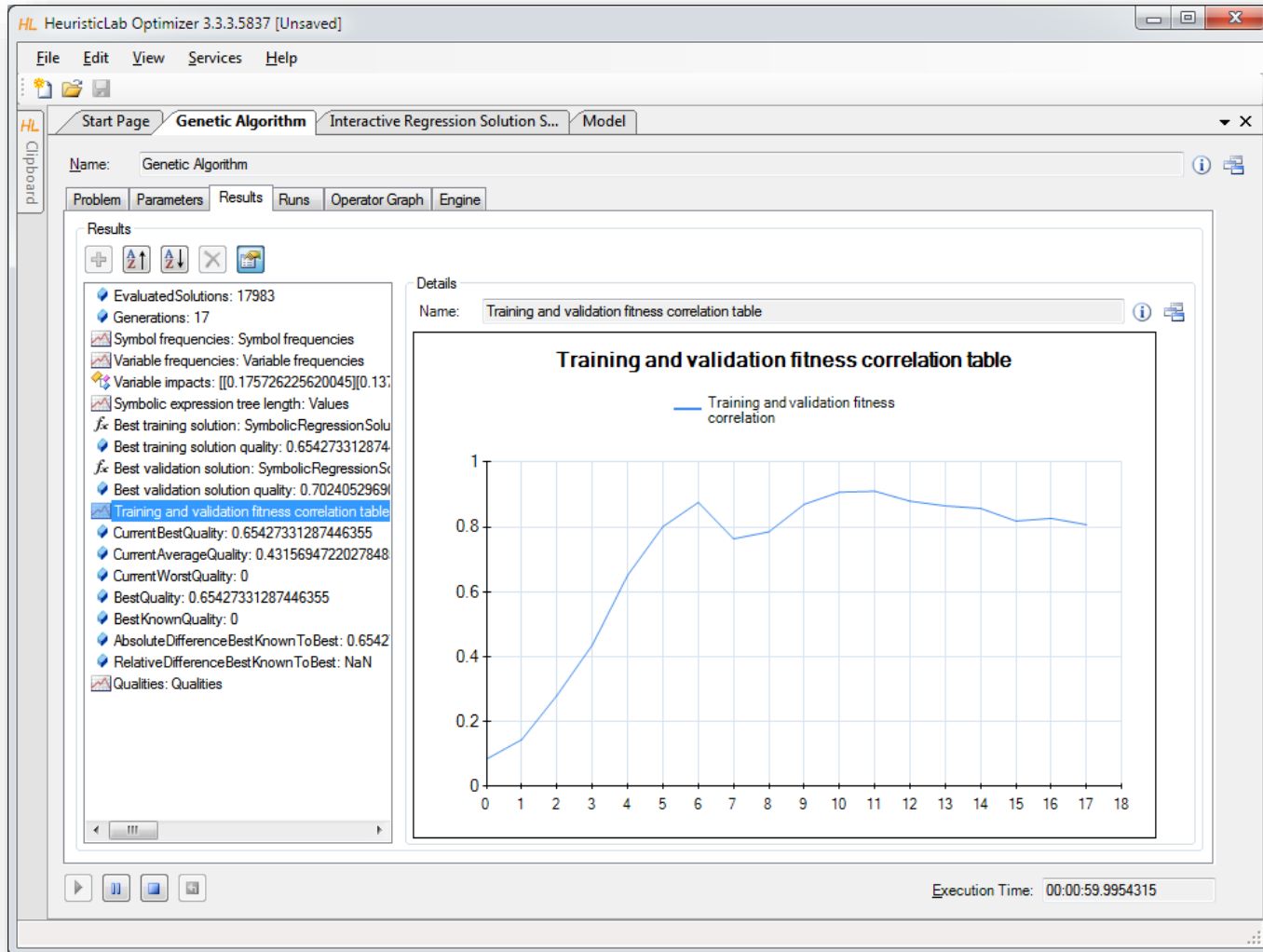
The "Details" panel shows the following information:

- 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 R<sup>2</sup> (test): 0.515136602295072
- Pearson's R<sup>2</sup> (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 ranges from -1.934 to 3.165, and the y-axis ranges from -1.934 to 3.165. The training samples are clustered around the diagonal line, indicating a strong correlation between estimated and target values.

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 (controller, etc.)
  - ...
- Cloud Computing
  - port HeuristicLab Hive to Windows Azure
- 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](mailto:heuristiclab@googlegroups.com)
  - write an e-mail to [support@heuristiclab.com](mailto: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

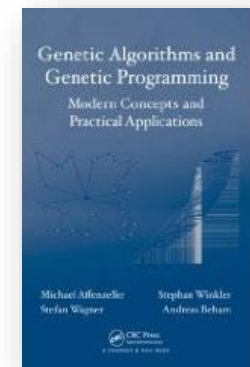
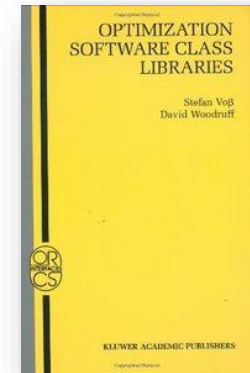
WWW: <http://heal.heuristiclab.com>





# 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**  
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- Detailed list of all publications of the HEAL research group: <http://research.fh-ooe.at/de/orgunit/356#showpublications>

# Questions & Answers



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