The Genetic and Evolutionary Computation Conference

Algorithm and Experiment Design with HeuristicLab

An Open Source Optimization Environment for Research and Education

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Instructor Biographies

- Stefan Wagner
  - MSc in computer science (2004)
    Johannes Kepler University Linz, Austria
  - PhD in technical sciences (2009)
    Johannes Kepler University Linz, Austria
  - Associate professor (2005 – 2009)
    Upper Austria University of Applied Sciences
  - Full professor for complex software systems (since 2009)
    Upper Austria University of Applied Sciences
  - Co-founder of the HEAL research group
  - Project manager and chief architect of HeuristicLab
  - http://heal.heuristiclab.com/team/wagner

- Gabriel Kronberger
  - MSc in computer science (2005)
    Johannes Kepler University Linz, Austria
  - PhD in technical sciences (2010)
    Johannes Kepler University Linz, Austria
  - Research assistant (since 2005)
    Upper Austria University of Applied Sciences
  - Member of the HEAL research group
  - Architect of HeuristicLab
  - http://heal.heuristiclab.com/team/kronberger

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Agenda

- Objectives of the Tutorial
- Introduction
- Where to get HeuristicLab?
- Plugin Infrastructure
- Graphical User Interface
- Available Algorithms & Problems
- Demonstration
- Some Additional Features
- Planned Features
- Team
- Suggested Readings
- Bibliography
- Questions & Answers

HeuristicLab

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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

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Introduction

HeuristicLab
A Paradigm-Independent and Extensible Environment for Heuristic Optimization

- 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 3.3.5 released in June 2011

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Where to get HeuristicLab?

- Download binaries
  - deployed as ZIP archives
  - latest stable version 3.3.5
    - released in June 2011
  - daily trunk build
  - http://dev.heuristiclab.com/download
- Check out sources
  - SVN repository
  - HeuristicLab 3.3.5 tag
    - http://dev.heuristiclab.com/svn/hl/core/tags/3.3.5
  - current development trunk
    - http://dev.heuristiclab.com/svn/hl/core/trunk
- License
  - GNU General Public License (Version 3)
- System requirements
  - Microsoft .NET Framework 4.0 Full Version
  - enough RAM and CPU power ;-)

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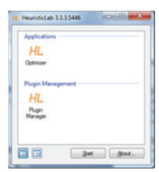
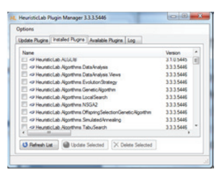
Plugin Infrastructure

- HeuristicLab consists of many assemblies
  - for example 74 plugins in HeuristicLab 3.3.3
  - 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



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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 (default) or moved (shift key)
  - enabled for collection items and content objects

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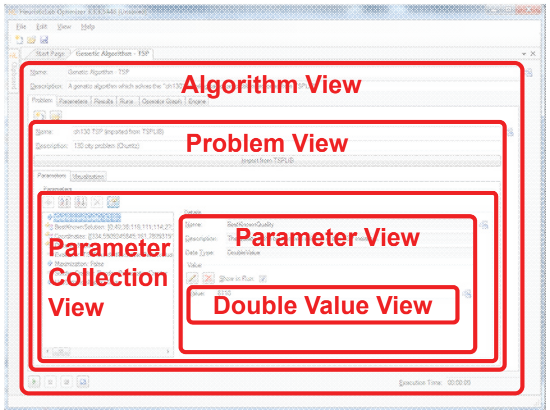
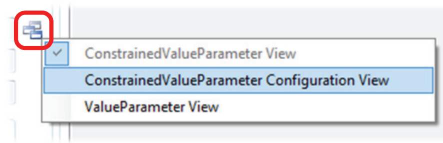
Graphical User Interface



Graphical User Interface

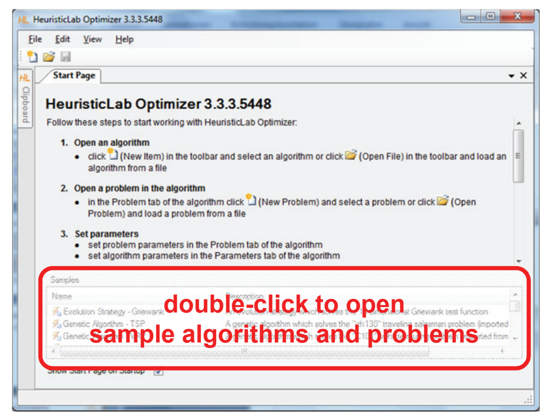
- ViewHost
  - control which hosts views
  - right-click on windows icon to switch views
  - double-click on windows icon to open another view
  - drag & drop windows icon to copy contents



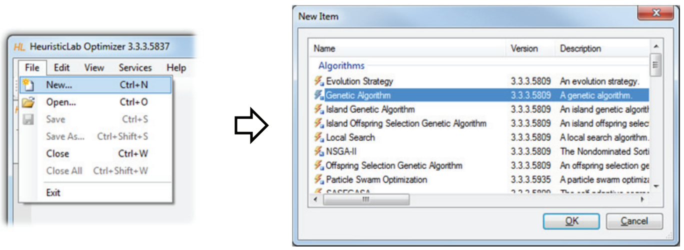
Available Algorithms & Problems

- Algorithms
  - Genetic Algorithm
  - Island Genetic Algorithm
  - Offspring Selection Genetic Algorithm
  - Island Offspring Selection Genetic Algorithm
  - SASEGASA
  - Evolution Strategy
  - NSGA-II
  - Particle Swarm Optimization
  - Local Search
  - Simulated Annealing
  - Tabu Search
  - Variable Neighborhood Search
  - Linear Regression
  - Linear Discriminant Analysis
  - Support Vector Machine
  - k-Means
  - User-defined Algorithm
- Problems
  - Single-Objective Test Function
  - Traveling Salesman Problem
  - Quadratic Assignment Problem
  - Vehicle Routing Problem
  - Scheduling
  - Knapsack
  - OneMax
  - Data Analysis
  - Regression
  - Symbolic Regression
  - Classification
  - Symbolic Classification
  - Clustering
  - Artificial Ant
  - External Evaluation Problem
  - User-defined Problem

HeuristicLab Optimizer



Create Algorithm



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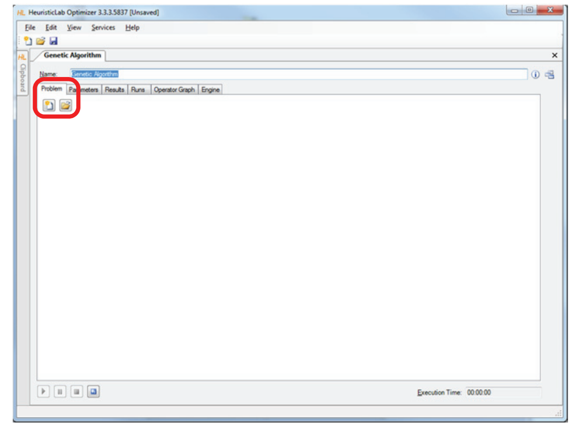
Create or Load Problem



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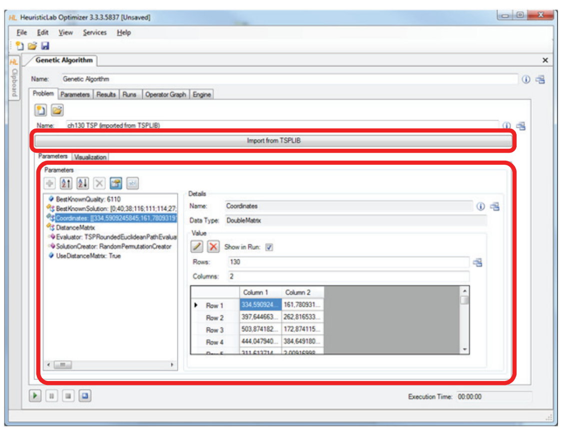
Import or Parameterize Problem Data



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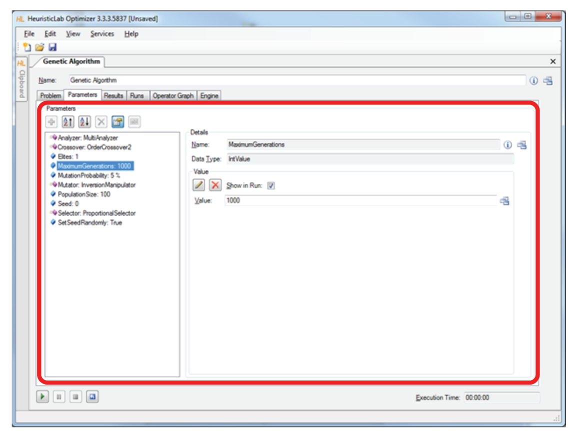
Parameterize Algorithm



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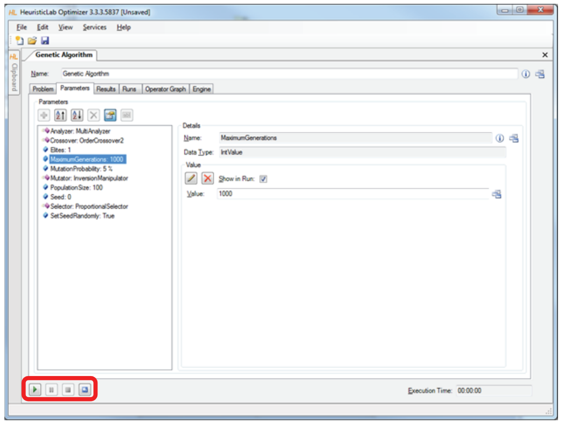
Start, Pause, Resume, Stop and Reset



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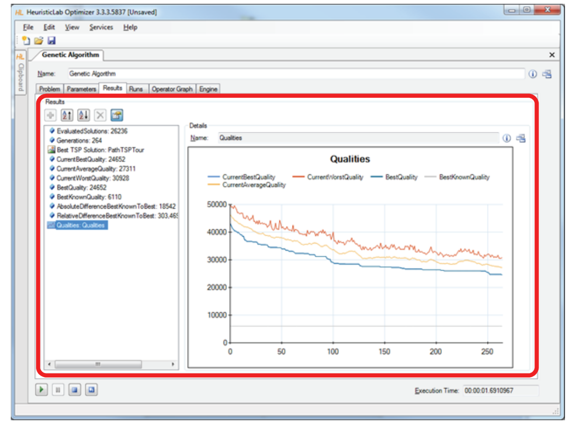
Inspect Results



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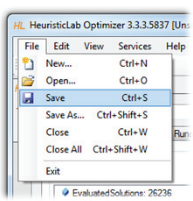
Save and Load

- 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



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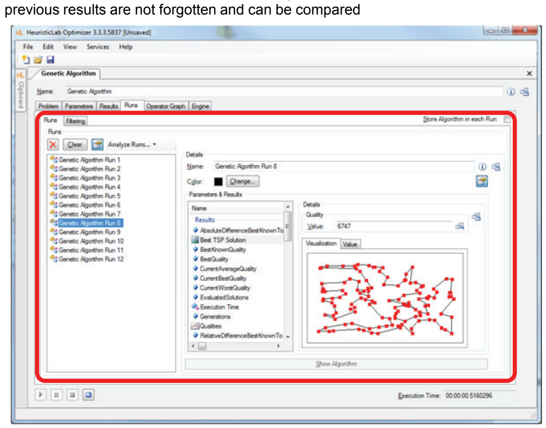
Compare Runs

- 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



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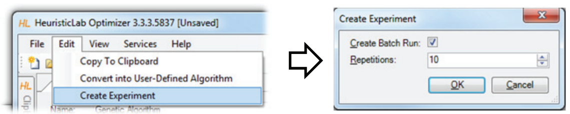
Create Batch Runs and Experiments

- 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



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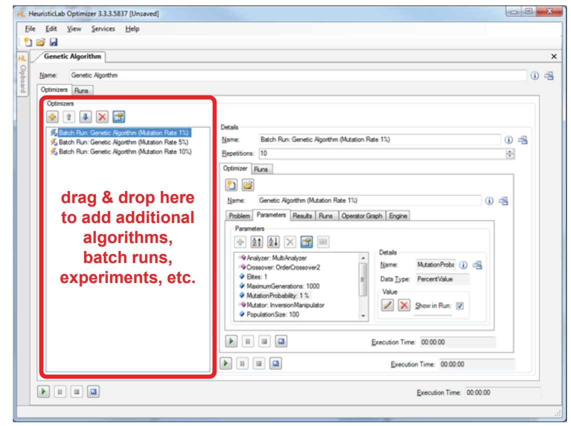
Create Batch Runs and Experiments



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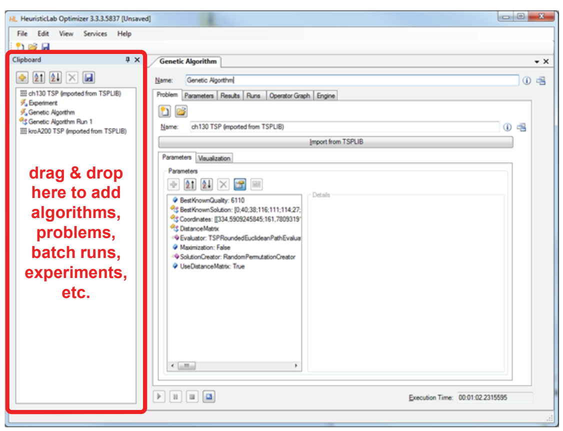
Clipboard



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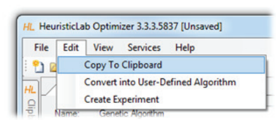
Clipboard

- 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

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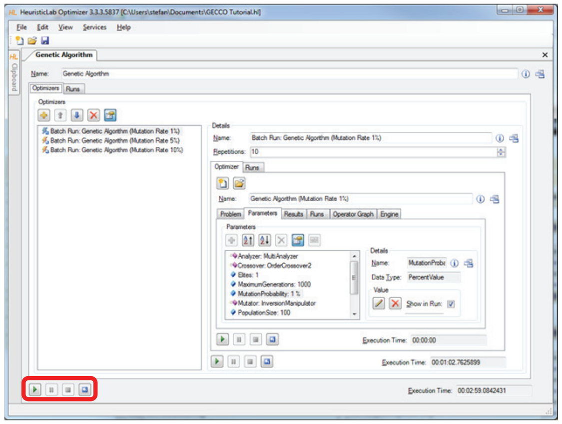
Start, Pause, Resume, Stop, Reset



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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

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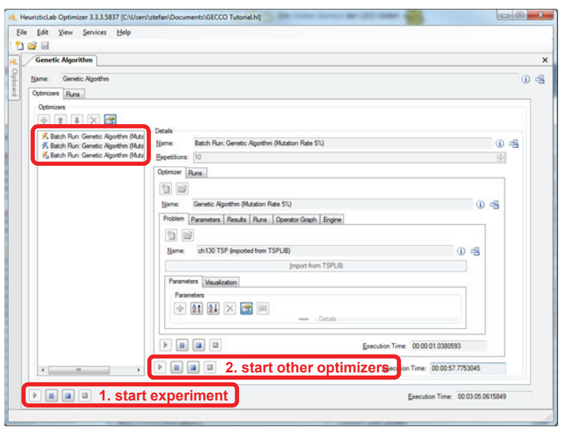
Parallel Execution of Experiments



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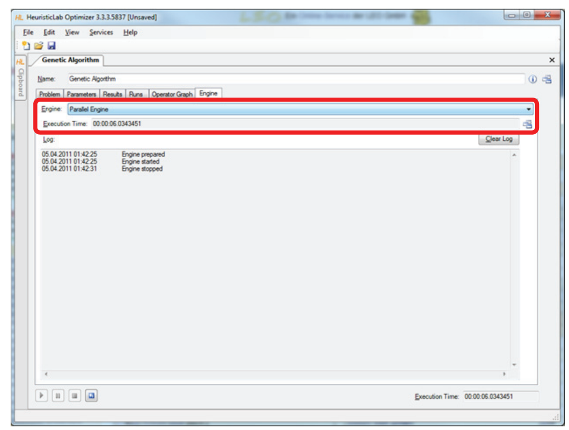
Parallel Execution of Algorithms



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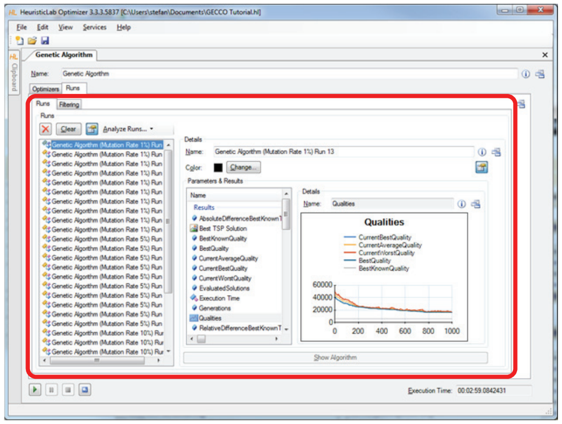
Compare Runs



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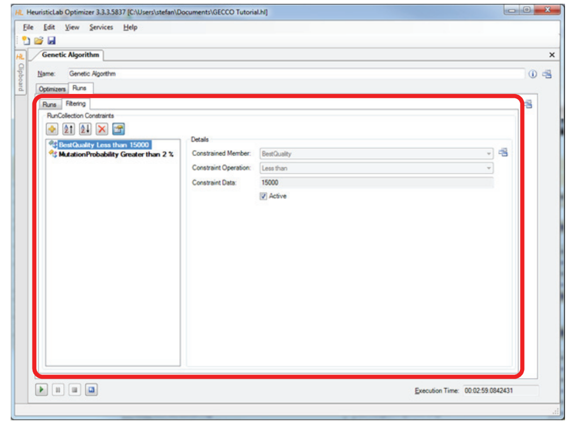
Filter Runs



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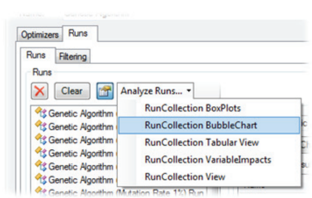
Analyze Runs

- 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



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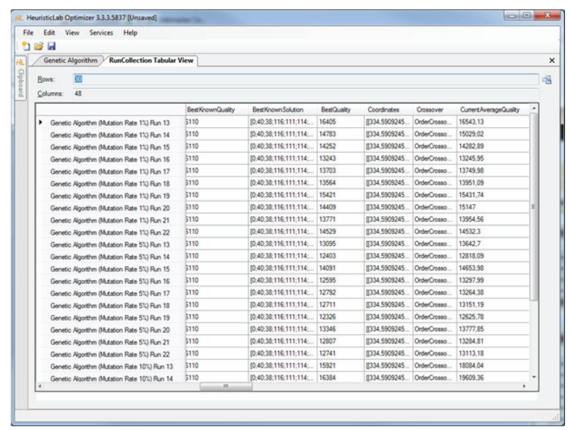
RunCollection Tabular View



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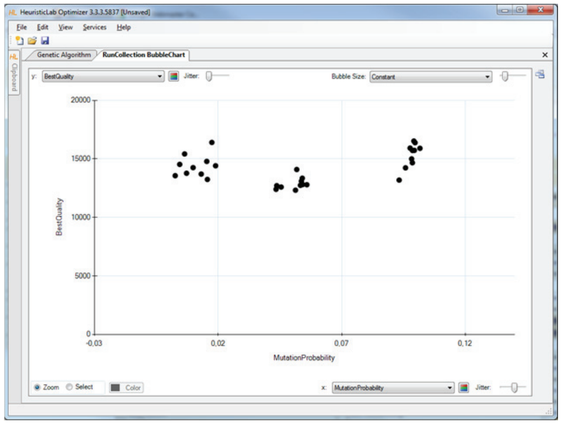
RunCollection Tabular View

- 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

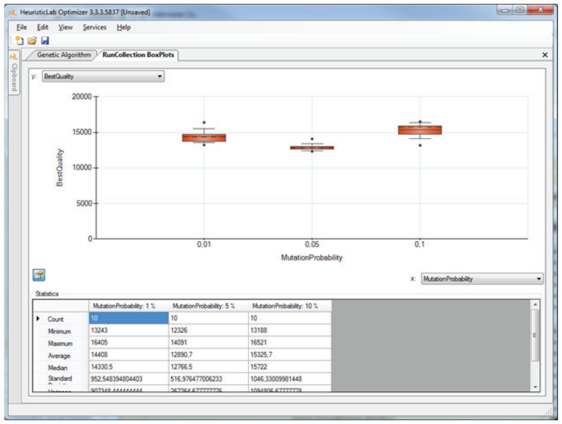
RunCollection BubbleChart



RunCollection 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

RunCollection BoxPlots



RunCollection 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)

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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
  - …

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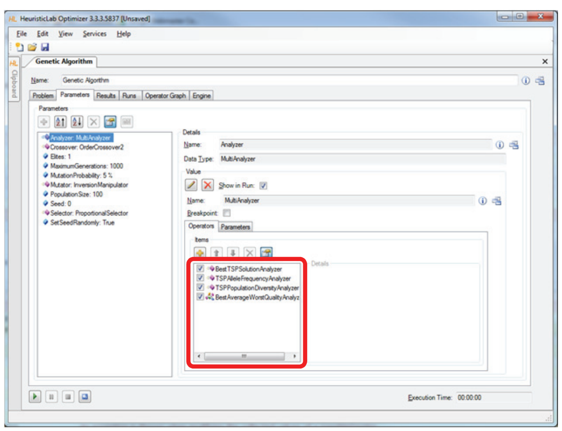
Analyzers



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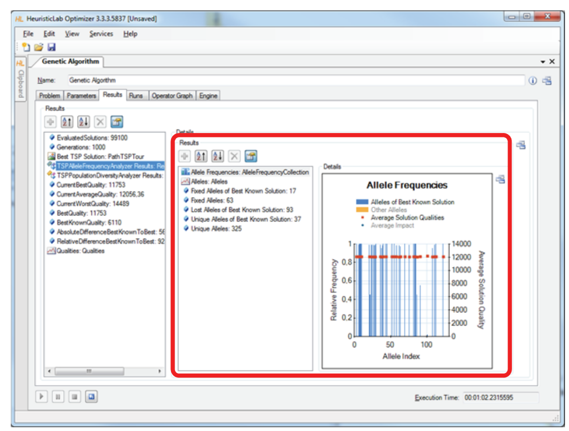
TSPAlleleFrequencyAnalyzer



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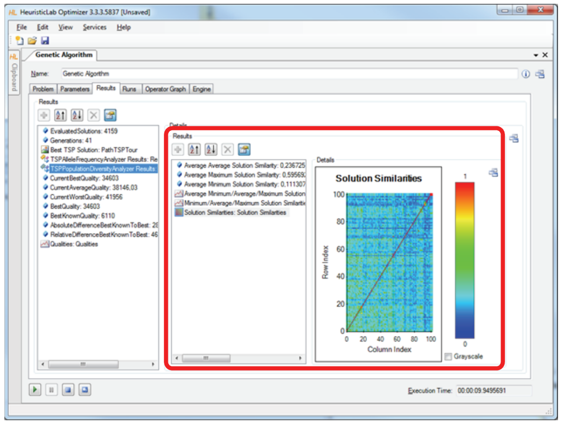
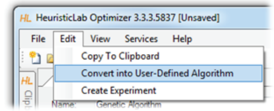
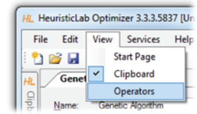
TSPPopulationDiversityAnalyzer



Building User-Defined Algorithms

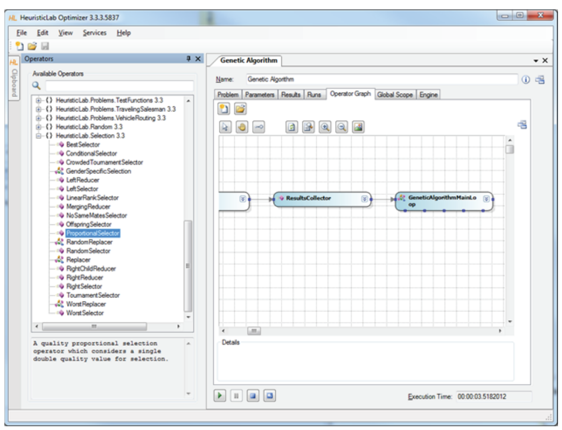
- Operator graphs
  - algorithms are represented as operator graphs
  - operator graphs of user-defined algorithms can be changed
  - algorithms can be defined in the graphical algorithm designer
  - use the menu to convert a standard algorithm into a user-defined algorithm



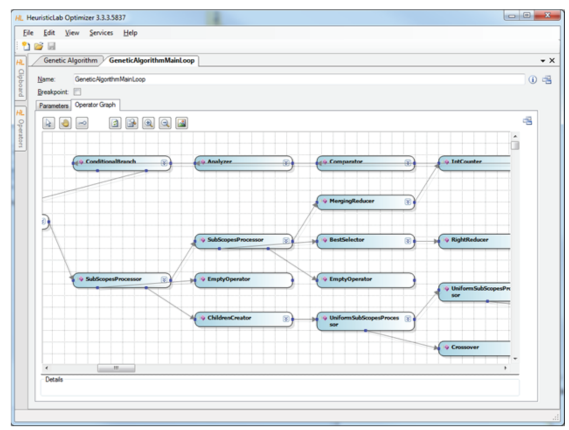


- Operators sidebar
  - drag & drop operators into an operator graph
- Programmable operators
  - add programmable operators in order to implement custom logic in an algorithm
  - no additional development environment needed
- Debug algorithms
  - use the debug engine to obtain detailed information during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

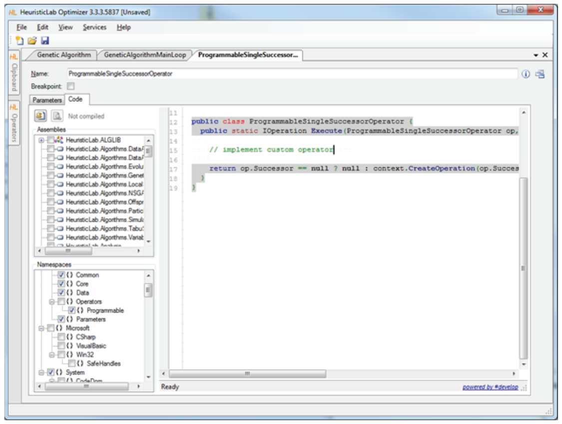
Building User-Defined Algorithms



Building User-Defined Algorithms



Programmable Operators



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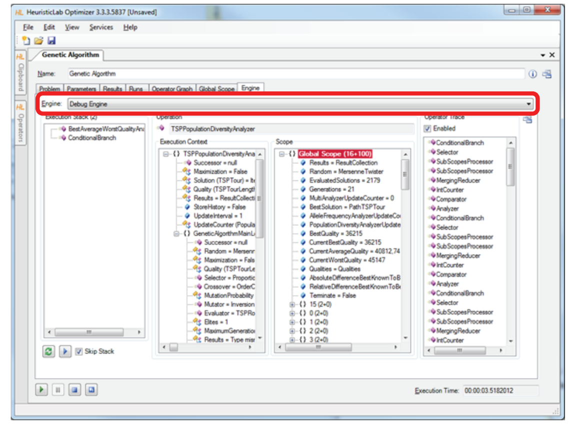
Debugging Algorithms



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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 $(y_1 \ldots y_N)^T$
- Goal: learn association of input variable values to labels
- Common tasks
  - Regression (real-valued labels)
  - Classification (discrete labels)
  - Clustering (no labels, group similar observations)

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Data-based Modeling Algorithms in HeuristicLab

- Symbolic regression and classification based on genetic programming
- External Libraries:
  - Support Vector Machines for Regression and Classification
  - Linear Regression
  - Linear Discriminate Analysis
  - K-Means clustering

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In the next 60 minutes: case studies

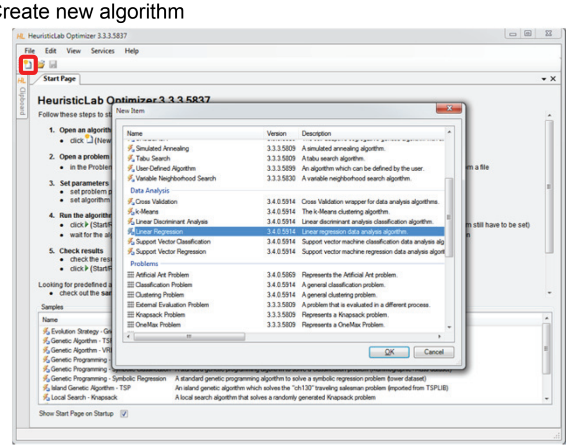
- Regression
  - Artificial benchmark problem dataset *Poly-10*
  - Algorithms:
    - Linear regression
    - Symbolic regression using Genetic Programming
- Classification
  - Real world medical *Mammographic Mass* dataset from the UCI Machine Learning Repository
  - Algorithms:
    - Symbolic classification

Case study: Regression

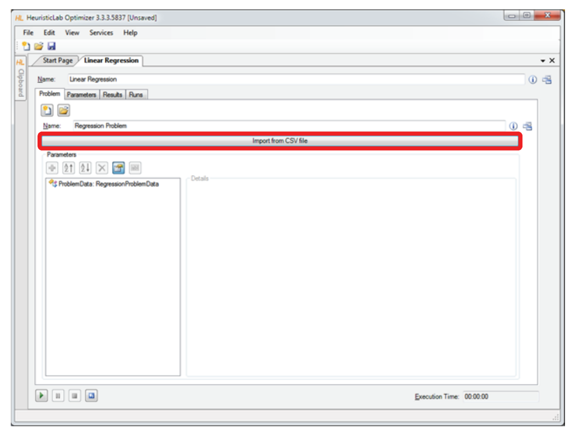
- Poly-10 benchmark problem dataset
  - 10 input variables $x_1 \ldots x_{10}$
  - $y = x_1 x_2 + x_3 x_4 + x_5 x_6 + x_1 x_7 x_9 + x_3 x_6 x_{10}$
  - Non-linear modeling approach necessary
  - Frequently used in GP literature
  - Download: http://dev.heuristiclab.com/AdditionalMaterial#GECCO2011

Linear Regression

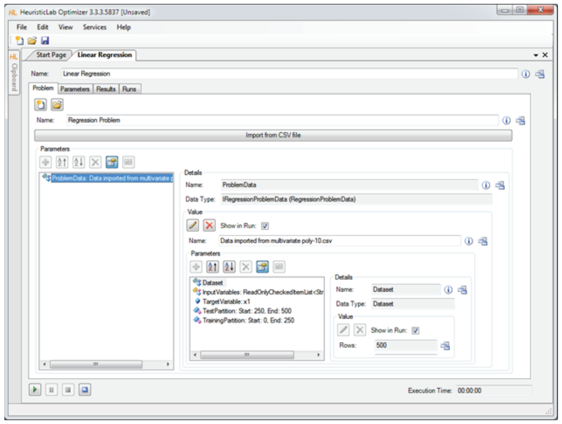
- Create new algorithm



Import Data from CSV-File



Inspect And Configure Dataset



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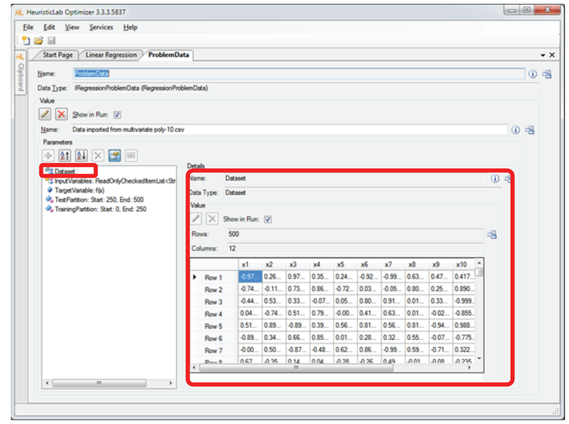
Inspect Imported Data



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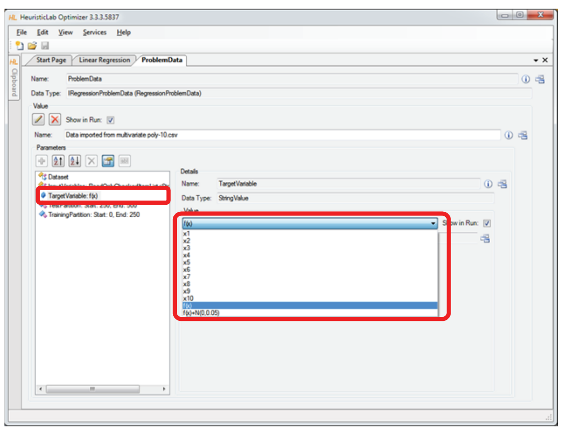
Set Target Variable



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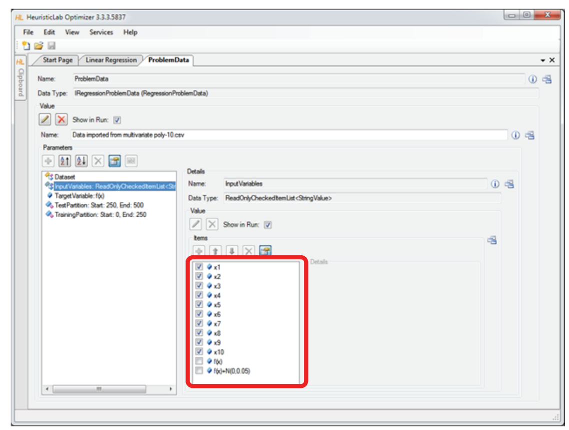
Select Input Variables



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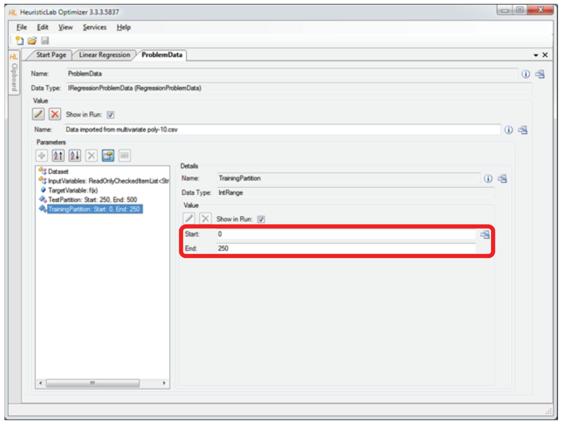
Configure Training and Test Partitions



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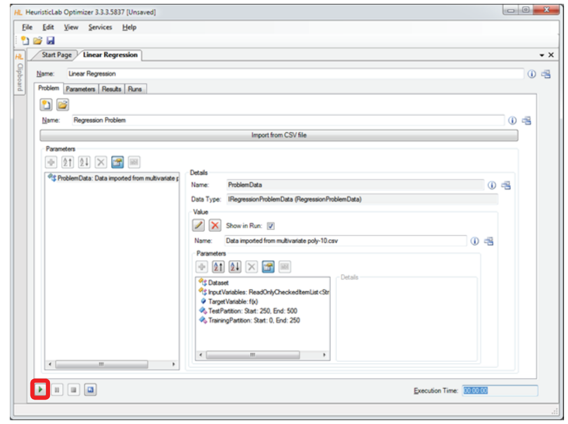
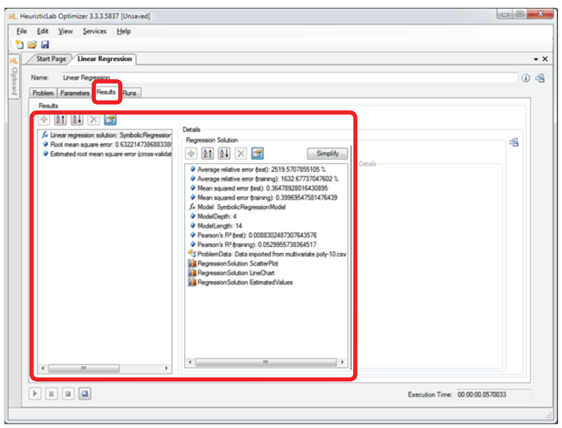
Run Linear Regression



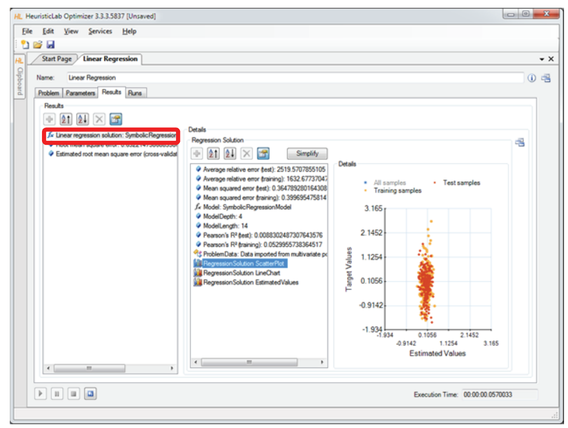
58

Inspect Results



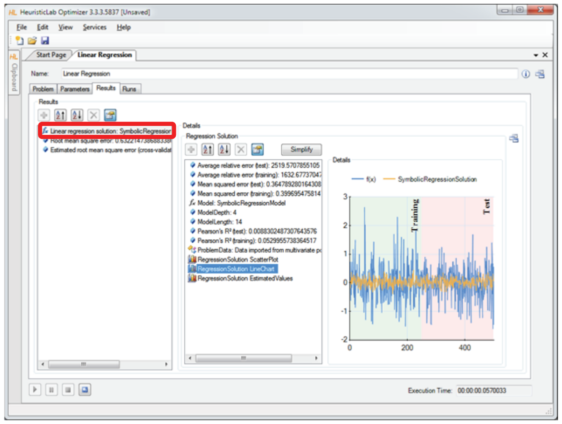
59

Inspect Scatterplot of Predicted and Target Values



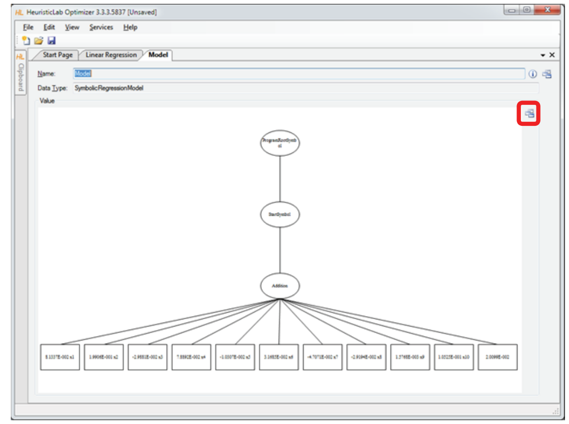
60

Inspect Linechart



61

Inspect Graphical Representation of Model



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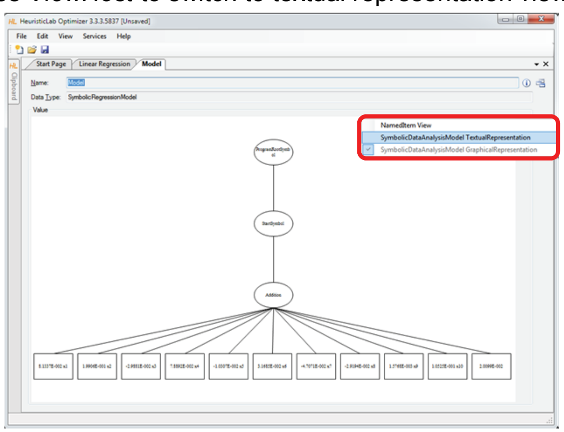
Textual Representations Are Also Available

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



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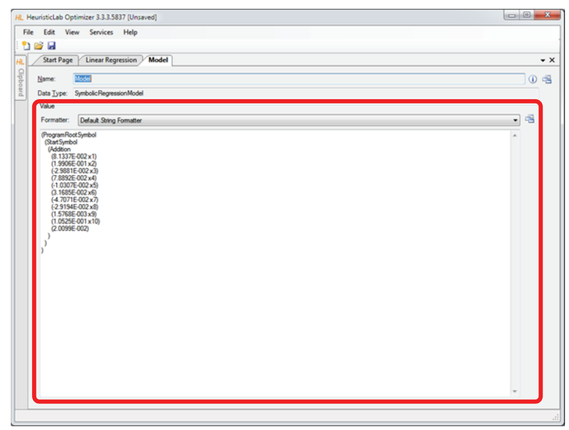
Default Textual Representation for Model Export



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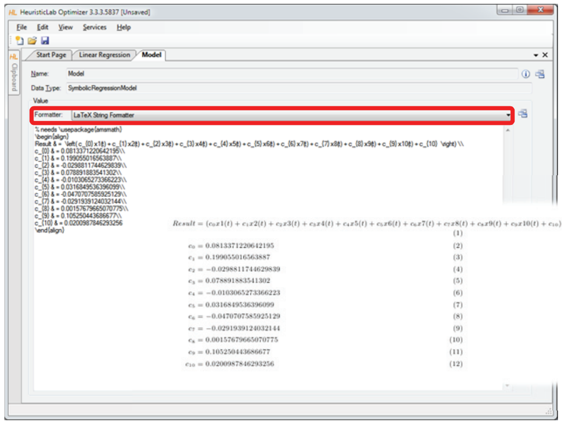
Textual Representation for Export to LaTeX



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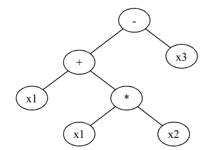
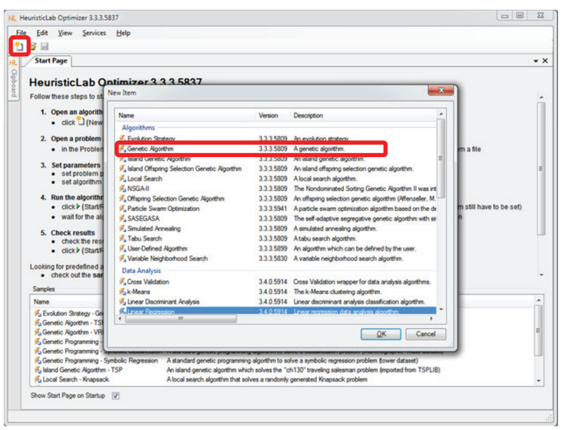
Nonlinear Modeling: Symbolic Regression

- 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



66

Create New Genetic Algorithm



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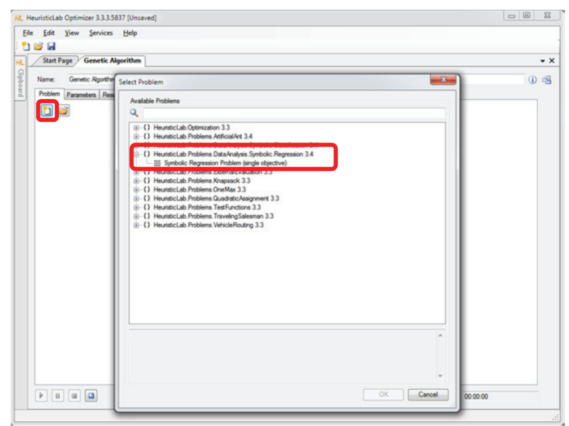
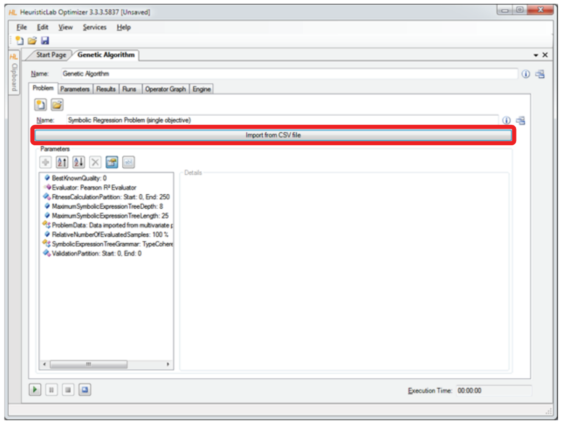
Create New Symbolic Regression Problem



68

Import Data



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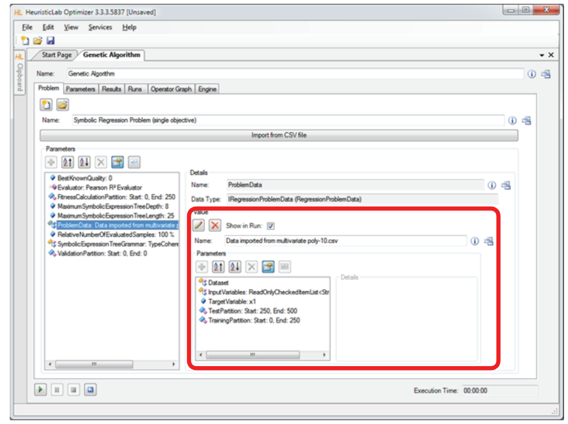
Inspect Data and Configure Dataset



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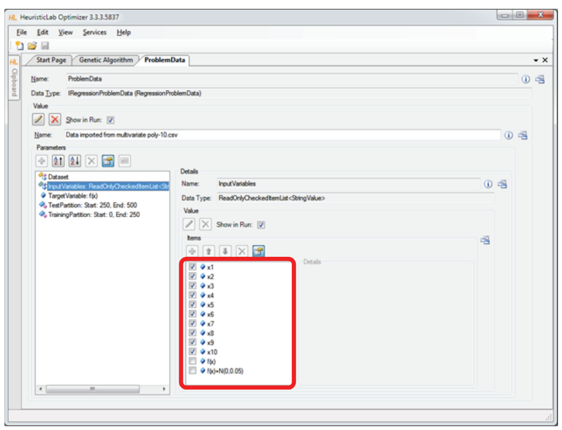
Set Target and Input Variables



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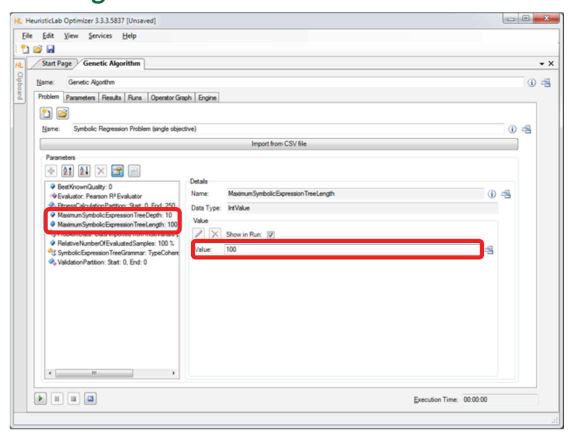
Configure Maximal Model Depth and Length



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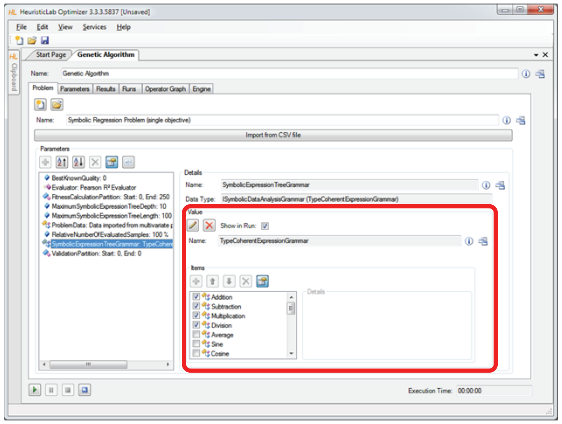
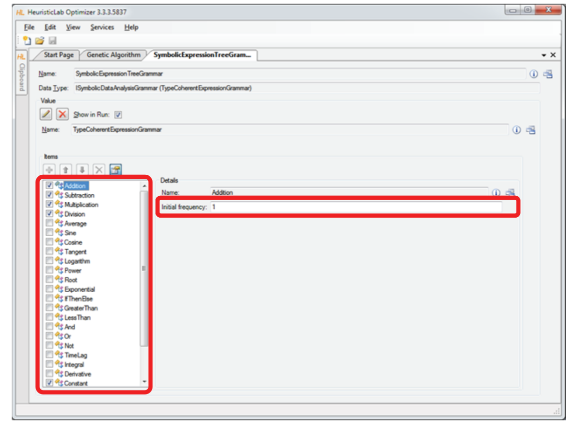
Configure Function Set (Grammar)



73

Configure Function Set (Grammar)



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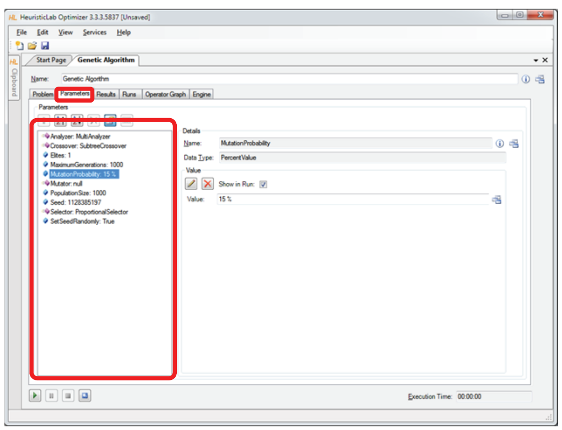
Configure Algorithm Parameters



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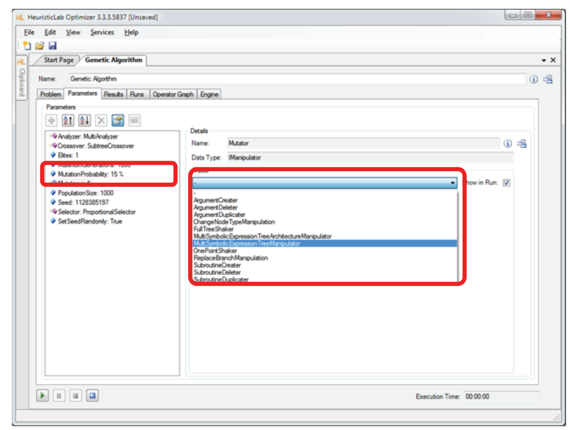
Configure Mutation Operator



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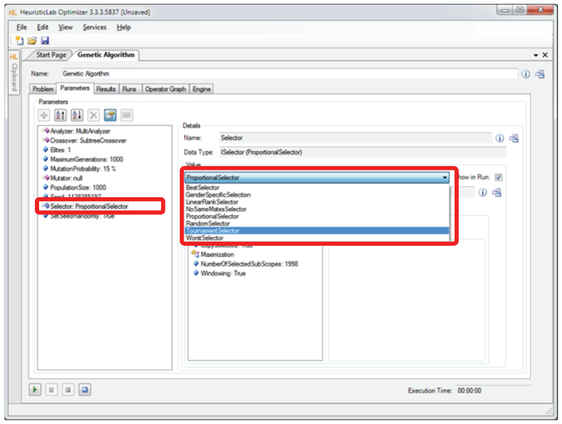
Configure Selection Operator



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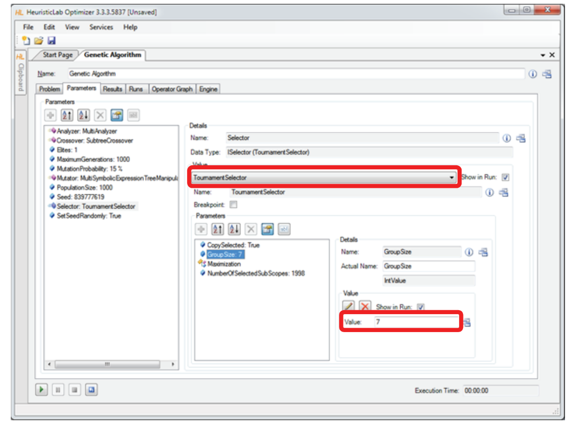
Configure Tournament Group Size



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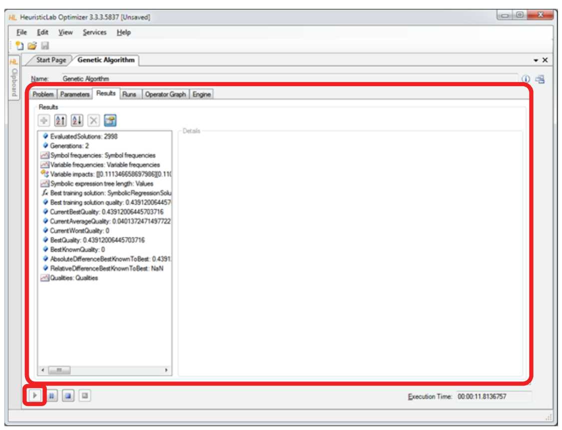
Start Algorithm and Inspect Results



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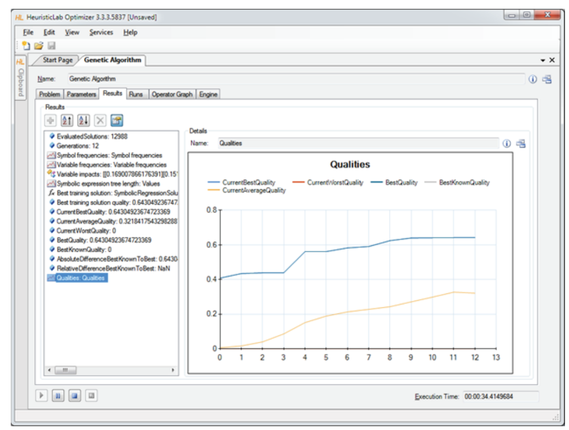
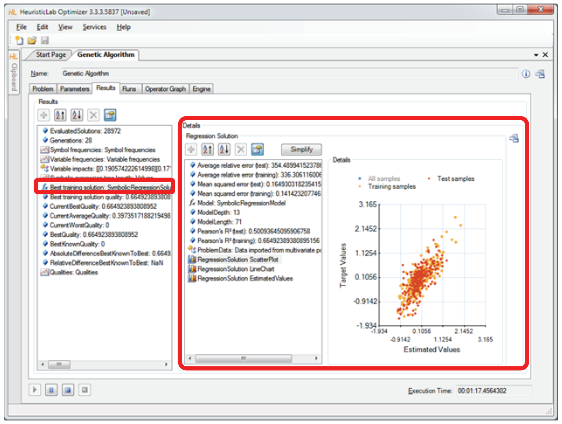
Inspect Quality Chart



80

Inspect Best Model on Training Partition



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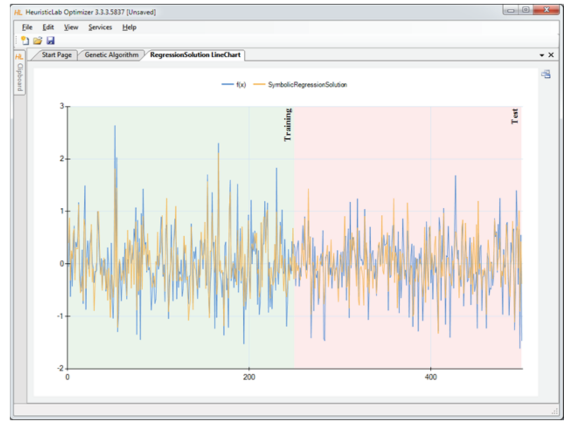
Inspect Linechart of Best Model on Trainingset



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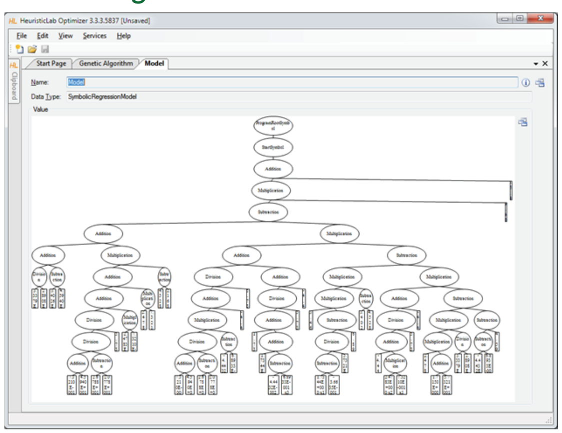
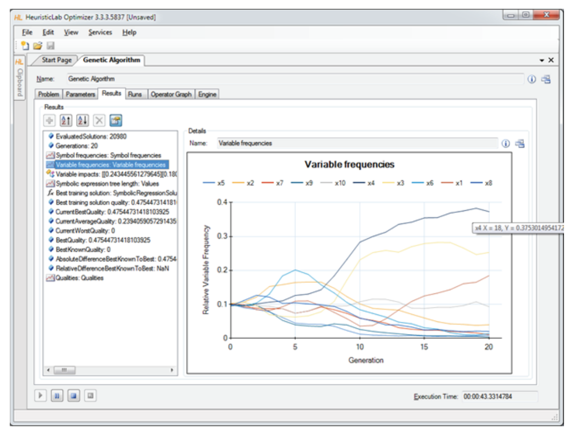
Inspect Structure of Best Model on Trainingset



83

Inspect Variable Frequency Chart



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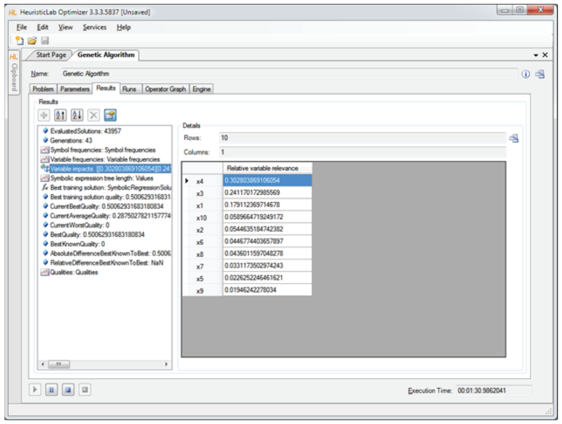
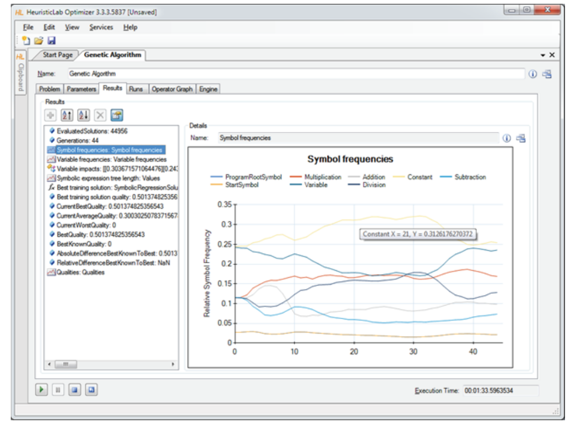
Inspect Variable Impacts



85

Inspect Symbol Frequencies



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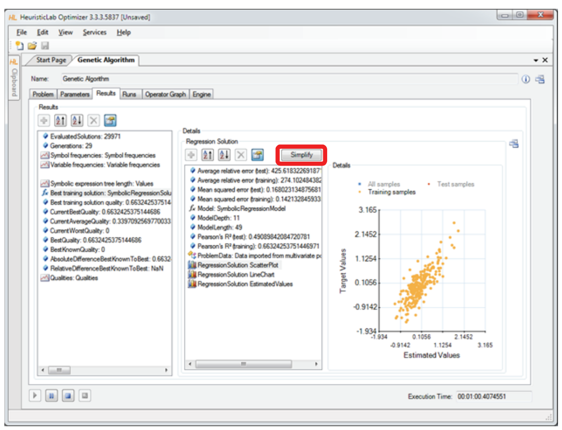
Detailed Model Analysis and Simplification



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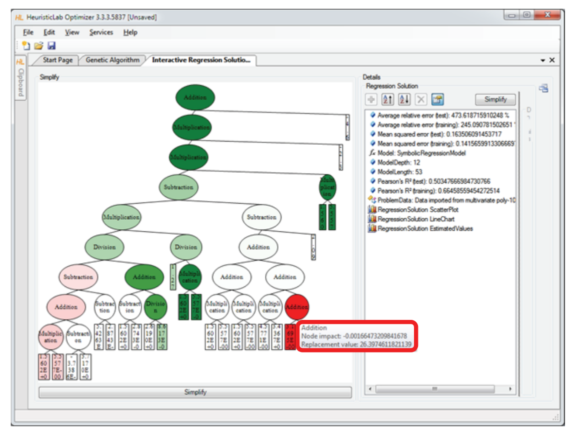
Symbolic Simplification and Node Impacts



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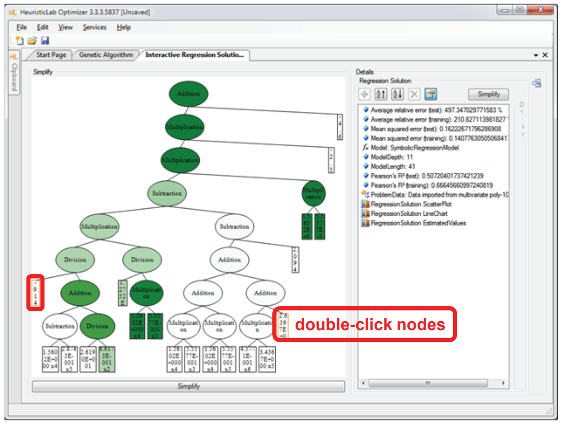
Manual Simplification



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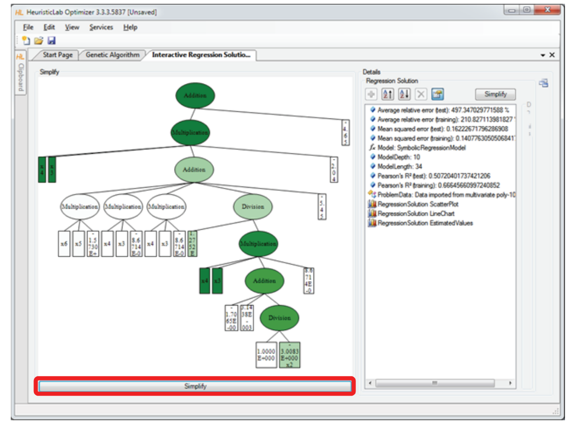
Automatic Symbolic Simplification



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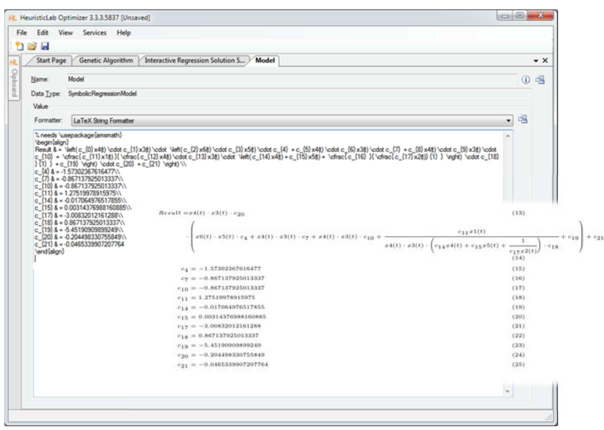
LaTeX Export



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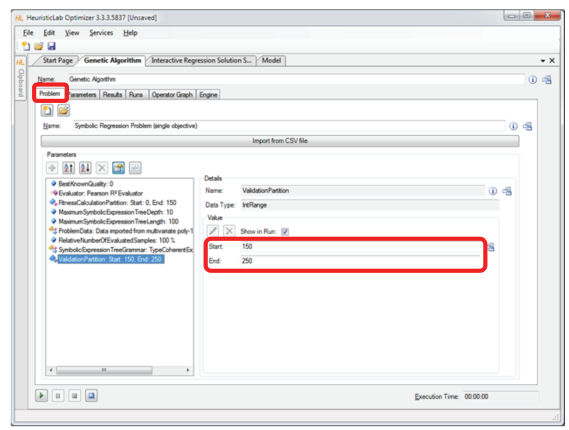
Configuration of Validation Partition



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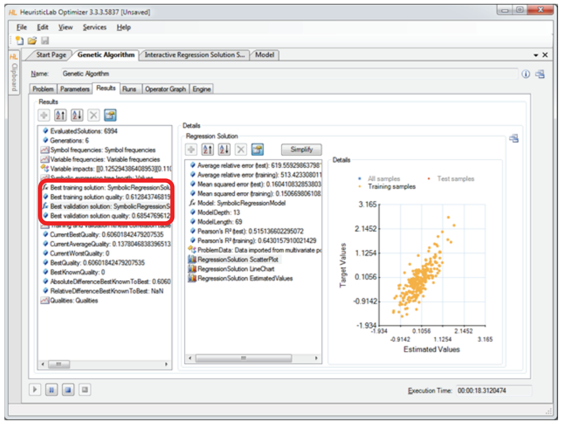
Inspect Best Model on Validation Partition



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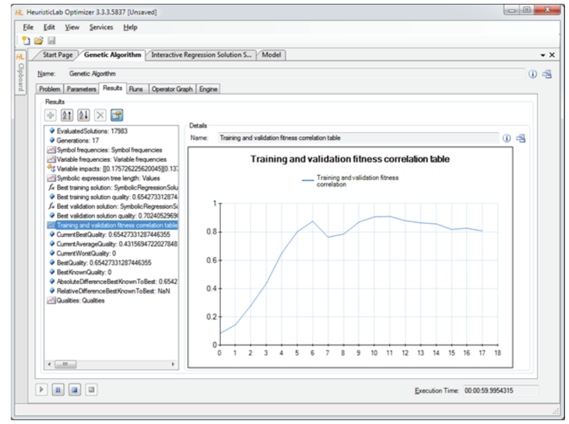
Inspect Linechart of Correltion of Training and Validation Fitness



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Case study: Classification

- Real world medical dataset (*Mammographic Mass*) from UCI Machine Learning Repository (Frank & Asuncion)
  - data from non-invasive mammography screening
  - variables:
    - patient age
    - visual features of inspected mass lesions: shape, margin, density
  - target variable: severity (malignant, benign)
  - Download: http://dev.heuristiclab.com/AdditionalMaterial#GECCO2011

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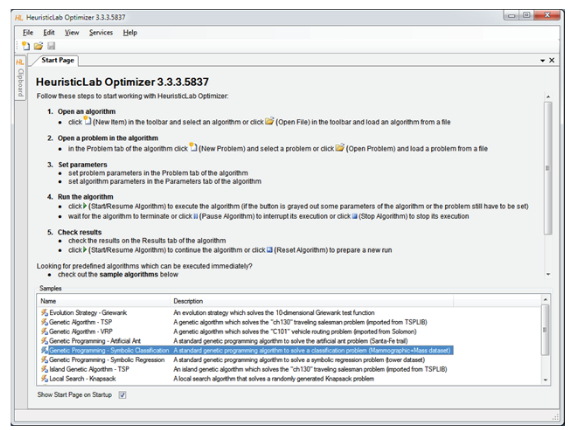
Open Sample



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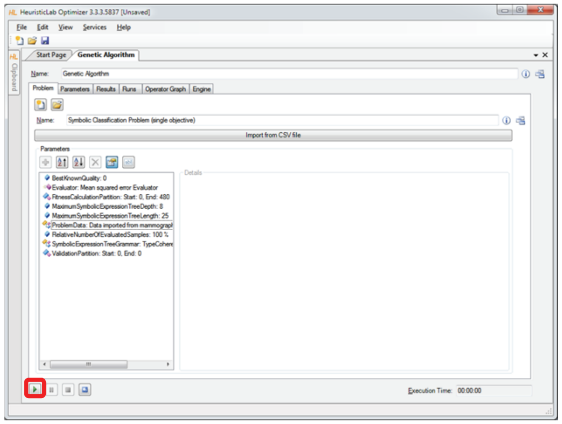
Configure and Run Algorithm



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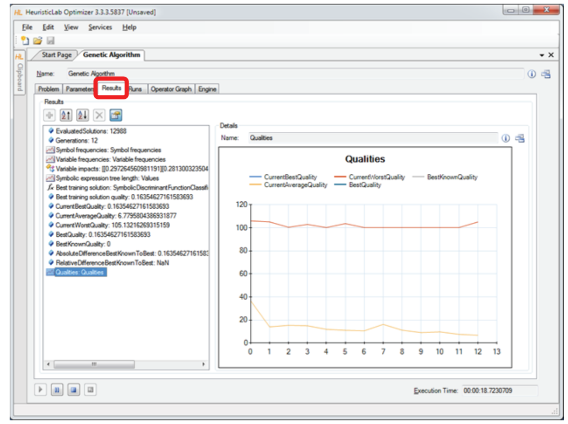
Inspect Quality Linechart



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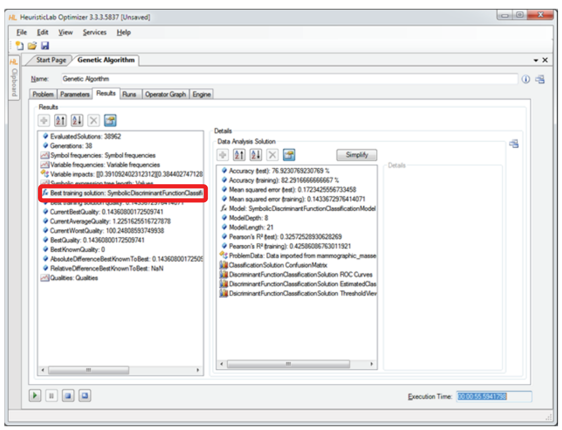
Inspect Best Training Solution



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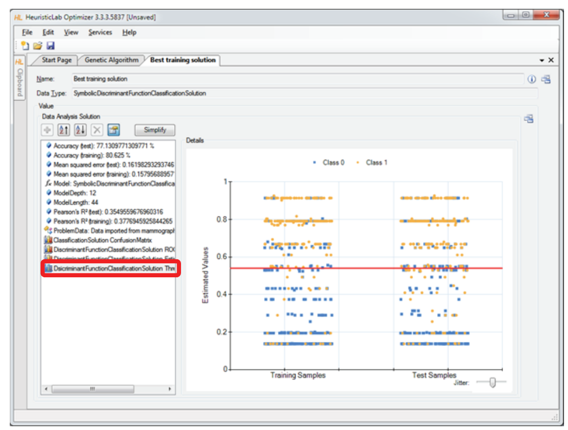
Inspect Model Output and Thresholds



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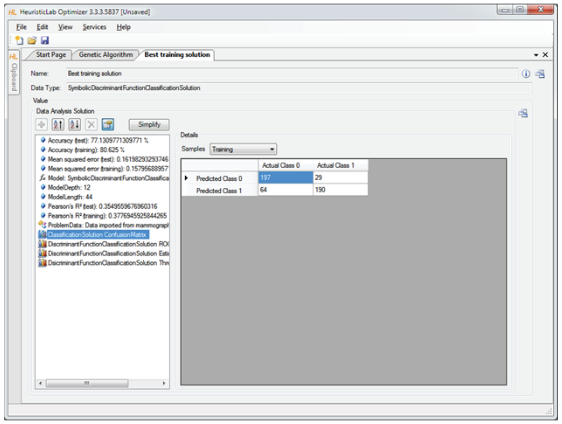
Inspect Confusion Matrix



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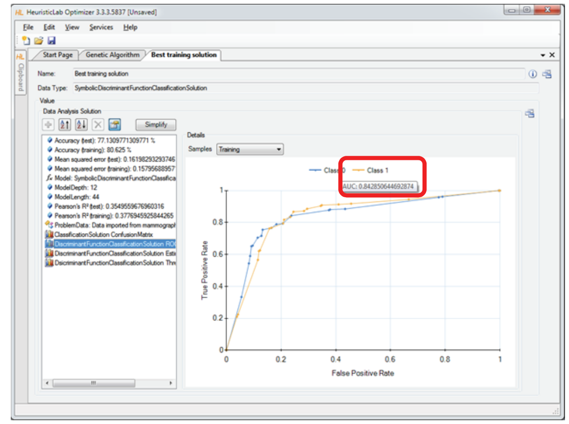
Inspect ROC curve



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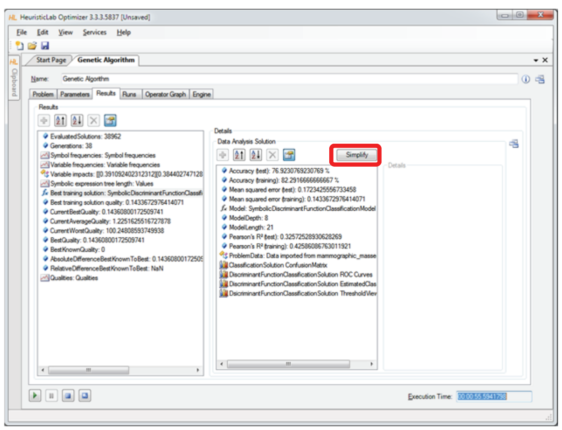
Analyse and Simplify Best Training Solution



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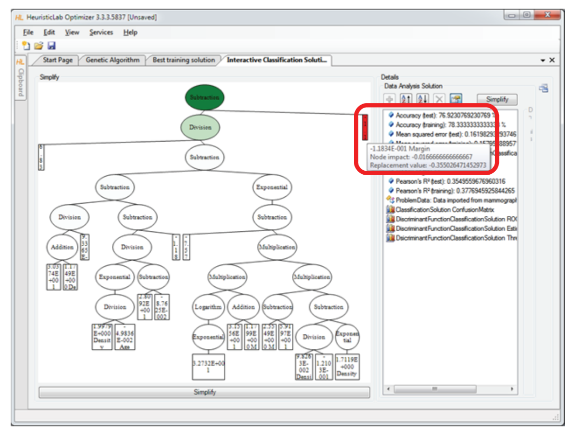
Analyse and Simplify Model



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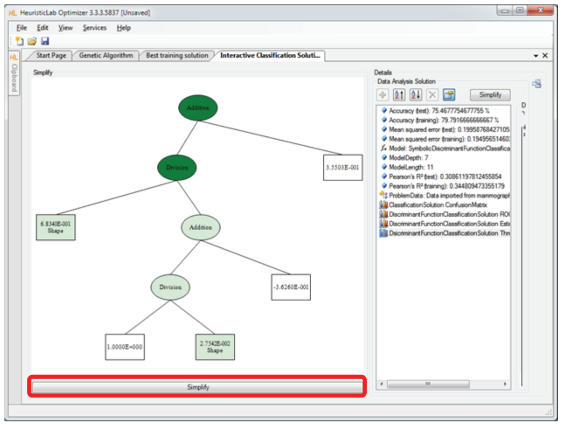
Symbolically Simplified Model



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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, 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

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Planned Features

- Algorithms & Problems
  - steady-state genetic algorithm
  - unified tabu search for vehicle routing
  - scatter search
  - …
- Cloud Computing
  - port HeuristicLab Hive to Windows Azure
- Linux
  - port HeuristicLab to run on Mono and Linux machines
- Have a look at the HeuristicLab roadmap
  - http://dev.heuristiclab.com/trac/hl/core/roadmap
- Any other ideas, requests or recommendations?
  - please write an e-mail to support@heuristiclab.com

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HeuristicLab Team

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HEAL Heuristic and Evolutionary Algorithms Laboratory

FH OBERÖSTERREICH

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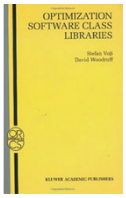
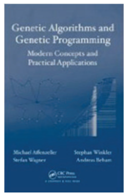
Suggested Readings

- 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



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  Adaptive and Natural Computing Algorithms, pp. 538-541
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  Benefits of plugin-based heuristic optimization software systems
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  Springer, 2007

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  Springer, 2009

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  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

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

Questions & Answers

http://dev.heuristiclab.com

support@heuristiclab.com