



2012



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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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>




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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

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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



- 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 3.3.6 released on January 3rd, 2012



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Where to get HeuristicLab?



- Download binaries
 - deployed as ZIP archives
 - latest stable version 3.3.6
 - released on January 3rd, 2012
 - daily trunk builds
 - <http://dev.heuristiclab.com/download>
- Check out sources
 - SVN repository
 - HeuristicLab 3.3.6 tag
 - <http://dev.heuristiclab.com/svn/hl/core/tags/3.3.6>
 - 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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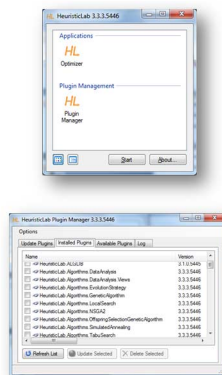
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Plugin Infrastructure



- HeuristicLab consists of many assemblies
 - 94 plugins in HeuristicLab 3.3.6
 - 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

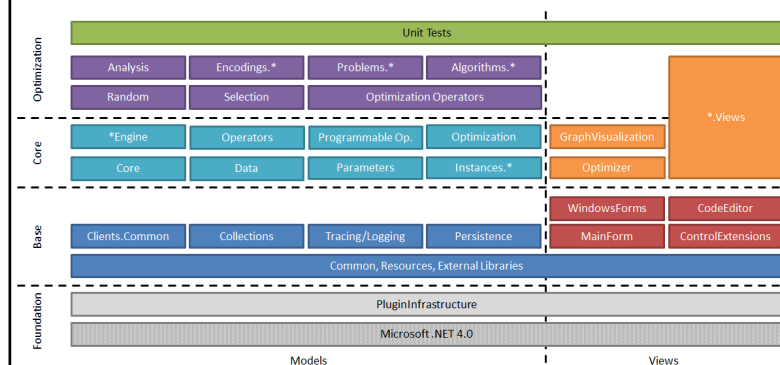


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Plugin Architecture



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Graphical User Interface



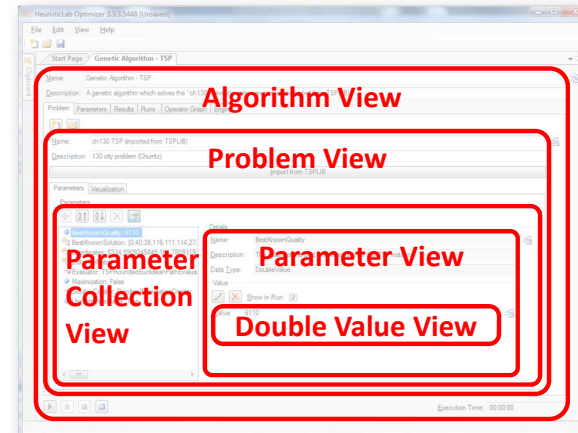
- HeuristicLab GUI is made up of views
 - views are visual representations of content objects
 - views are composed in the same way as their content
 - views and content objects are loosely coupled
 - multiple different views may exist for the same content
- Drag & Drop
 - views support drag & drop operations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

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Graphical User Interface



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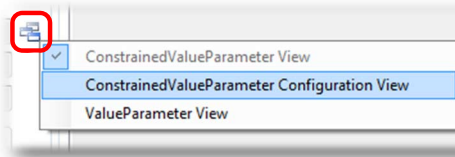
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Graphical User Interface



- 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



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Available Algorithms & Problems



Algorithms

- Evolution Strategy
- Genetic Algorithm
- Genetic Programming
- Island Genetic Algorithm
- Island Offspring Selection Genetic Algorithm
- Local Search
- NSGA-II
- Offspring Selection Genetic Algorithm
- Particle Swarm Optimization
- Robust Taboo Search
- SASEGASA
- Simulated Annealing
- Tabu Search
- User-defined Algorithm
- Variable Neighborhood Search
- Performance Benchmarks
- Cross Validation
- k-Means
- Linear Discriminant Analysis
- Linear Regression
- Multinomial Logit Classification
- Nearest Neighbor Regression and Classification
- Neural Network Regression and Classification
- Random Forest Regression and Classification
- Support Vector Regression and Classification

Problems

- Artificial Ant
- Classification
- Clustering
- External Evaluation Problem
- Knapsack
- OneMax
- Quadratic Assignment
- Regression
- Single-Objective Test Function
- Symbolic Classification
- Symbolic Regression
- Traveling Salesman
- User-defined Problem
- Vehicle Routing

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Demonstration Part I: Working with HeuristicLab



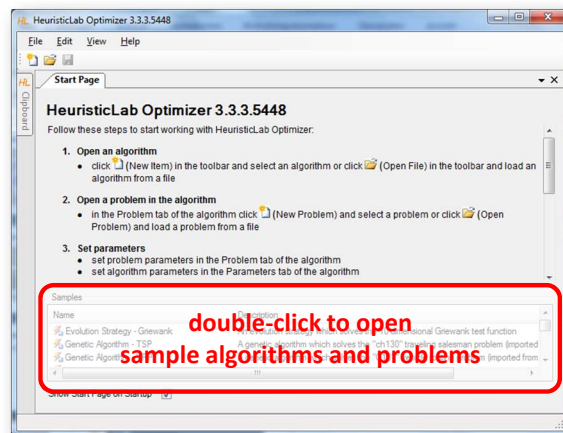
- Create, Parameterize and Execute Algorithms
- Save and Load Items
- Create Batch Runs and Experiments
- Multi-core CPUs and Parallelization
- Analyze Runs
- Analyzers
- Building User-Defined Algorithms

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HeuristicLab Optimizer

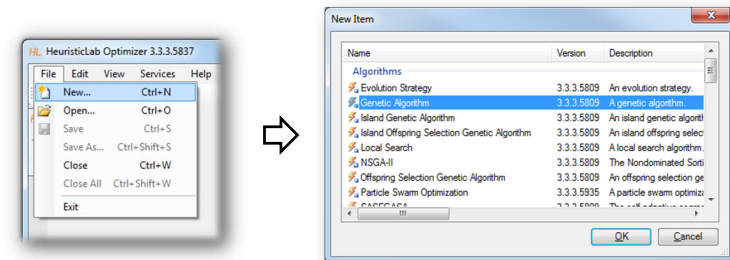


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Create Algorithm

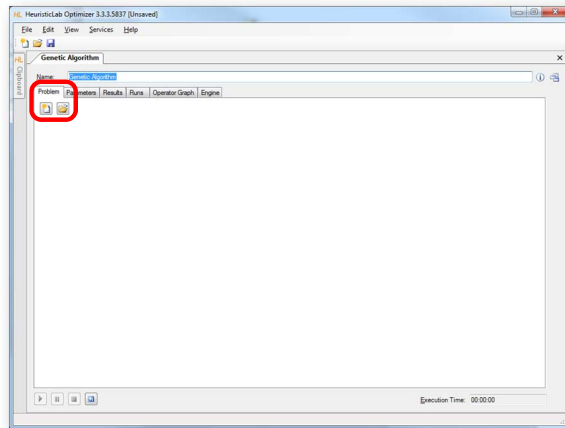


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Create or Load Problem

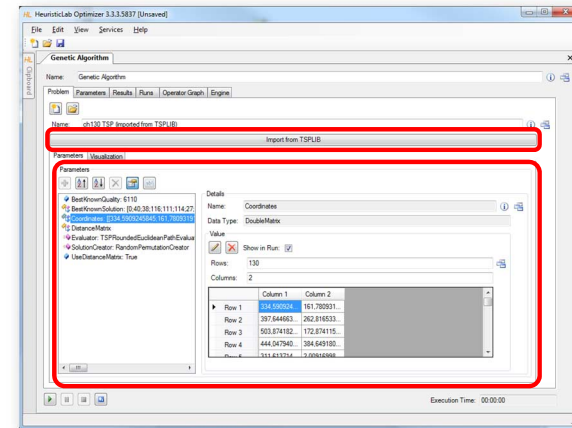


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Import or Parameterize Problem Data

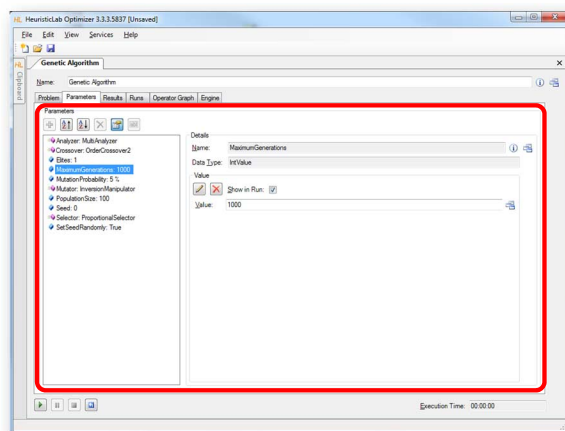


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Parameterize Algorithm

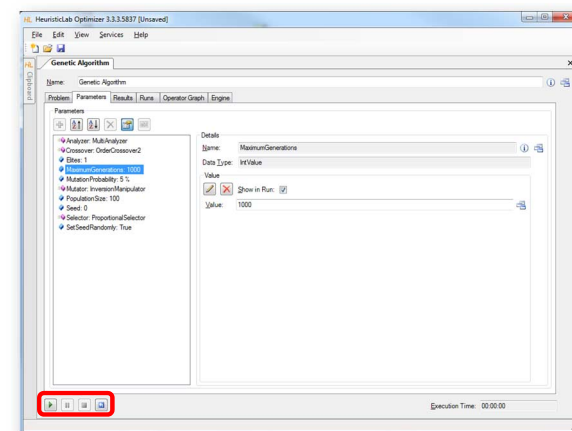


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Start, Pause, Resume, Stop and Reset

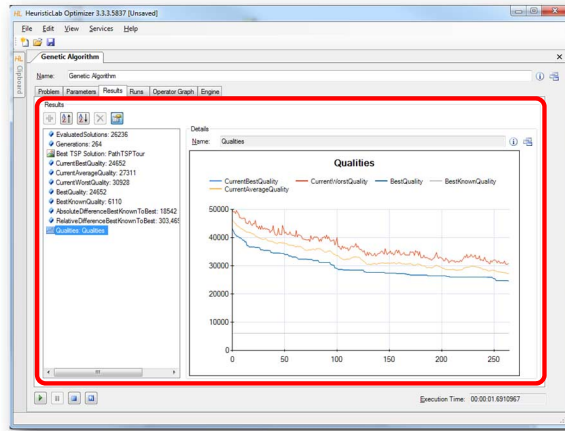


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Inspect Results



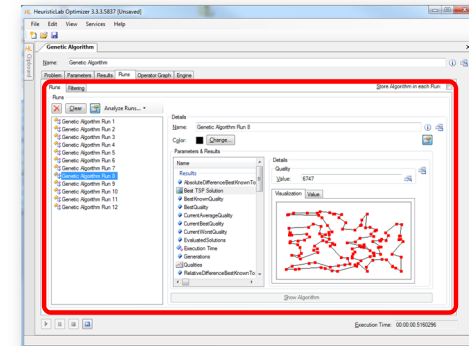
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Compare Runs

- 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



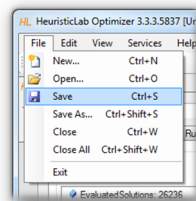
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Save and Load

- 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



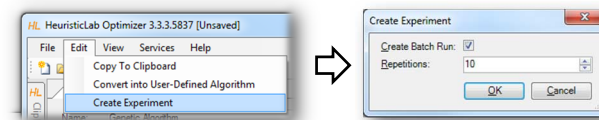
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Create Batch Runs and Experiments

- 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

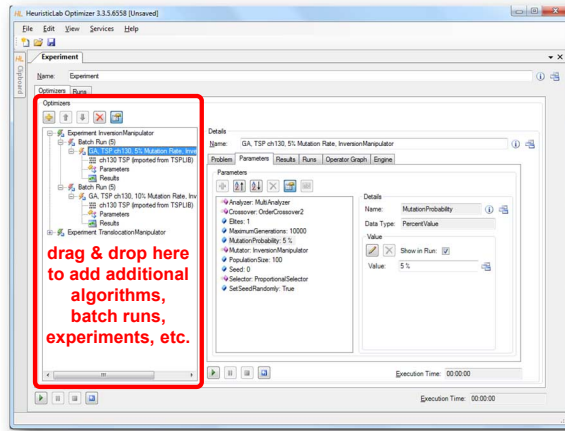


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Create Batch Runs and Experiments

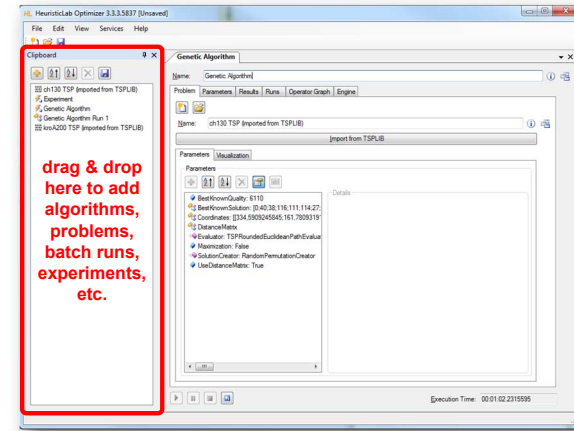


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Clipboard



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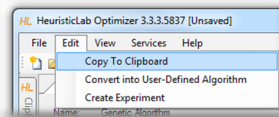
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Clipboard



- 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



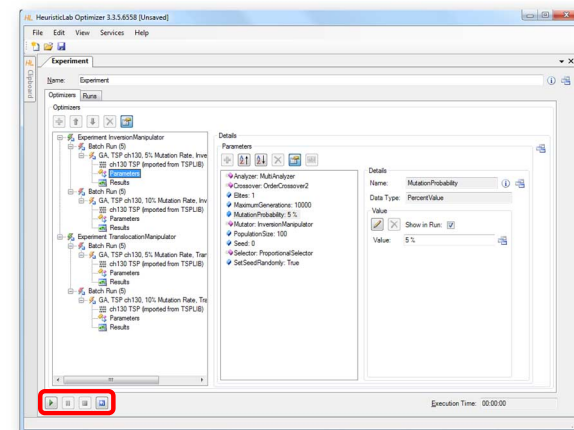
- Show items
 - double-click on an item in the clipboard to show its view
- Save and restore clipboard content
 - click on the save button to write the clipboard content to disk
 - clipboard is automatically restored when HeuristicLab is started the next time

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Start, Pause, Resume, Stop, Reset

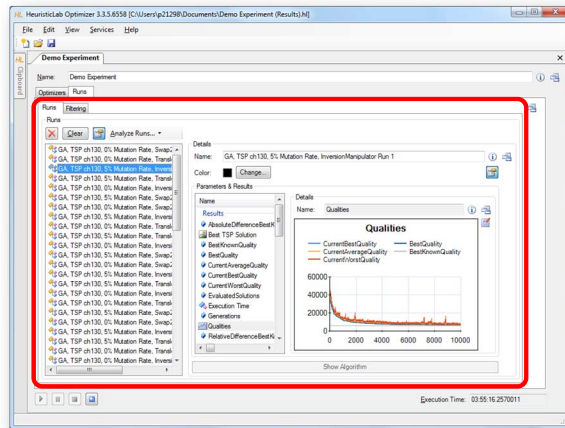


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Compare Runs



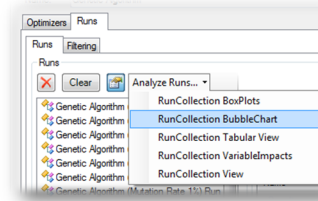
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Analyze Runs

- 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

	BestKnownQuality	BestKnownSolution	BestQuality	Coordinates	Crossover	CurrentAverageQuality
Genetic Algorithm (Mutation Rate 1%) Run 13	3110	[0.40.38.116.111.114...	16405	[334.5900245...	OrderCrossover...	16543.13
Genetic Algorithm (Mutation Rate 1%) Run 14	3110	[0.40.38.116.111.114...	14783	[334.5900245...	OrderCrossover...	16020.02
Genetic Algorithm (Mutation Rate 1%) Run 15	3110	[0.40.38.116.111.114...	14292	[334.5900245...	OrderCrossover...	14209.89
Genetic Algorithm (Mutation Rate 1%) Run 16	3110	[0.40.38.116.111.114...	13243	[334.5900245...	OrderCrossover...	13245.95
Genetic Algorithm (Mutation Rate 1%) Run 17	3110	[0.40.38.116.111.114...	13703	[334.5900245...	OrderCrossover...	13749.98
Genetic Algorithm (Mutation Rate 1%) Run 18	3110	[0.40.38.116.111.114...	13564	[334.5900245...	OrderCrossover...	13591.09
Genetic Algorithm (Mutation Rate 1%) Run 19	3110	[0.40.38.116.111.114...	15621	[334.5900245...	OrderCrossover...	15625.74
Genetic Algorithm (Mutation Rate 1%) Run 20	3110	[0.40.38.116.111.114...	14409	[334.5900245...	OrderCrossover...	15147
Genetic Algorithm (Mutation Rate 1%) Run 21	3110	[0.40.38.116.111.114...	13771	[334.5900245...	OrderCrossover...	13564.56
Genetic Algorithm (Mutation Rate 1%) Run 22	3110	[0.40.38.116.111.114...	14529	[334.5900245...	OrderCrossover...	14332.3
Genetic Algorithm (Mutation Rate 1%) Run 13	3110	[0.40.38.116.111.114...	13895	[334.5900245...	OrderCrossover...	13642.7
Genetic Algorithm (Mutation Rate 1%) Run 14	3110	[0.40.38.116.111.114...	12403	[334.5900245...	OrderCrossover...	12514.08
Genetic Algorithm (Mutation Rate 1%) Run 15	3110	[0.40.38.116.111.114...	14091	[334.5900245...	OrderCrossover...	14053.98
Genetic Algorithm (Mutation Rate 1%) Run 16	3110	[0.40.38.116.111.114...	12895	[334.5900245...	OrderCrossover...	13207.99
Genetic Algorithm (Mutation Rate 1%) Run 17	3110	[0.40.38.116.111.114...	12782	[334.5900245...	OrderCrossover...	13204.38
Genetic Algorithm (Mutation Rate 1%) Run 18	3110	[0.40.38.116.111.114...	12711	[334.5900245...	OrderCrossover...	13115.19
Genetic Algorithm (Mutation Rate 1%) Run 19	3110	[0.40.38.116.111.114...	12326	[334.5900245...	OrderCrossover...	12625.78
Genetic Algorithm (Mutation Rate 1%) Run 20	3110	[0.40.38.116.111.114...	13346	[334.5900245...	OrderCrossover...	13777.85
Genetic Algorithm (Mutation Rate 1%) Run 21	3110	[0.40.38.116.111.114...	12807	[334.5900245...	OrderCrossover...	13284.81
Genetic Algorithm (Mutation Rate 1%) Run 22	3110	[0.40.38.116.111.114...	12341	[334.5900245...	OrderCrossover...	13115.10
Genetic Algorithm (Mutation Rate 10%) Run 13	3110	[0.40.38.116.111.114...	15921	[334.5900245...	OrderCrossover...	18084.64
Genetic Algorithm (Mutation Rate 10%) Run 14	3110	[0.40.38.116.111.114...	16384	[334.5900245...	OrderCrossover...	18028.36

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RunCollection Tabular View

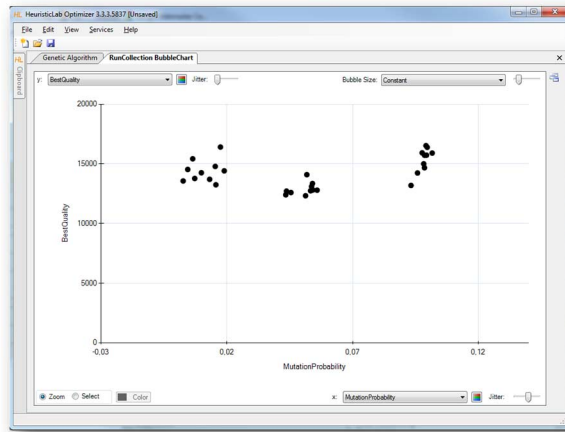
- Sort columns
 - click on column header to sort column
 - Ctrl-click on column header to sort multiple columns
- Show or hide columns
 - right-click on table to open dialog to show or hide columns
- Compute statistical values
 - select multiple numerical values to see count, sum, minimum, maximum, average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

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RunCollection BubbleChart



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RunCollection BubbleChart



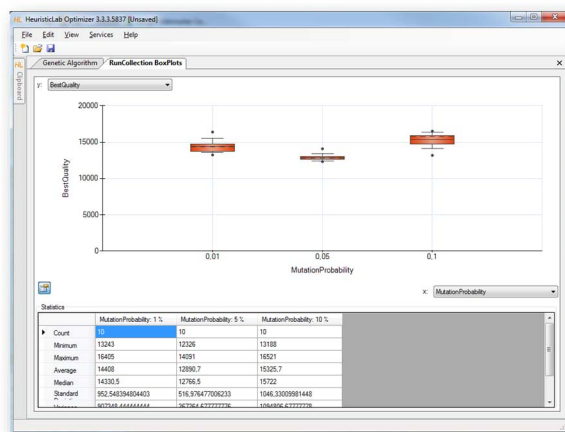
- Choose values to plot
 - choose which values to show on the x-axis, the y-axis and as bubble size
 - possible values are all parameter settings and results
- Add jitter
 - add jitter to separate overlapping bubbles
- Zoom in and out
 - click on Zoom and click and drag in the chart area to zoom in
 - 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

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RunCollection BoxPlots



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RunCollection BoxPlots



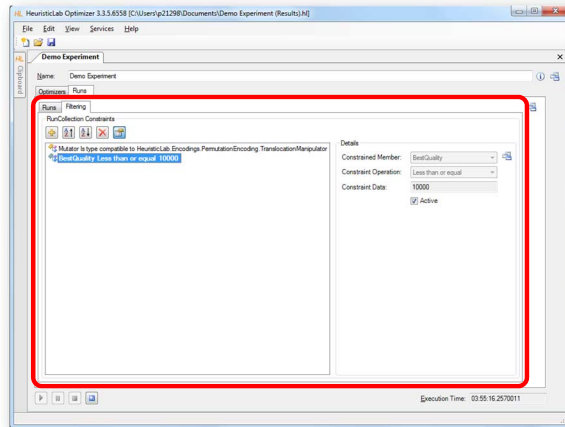
- Choose values to plot
 - choose which values to show on the x-axis and y-axis
 - possible values are all parameter settings and results
- Zoom in and out
 - click on Zoom and click and drag in the chart area to zoom in
 - double click on the chart area background or on the circle buttons beside the 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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Filter Runs



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Multi-core CPUs and Parallelization



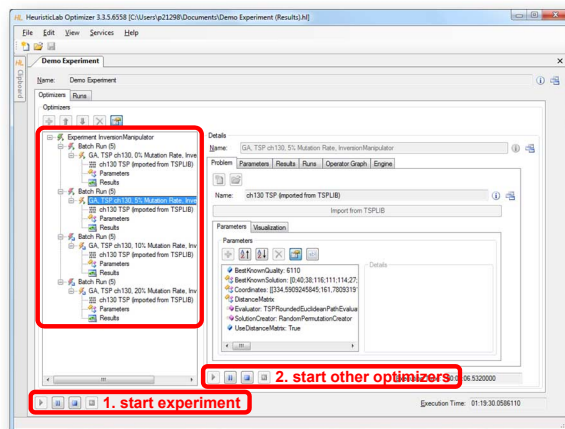
- Parallel execution of optimizers in experiments
 - optimizers in an experiment are executed sequentially from top to bottom per default
 - experiments support parallel execution of their optimizers
 - select a not yet executed optimizer and start it manually to utilize another core
 - execution of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

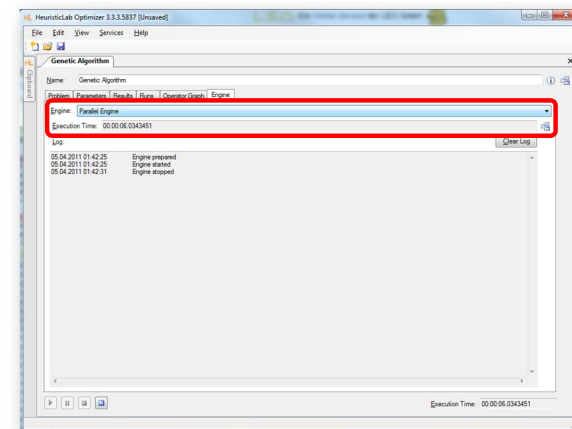


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Parallel Execution of Algorithms



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Analyzers



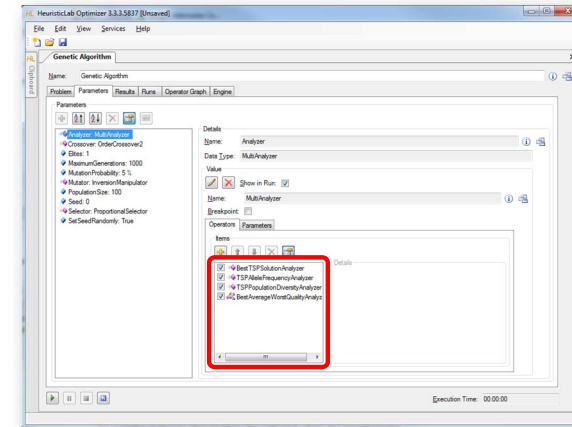
- Special operators for analysis purposes
 - are executed after each iteration
 - serve as general purpose extension points of algorithms
 - can be selected and parameterized in the algorithm
 - perform algorithm-specific and/or problem-specific tasks
 - some analyzers are quite costly regarding runtime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

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Analyzers

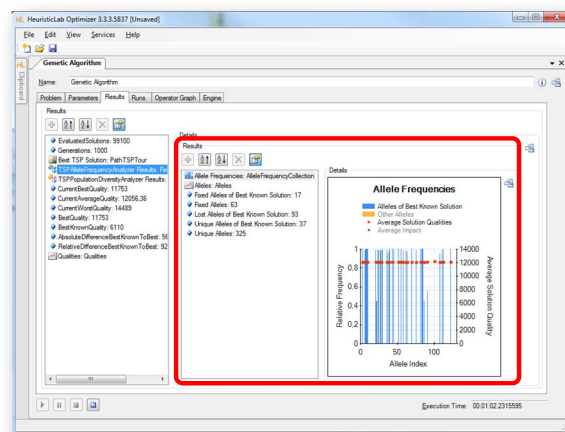


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TSPAlleleFrequencyAnalyzer

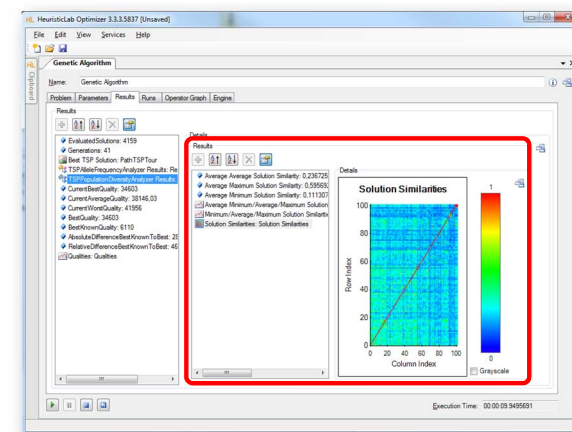


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TSPPopulationDiversityAnalyzer



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-
- Figure 1 shows two screenshots of the HeuristicLab Optimizer 3.3.3.5837 interface. The left screenshot shows the 'File' menu with 'Convert into User-Defined Algorithm' highlighted. The right screenshot shows the 'Genetic' menu with 'Operators' highlighted.

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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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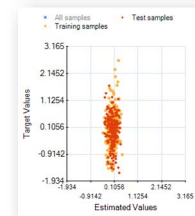
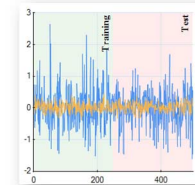
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Case Studies



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



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Case Study: Regression



- Poly-10 benchmark problem dataset
 - 10 input variables $x_1 \dots x_{10}$
 - $y = x_1 \cdot x_2 + x_3 \cdot x_4 + x_5 \cdot x_6 + x_1 \cdot x_7 \cdot x_9 + x_3 \cdot x_6 \cdot x_{10}$
 - non-linear modeling approach necessary
 - frequently used in GP literature
 - download <http://dev.heuristiclab.com/AdditionalMaterial#GECCO2012>

GECCO 2012

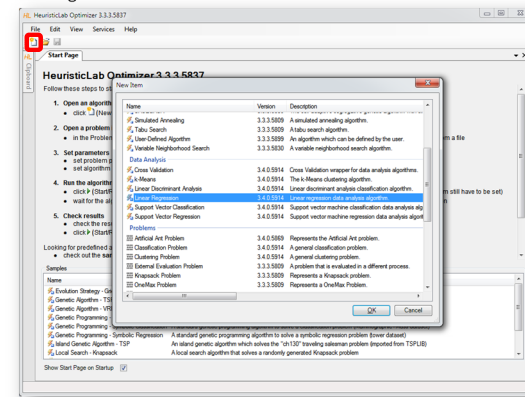
<http://dev.heuristiclab.com>

55

Linear Regression



- Create new algorithm

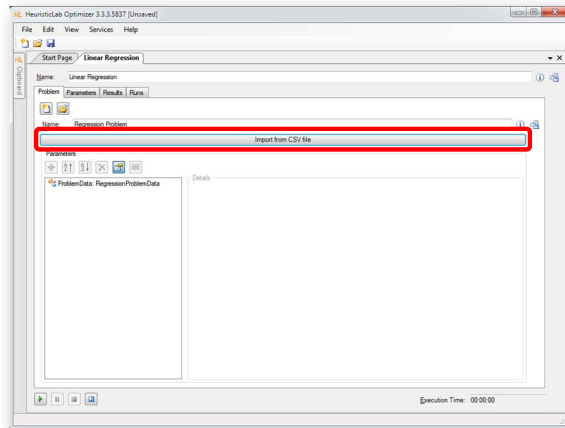


GECCO 2012

<http://dev.heuristiclab.com>

56

Import Data from CSV-File

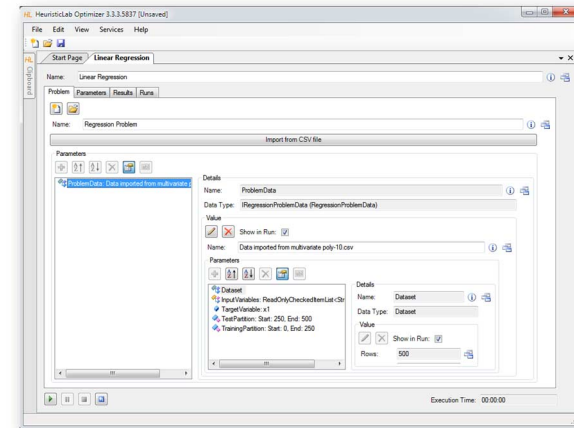


GECCO 2012

<http://dev.heuristiclab.com>

57

Inspect and Configure Dataset

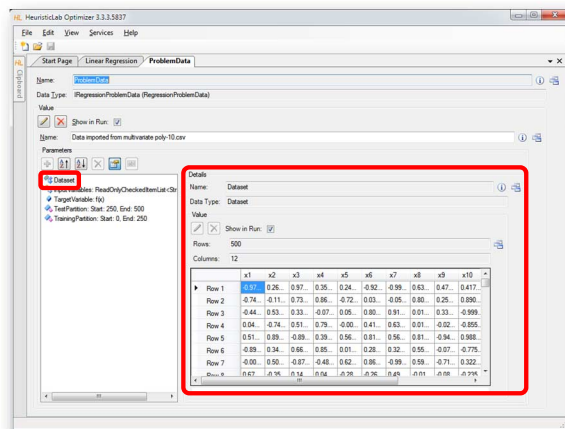


GECCO 2012

<http://dev.heuristiclab.com>

58

Inspect Imported Data

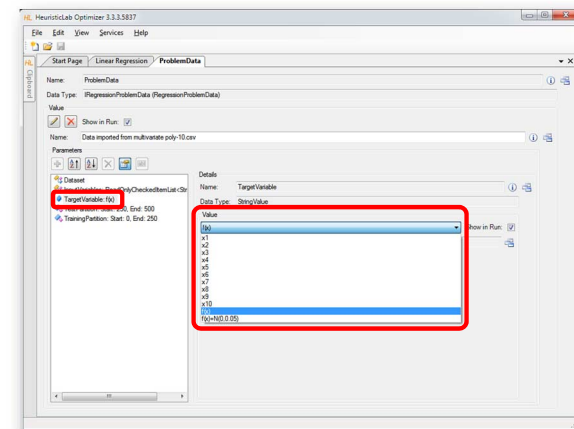


GECCO 2012

<http://dev.heuristiclab.com>

59

Set Target Variable

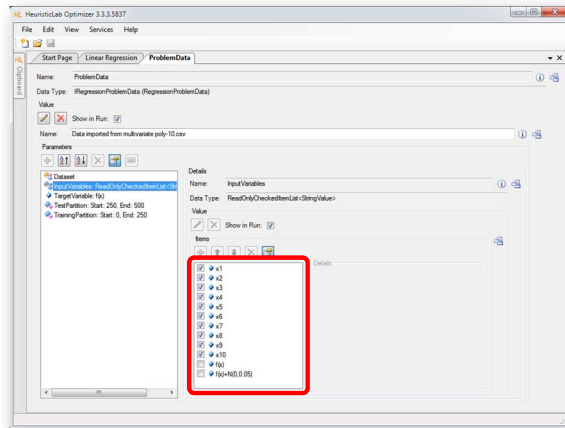


GECCO 2012

<http://dev.heuristiclab.com>

60

Select Input Variables

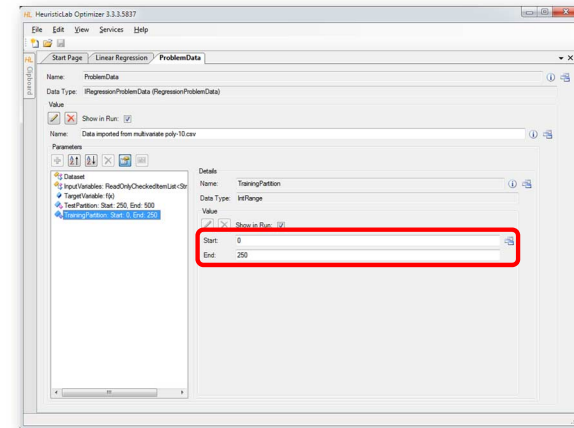


GECCO 2012

<http://dev.heuristiclab.com>

61

Configure Training and Test Partitions

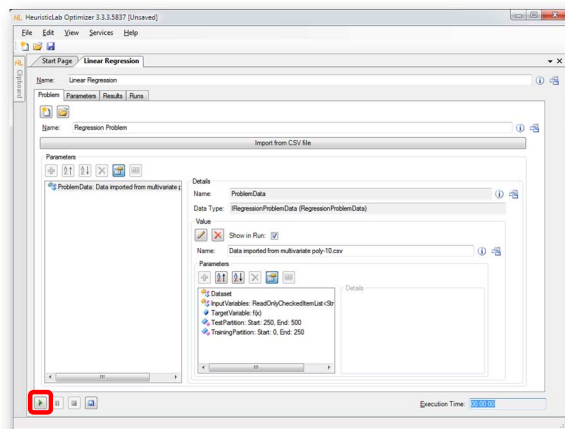


GECCO 2012

<http://dev.heuristiclab.com>

62

Run Linear Regression

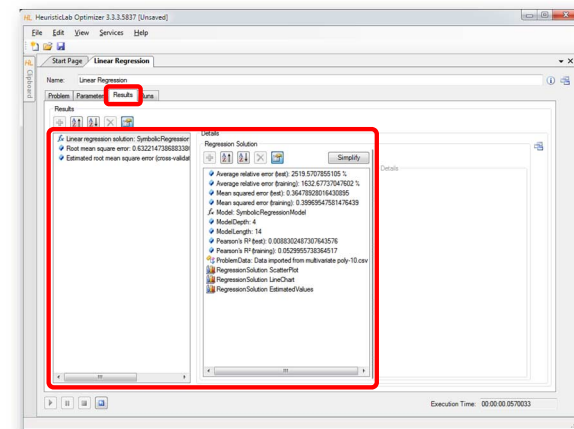


GECCO 2012

<http://dev.heuristiclab.com>

63

Inspect Results

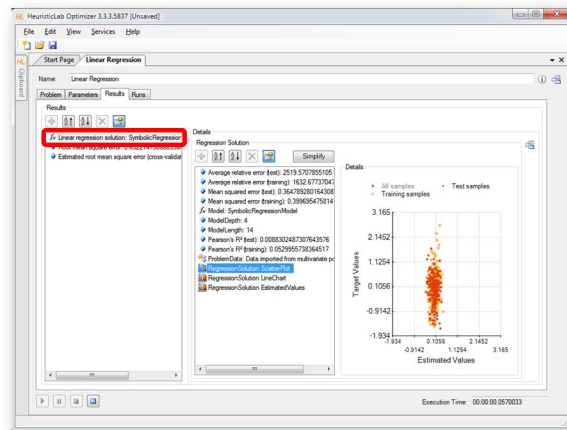


GECCO 2012

<http://dev.heuristiclab.com>

64

Inspect Scatterplot of Predicted and Target Values

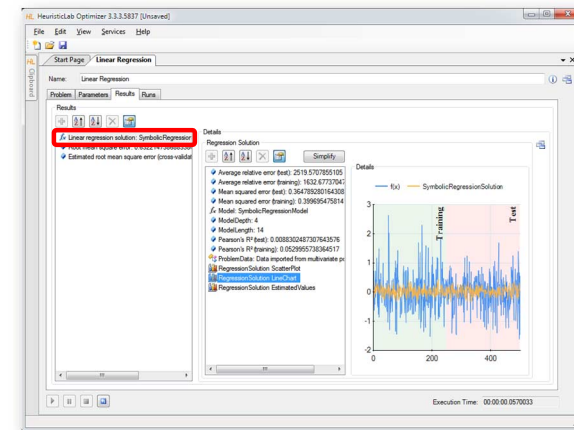


GECCO 2012

<http://dev.heuristiclab.com>

65

Inspect Linechart

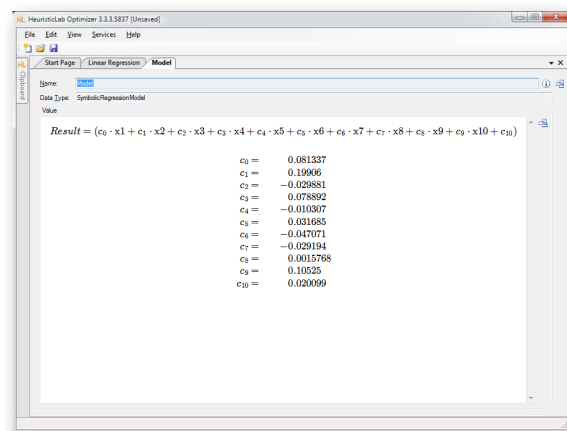


GECCO 2012

<http://dev.heuristiclab.com>

66

Inspect the Model



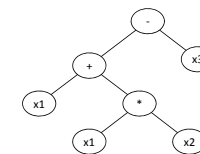
GECCO 2012

<http://dev.heuristiclab.com>

67

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



GECCO 2012

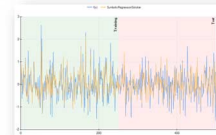
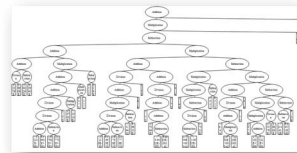
<http://dev.heuristiclab.com>

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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

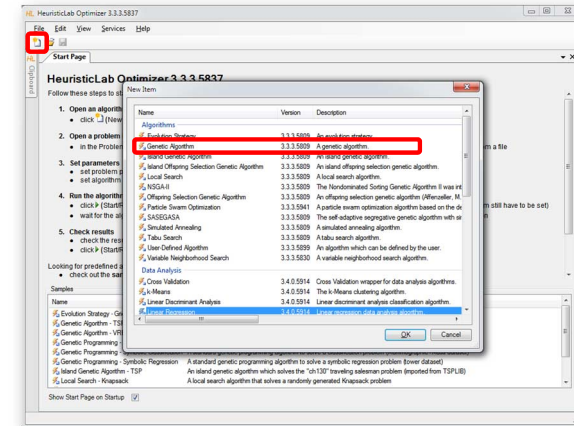


GECCO 2012

<http://dev.heuristiclab.com>

69

Create New Genetic Algorithm

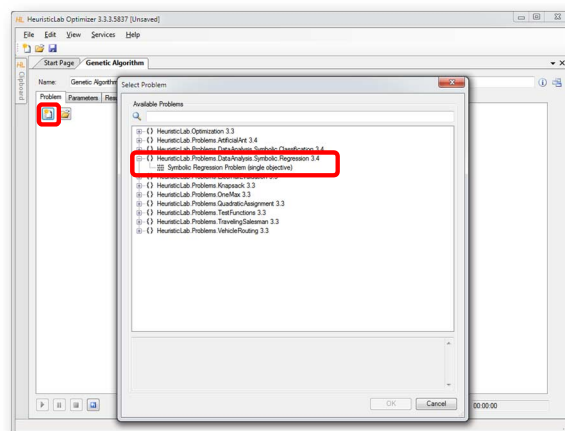


GECCO 2012

<http://dev.heuristiclab.com>

70

Create New Symbolic Regression Problem

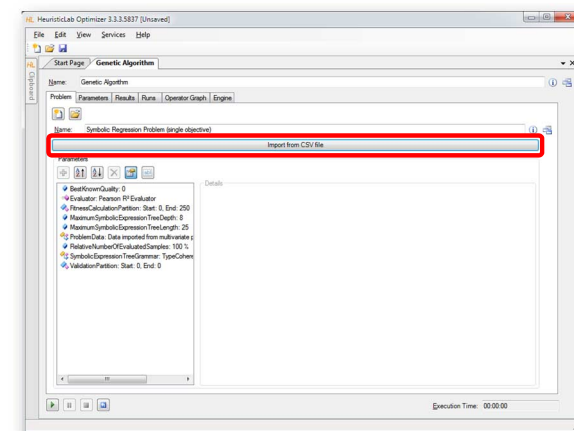


GECCO 2012

<http://dev.heuristiclab.com>

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Import Data

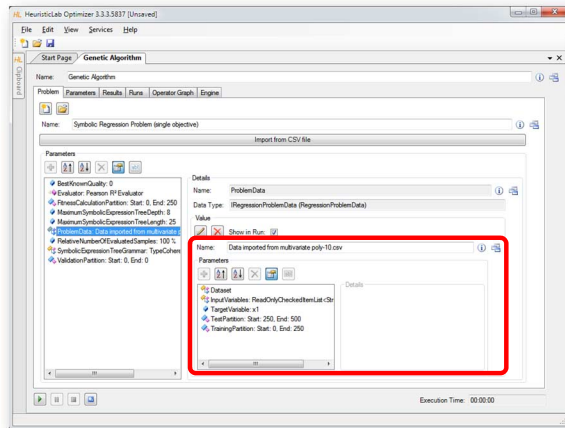


GECCO 2012

<http://dev.heuristiclab.com>

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Inspect Data and Configure Dataset

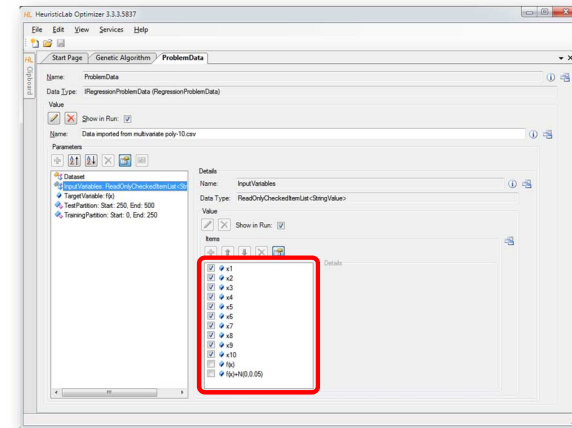


GECCO 2012

<http://dev.heuristiclab.com>

73

Set Target and Input Variables

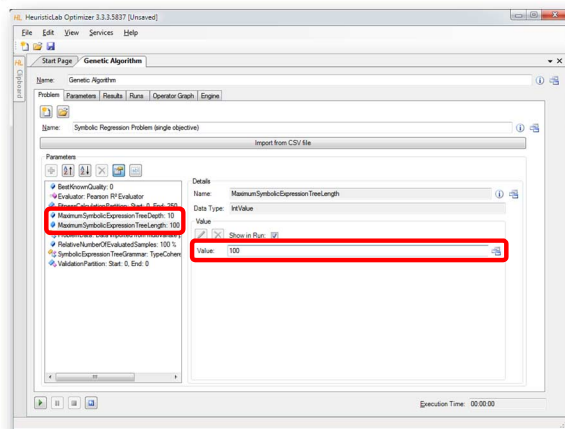


GECCO 2012

<http://dev.heuristiclab.com>

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Configure Maximal Model Depth and Length

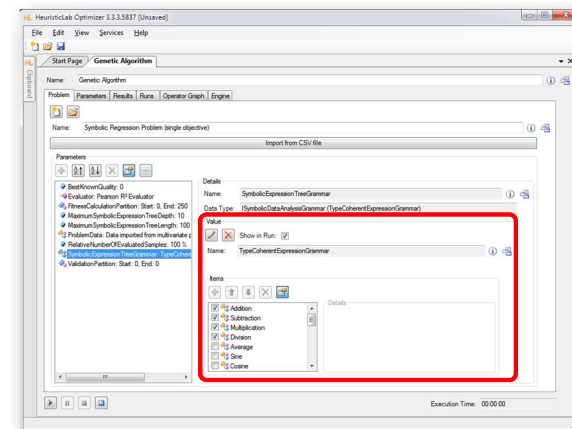


GECCO 2012

<http://dev.heuristiclab.com>

75

Configure Function Set (Grammar)

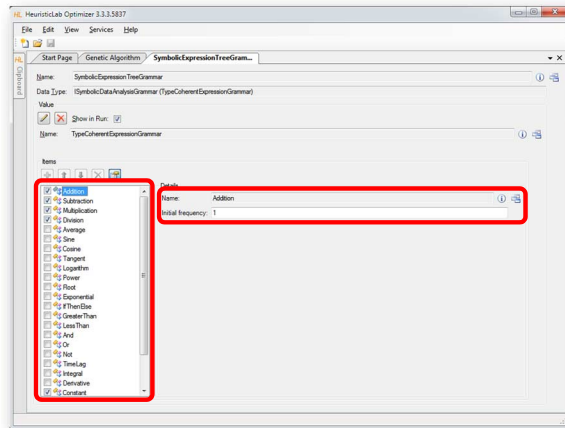


GECCO 2012

<http://dev.heuristiclab.com>

76

Configure Function Set (Grammar)

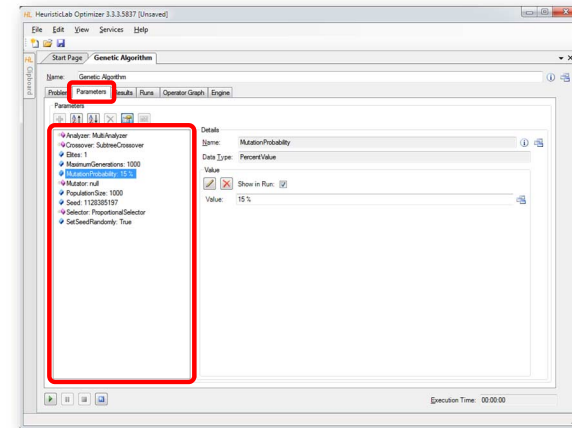


GECCO 2012

<http://dev.heuristiclab.com>

77

Configure Algorithm Parameters

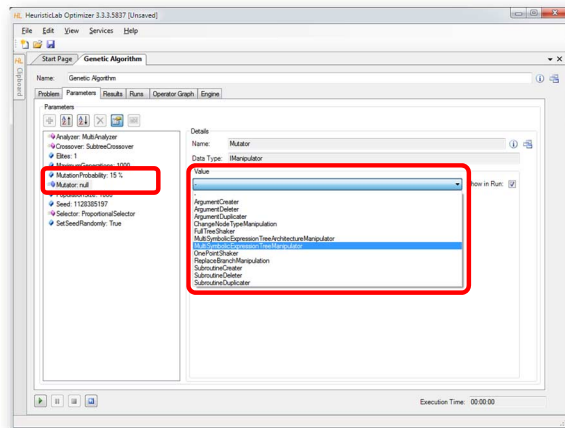


GECCO 2012

<http://dev.heuristiclab.com>

78

Configure Mutation Operator

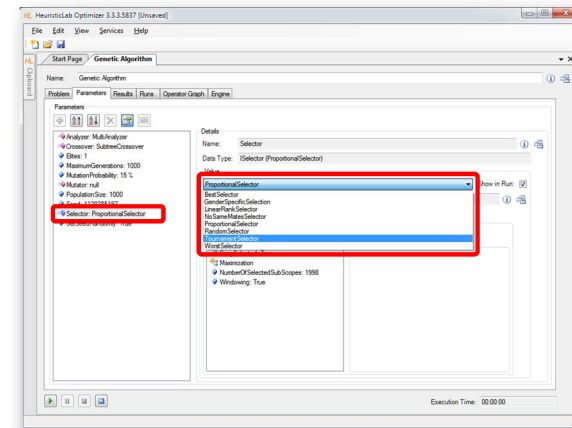


GECCO 2012

<http://dev.heuristiclab.com>

79

Configure Selection Operator

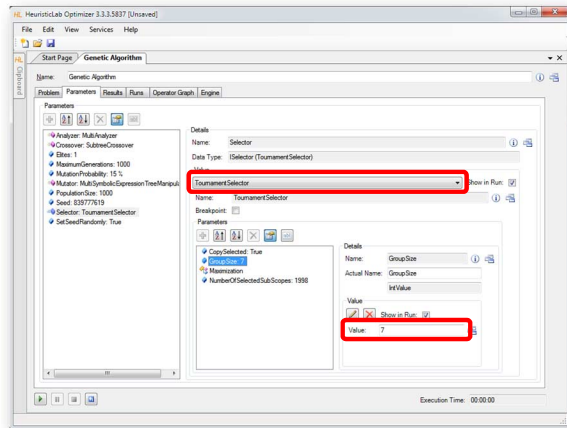


GECCO 2012

<http://dev.heuristiclab.com>

80

Configure Tournament Group Size

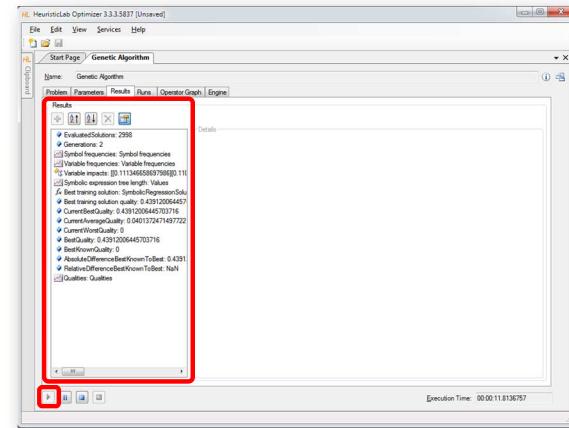


GECCO 2012

<http://dev.heuristiclab.com>

81

Start Algorithm and Inspect Results

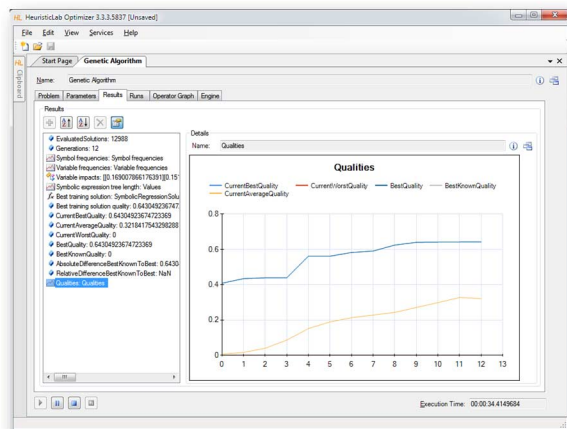


GECCO 2012

<http://dev.heuristiclab.com>

82

Inspect Quality Chart

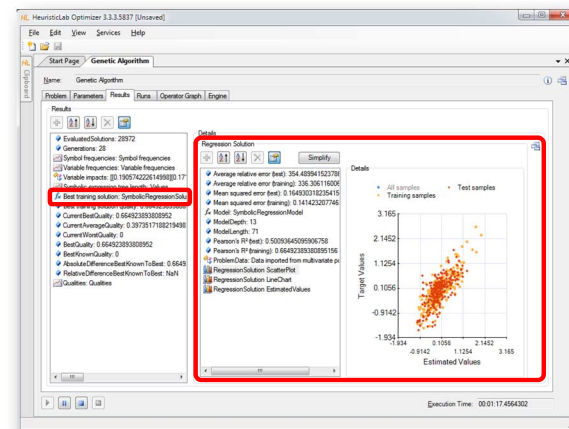


GECCO 2012

<http://dev.heuristiclab.com>

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Inspect Best Model on Training Partition

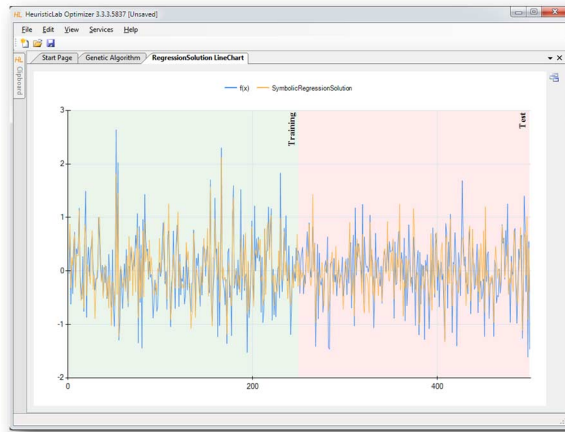


GECCO 2012

<http://dev.heuristiclab.com>

84

Inspect Linechart of Best Model on Training Partition

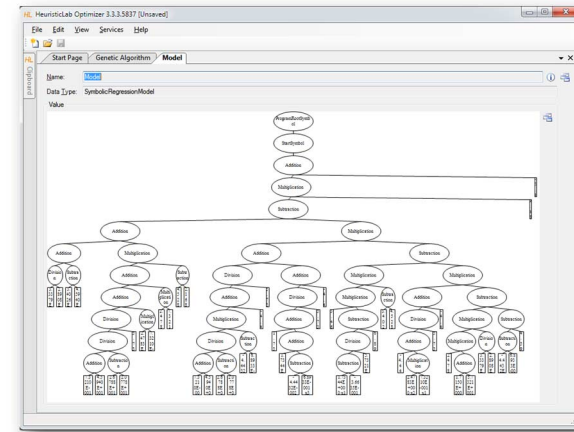


GECCO 2012

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Inspect Structure of Best Model on Training Partition



GECCO 2012

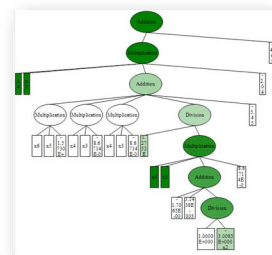
<http://dev.heuristiclab.com>

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Model Simplification and Export



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



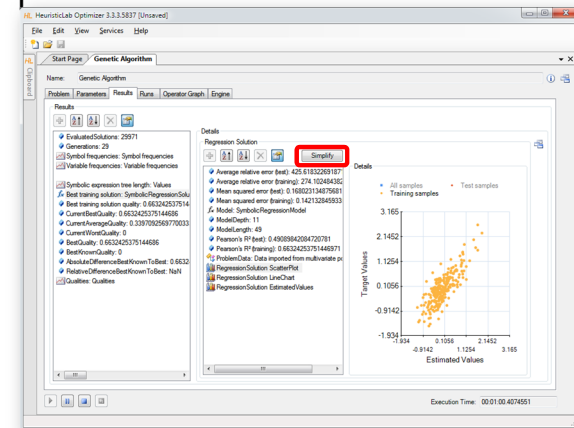
$$\text{Result} = \frac{a(0) \cdot a(1) \cdot a(2) \cdot a(3) \cdot a(4) \cdot a(5) \cdot a(6) \cdot a(7) \cdot a(8) \cdot a(9) \cdot a(10) \cdot a(11) \cdot a(12) \cdot a(13) \cdot a(14) \cdot a(15) \cdot a(16) \cdot a(17) \cdot a(18) \cdot a(19) \cdot a(20) \cdot a(21) \cdot a(22) \cdot a(23) \cdot a(24) \cdot a(25) \cdot a(26) \cdot a(27) \cdot a(28) \cdot a(29) \cdot a(30) \cdot a(31) \cdot a(32) \cdot a(33) \cdot a(34) \cdot a(35) \cdot a(36) \cdot a(37) \cdot a(38) \cdot a(39) \cdot a(40) \cdot a(41) \cdot a(42) \cdot a(43) \cdot a(44) \cdot a(45) \cdot a(46) \cdot a(47) \cdot a(48) \cdot a(49) \cdot a(50) \cdot a(51) \cdot a(52) \cdot a(53) \cdot a(54) \cdot a(55) \cdot a(56) \cdot a(57) \cdot a(58) \cdot a(59) \cdot a(60) \cdot a(61) \cdot a(62) \cdot a(63) \cdot a(64) \cdot a(65) \cdot a(66) \cdot a(67) \cdot a(68) \cdot a(69) \cdot a(70) \cdot a(71) \cdot a(72) \cdot a(73) \cdot a(74) \cdot a(75) \cdot a(76) \cdot a(77) \cdot a(78) \cdot a(79) \cdot a(80) \cdot a(81) \cdot a(82) \cdot a(83) \cdot a(84) \cdot a(85) \cdot a(86) \cdot a(87) \cdot a(88) \cdot a(89) \cdot a(90) \cdot a(91) \cdot a(92) \cdot a(93) \cdot a(94) \cdot a(95) \cdot a(96) \cdot a(97) \cdot a(98) \cdot a(99)}{a(0) \cdot a(1) \cdot a(2) \cdot a(3) \cdot a(4) \cdot a(5) \cdot a(6) \cdot a(7) \cdot a(8) \cdot a(9) \cdot a(10) \cdot a(11) \cdot a(12) \cdot a(13) \cdot a(14) \cdot a(15) \cdot a(16) \cdot a(17) \cdot a(18) \cdot a(19) \cdot a(20) \cdot a(21) \cdot a(22) \cdot a(23) \cdot a(24) \cdot a(25) \cdot a(26) \cdot a(27) \cdot a(28) \cdot a(29) \cdot a(30) \cdot a(31) \cdot a(32) \cdot a(33) \cdot a(34) \cdot a(35) \cdot a(36) \cdot a(37) \cdot a(38) \cdot a(39) \cdot a(40) \cdot a(41) \cdot a(42) \cdot a(43) \cdot a(44) \cdot a(45) \cdot a(46) \cdot a(47) \cdot a(48) \cdot a(49) \cdot a(50) \cdot a(51) \cdot a(52) \cdot a(53) \cdot a(54) \cdot a(55) \cdot a(56) \cdot a(57) \cdot a(58) \cdot a(59) \cdot a(60) \cdot a(61) \cdot a(62) \cdot a(63) \cdot a(64) \cdot a(65) \cdot a(66) \cdot a(67) \cdot a(68) \cdot a(69) \cdot a(70) \cdot a(71) \cdot a(72) \cdot a(73) \cdot a(74) \cdot a(75) \cdot a(76) \cdot a(77) \cdot a(78) \cdot a(79) \cdot a(80) \cdot a(81) \cdot a(82) \cdot a(83) \cdot a(84) \cdot a(85) \cdot a(86) \cdot a(87) \cdot a(88) \cdot a(89) \cdot a(90) \cdot a(91) \cdot a(92) \cdot a(93) \cdot a(94) \cdot a(95) \cdot a(96) \cdot a(97) \cdot a(98) \cdot a(99)}$$

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Detailed Model Analysis and Simplification

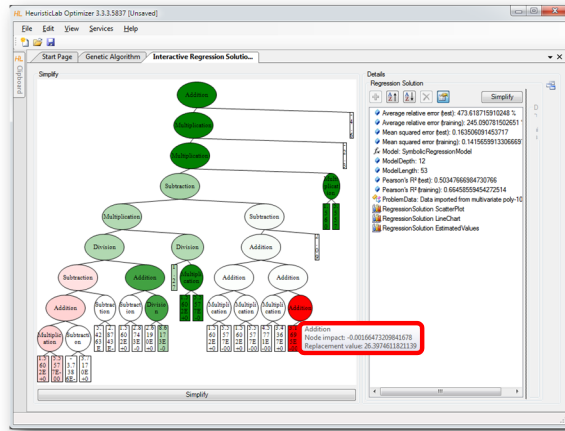


GECCO 2012

<http://dev.heuristiclab.com>

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Symbolic Simplification and Node Impacts

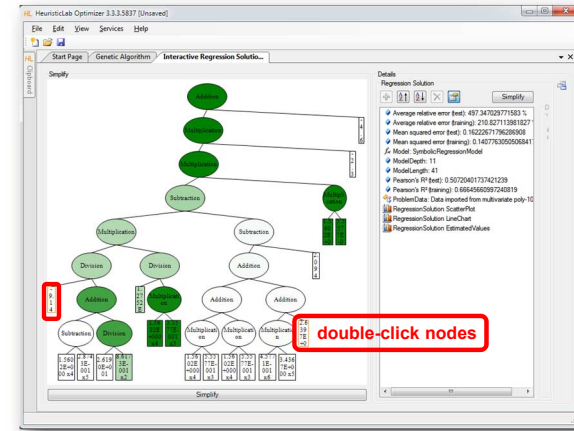


GECCO 2012

<http://dev.heuristiclab.com>

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Manual Simplification

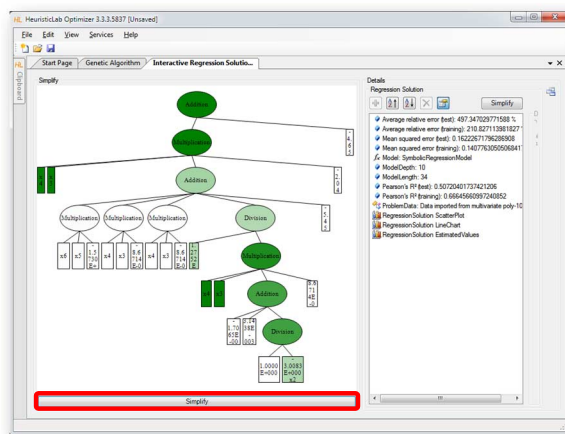


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<http://dev.heuristiclab.com>

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Automatic Symbolic Simplification



GECCO 2012

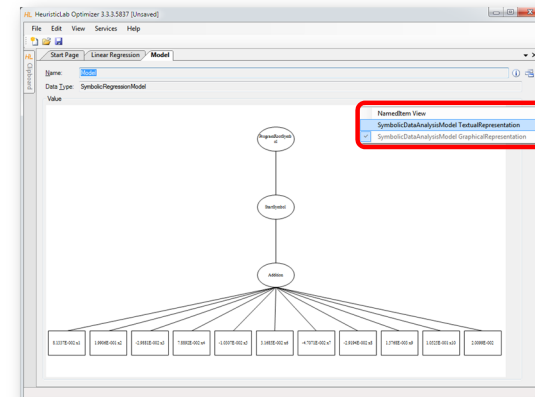
<http://dev.heuristiclab.com>

91

Textual Representations Are Also Available



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

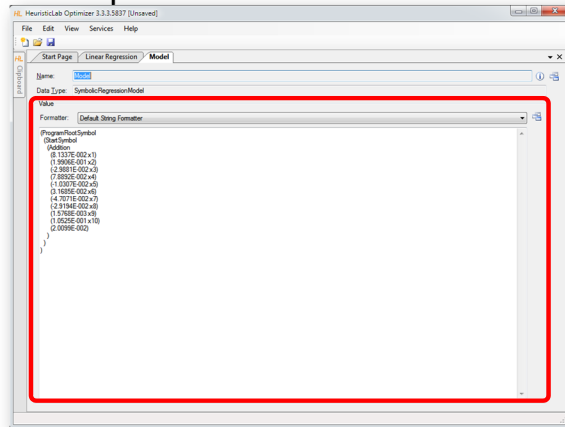


GECCO 2012

<http://dev.heuristiclab.com>

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Default Textual Representation for Model Export

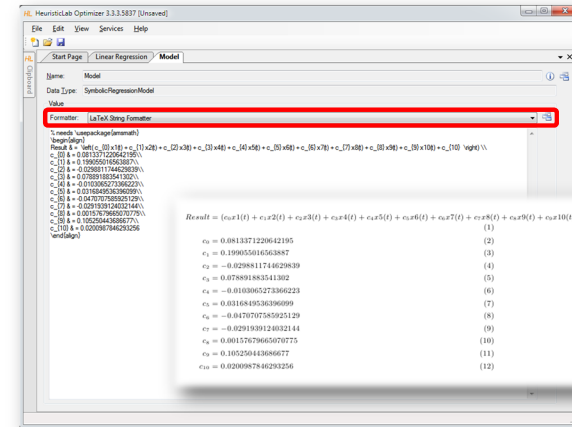


GECCO 2012

<http://dev.heuristiclab.com>

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Textual Representation for Export to LaTeX

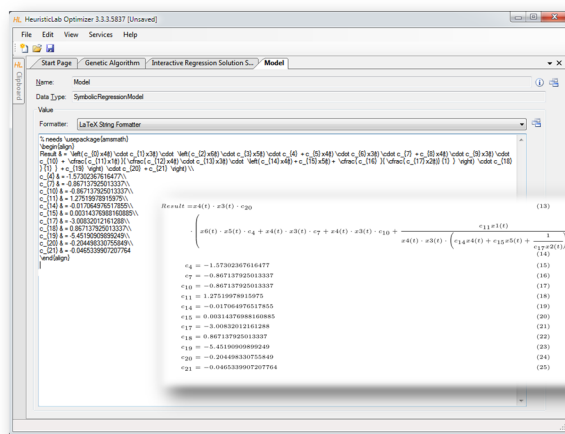


GECCO 2012

<http://dev.heuristiclab.com>

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LaTeX Export



GECCO 2012

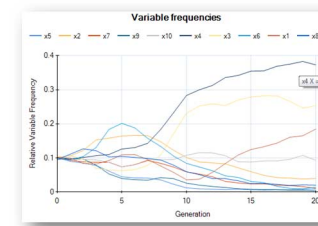
<http://dev.heuristiclab.com>

95

Variable Relevance Analysis



- Which variables are important to predict classes correctly?
- Demonstration
 - Variable frequency analyzer
 - symbol frequency analyzer
 - variable impacts



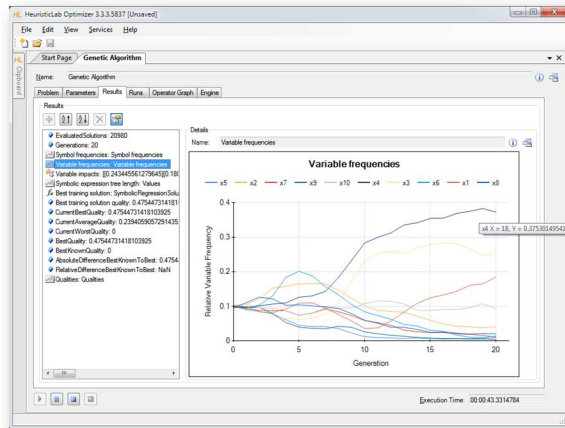
	Relative variable relevance
x4	0.3028038659106054
x3	0.241170172985569
x1	0.179112369714678
x10	0.0589664719249172
x2	0.0544635184742382
x6	0.0446774403657897
x8	0.0436011597048278
x7	0.0331173502974243
x5	0.0226252246461621
x9	0.01946242278034

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<http://dev.heuristiclab.com>

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Inspect Variable Frequency Chart

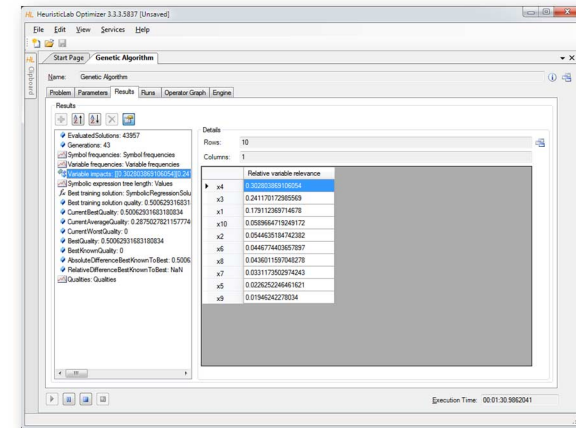


GECCO 2012

<http://dev.heuristiclab.com>

97

Inspect Variable Impacts

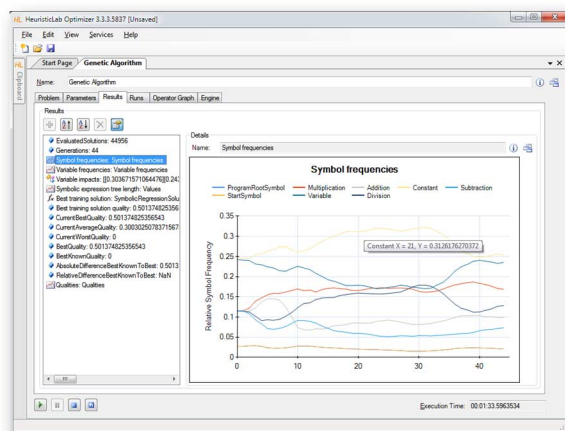


GECCO 2012

<http://dev.heuristiclab.com>

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Inspect Symbol Frequencies



GECCO 2012

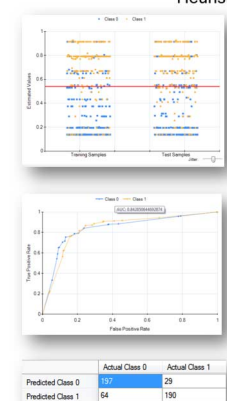
<http://dev.heuristiclab.com>

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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



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<http://dev.heuristiclab.com>

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Case Study: Classification



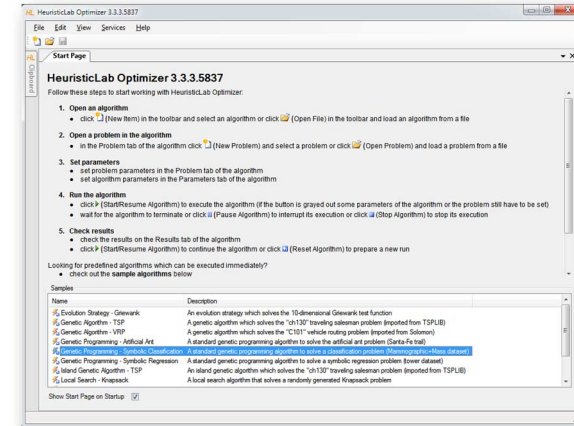
- Real world medical dataset (*Mammographic Mass*) from UCI Machine Learning Repository
 - data from non-invasive mammography screening
 - variables:
 - patient age
 - visual features of inspected mass lesions: shape, margin, density
 - target variable: severity (malignant, benign)
- download
 - <http://dev.heuristiclab.com/AdditionalMaterial#GECCO2012>

GECCO 2012

<http://dev.heuristiclab.com>

101

Open Sample

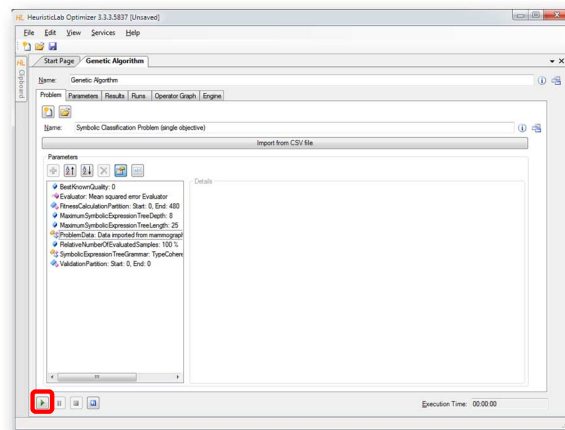


GECCO 2012

<http://dev.heuristiclab.com>

102

Configure and Run Algorithm

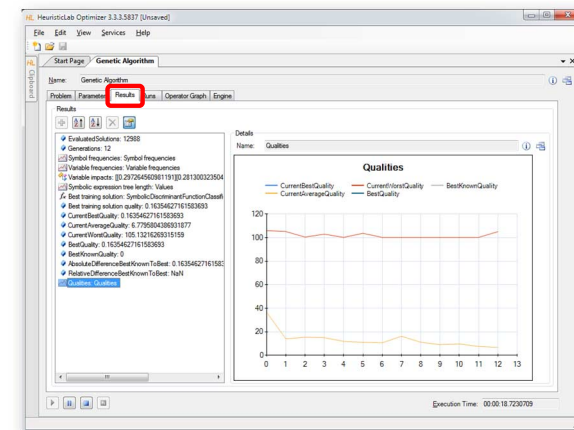


GECCO 2012

<http://dev.heuristiclab.com>

103

Inspect Quality Linechart

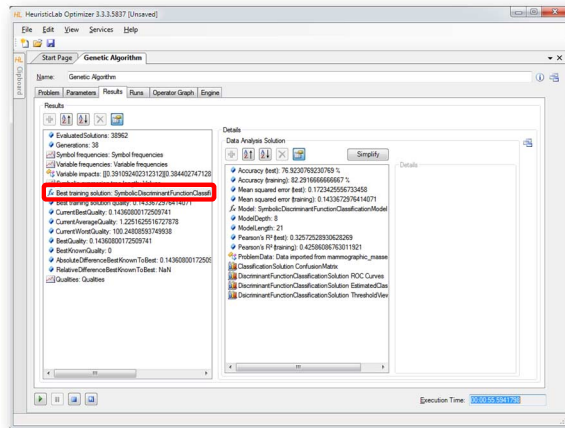


GECCO 2012

<http://dev.heuristiclab.com>

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Inspect Best Training Solution

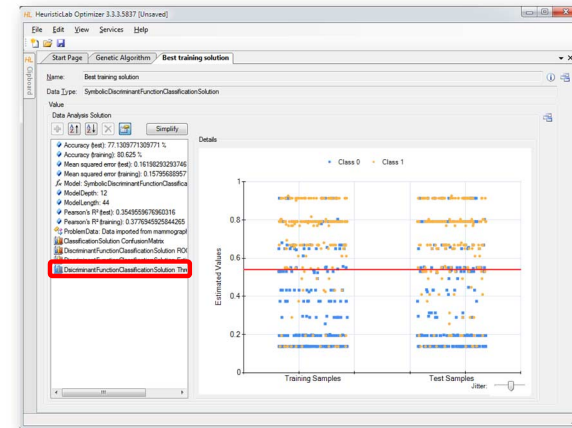


GECCO 2012

<http://dev.heuristiclab.com>

105

Inspect Model Output and Thresholds

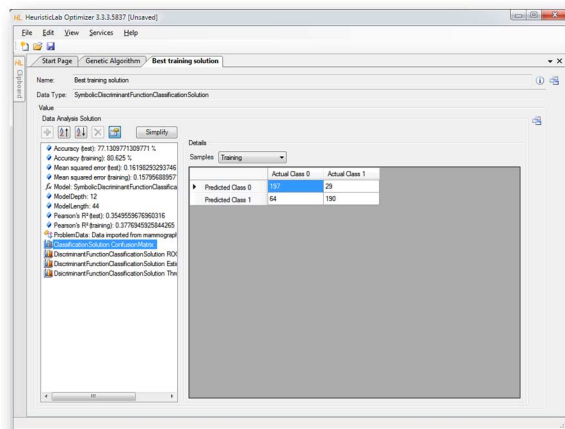


GECCO 2012

<http://dev.heuristiclab.com>

106

Inspect Confusion Matrix

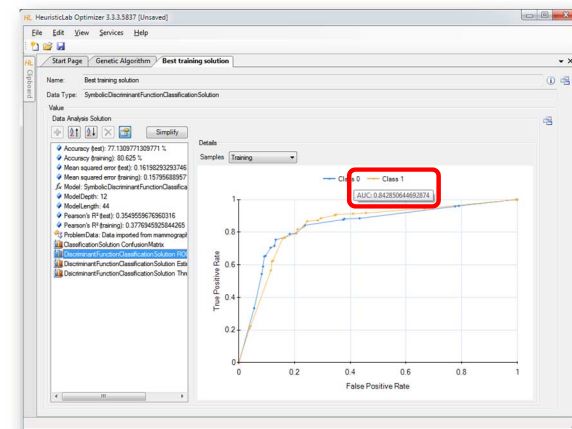


GECCO 2012

<http://dev.heuristiclab.com>

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Inspect ROC Curve



GECCO 2012

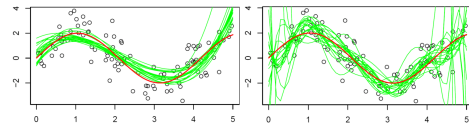
<http://dev.heuristiclab.com>

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Validation of Results

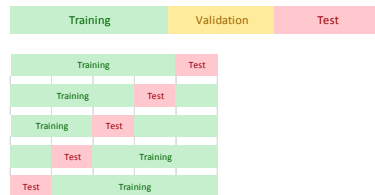


- Overfitting = memorizing data



- Strategies to reduce overfitting

- validation partition
- cross-validation



GECCO 2012

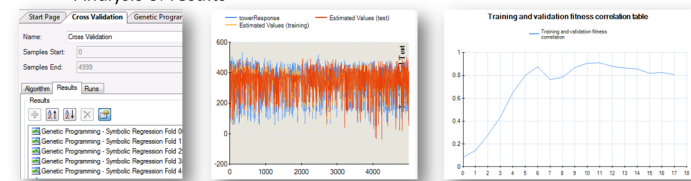
<http://dev.heuristiclab.com>

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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

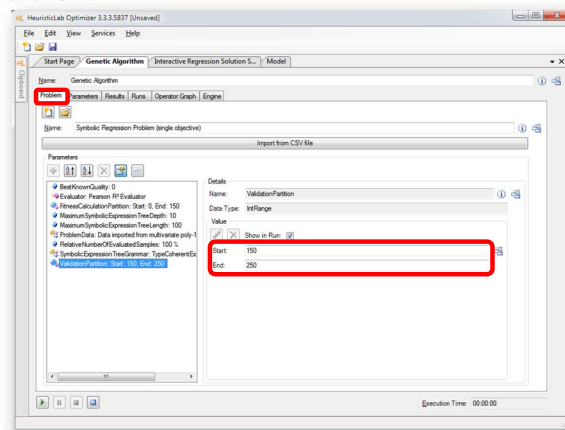


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Configuration of Validation Partition

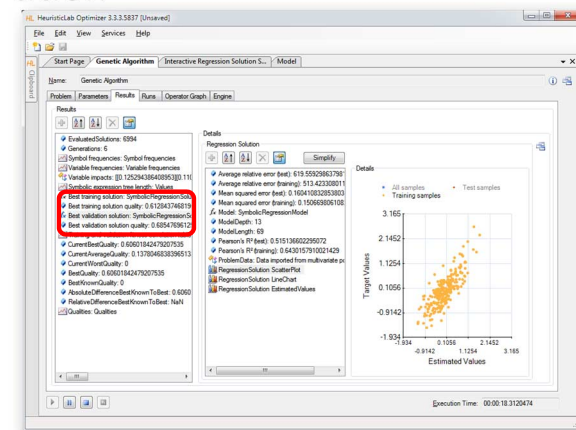


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Inspect Best Model on Validation Partition

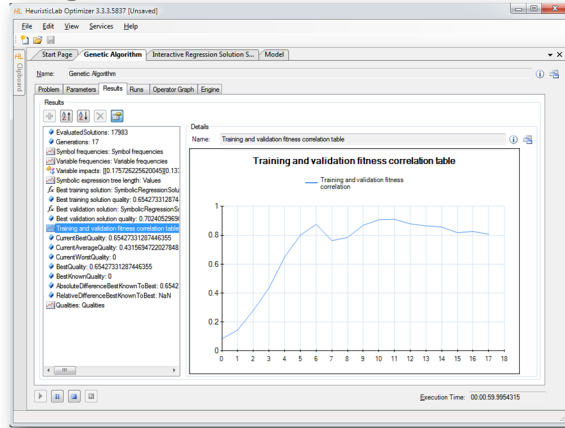


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Inspect Linechart of Correlation of Training and Validation Fitness



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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

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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?
 - join our HeuristicLab Google group heuristiclab@googlegroups.com or
 - write an e-mail to support@heuristiclab.com

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HeuristicLab Team



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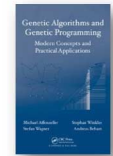
Suggested Readings



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

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Questions & Answers



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