$\begin{array}{c} \text{GPLAB} \\ \text{A Genetic Programming Toolbox for MATLAB} \end{array}$

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> Version 2 May 2004

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Chapter 1

Introduction

MATLAB [1] is a widely used programming environment available for a large number of computer platforms. Its programming language is simple and easy to learn, yet fast and powerful in mathematical calculus. Furthermore, its extensive and straightforward data visualization tools make it a very appealing programming environment. Toolboxes are collections of optimized, application-specific functions, which extend the MATLAB environment and provide a solid foundation on which to build.

GPLAB is a genetic programming toolbox for MATLAB. Versatile, generalist and easily extendable, it can be used by all types of users, from the layman to the advanced researcher. It was tested on different MATLAB versions and computer platforms, namely versions 5.2 and 6.5 for Windows and versions 5.3 and 6.5 for Linux. This manual is accompanied by a zip file containing all the functions that form the toolbox, released under GNU General Public Licence. Both are freely available for download at http://gplab.sourceforge.net/.

Chapter 2 describes the operational structure of GPLAB. Details on the available parameters and state variables are found in Chaps. 3 and 4 respectively. Chapter 5 shows the available offline graphical capabilities of GPLAB, and Chapter 6 presents a summary of all toolbox functions, divided in functional groups.

1.1 Update from version 1.x

GPLAB is slowly growing and (hopefully) improving. The changes are always biased towards my own work, but I also try to incorporate different things that I have come to realize other users need. Here are the major changes from version 1.x:

 Added possibility of performing cross-validation during the evolutionary process, by using an additional data set, called test data set. Added function to evaluate an individual in a different data set, to obtain fitness value or simply do predictions.

- Added variations to the dynamic maximum tree depth technique [11] the heavy dynamic limit and the dynamic limit on tree size (number of nodes). Some of these have also resulted in variations to the tree initialization procedures [12]. Added the possibility of removing the strict limit on depth (or size).
- Removed tree structure (depth, size) validation procedures from the genetic operators. Now the genetic operators simply create the new individuals and these will be passed through validation filters elsewhere. Building new genetic operators has become much easier.
- Removed the need for the user to set the dynamic depth parameter it is automatically set, now.
- Improved online graphics. Four different online plots are available now fitness (added stardard deviation and cross validation measures), operators (added reproduction and cloning frequencies), diversity (added hamming diversity and possibility to use several measures at the same time), complexity (depth and size information is more complete, intron percentage and tree fill rate are included when available).
- Added more offline graphics, like the drawing of the pareto front and of the evolved trees.
- Fitness values are now rounded to a certain precision (number of decimal places determined by parameter) to avoid faulty fitness comparisons due to rounding errors.

And some of the minor changes (at least the ones I haven't forgotten to mention):

- Data files for training (and optionally testing) do not need to be located in your working directory any longer.
- Importing data files does not change the order of the fitness cases any longer it just removes repeated occurrences.

1.2 Acknowledgements

I would like to address a big thank you to Henrik Schumann-Olsen, Jens T. Thielemann and Oddvar Kloster at SINTEF (http://www.sintef.no) for the extensive additional code they have provided for GPLAB version 1. I have integrated most of its goodies in this new version of GPLAB, but some are still missing, like the powerful feature of building multiple trees. I intend to integrate it also - no promises when, though. Many other users have steadily provided a wealth of comments and suggestions - thank you all, particularly Mehrashk Meidani (mehrashk@yahoo.com) at Shiraz University for helping me with a protected function (mypower.m). I have also used an utilitarian function (fixdec.m) written by Peter J. Acklam (http://home.online.no/~pjacklam).

Chapter 2

Operational structure

The architecture of GPLAB follows a highly modular and parameterized structure, which different users may use at various levels of depth and insight. What follows is a visual description of this structure, along with brief explanations of some operation details and control parameters, algorithm's variables, a summary of three usage profiles appropriate for different types of users, and details on how to deal with "plug and play functions".

2.1 Main modules

Figure 2.1 shows the operational structure of GPLAB. There are three main operation modules, namely SET VARS, GEN POP, and GENERATION, and each represents an interaction point with the user. Inside each main module the sub-modules are executed from top to bottom, the same happening inside INITIAL PROBS and ADAPT PROBS. The description of these two can be found in Sects. 3.13 and 3.12 respectively. Any module with a question mark can be skipped, depending on the parameter indicated above it. Each module may use one or more parameters and one or more user functions. User functions implement alternative or collective procedures for realizing a module, and they behave as plug and play devices.

2.1.1 GEN POP

This module generates the initial population (INIT POP) and calculates its fitness (FITNESS). The individuals in GPLAB are tree structures initialized with one of three available initialization methods - Full, Grow, Ramped Half-and-Half [8]. The functions available to build the trees include the if-then-else statement and some protected functions, plus any MATLAB function that verifies closure. The terminals include a random number generator and all the variables necessary, created in runtime. Fitness is, by default, the sum of absolute differences between the obtained and expected results in all fitness cases. The lower the

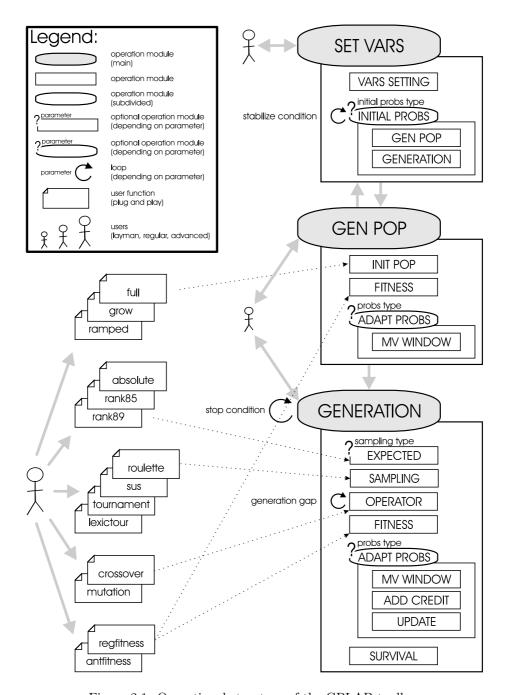


Figure 2.1: Operational structure of the GPLAB toolbox $\,$

fitness value, the better the individual. This is the standard for symbolic regression and parity problems ("regfitness" in Fig. 2.1), but GPLAB accepts any other plug and play function to calculate fitness, like the function for artificial ant problems, also provided ("antfitness").

GEN POP is called by the user. It starts by requesting some parameter initializations to SET VARS, and finishes by passing the execution to GENERATION. If the user only requests the creation of the initial generation, GENERATION is not used.

2.1.2 GENERATION

This module creates a new generation of individuals by applying the genetic operators to the previous population (OPERATORS). Standard tree crossover and tree mutation are the two genetic operators available as plug and play functions. They must have a pool of parents to choose from, created by a SAM-PLING method, which may or may not base its choice on the EXPECTED number of offspring of each individual. Four sampling methods (Roulette [6], SUS [3], Tournament [4], Lexicographic Parsimony Pressure Tournament [9]) and three methods for calculating the expected number of offspring (Absolute [7], Rank85 [2], Rank89 [10]) are available as plug and play functions, and any combination of the two can be used. The genetic operators create new individuals until a new population is filled, a number determined by the generation gap (see Sect. 3.10).

Calculating fitness is followed by the SURVIVAL module, where the individuals that enter the new generation are chosen according to the elitism level parameter. The GENERATION module repeats itself until the stop condition is fulfilled, or when the maximum generation is reached. Several stop conditions can be used simultaneously (see Sect. 3.14). This module can be called either by the user or by GEN POP.

2.1.3 SET VARS

This module either initializes the parameters with the default values or updates them with the user settings. Besides the parameters directly related to the execution of the algorithm, other parameters affect the output of its results (see Chap. 3 for a description of all parameters). SET VARS can be called either by the user or by a request for parameter initialization from GEN POP.

2.2 Working variables

GPLAB uses a vast number of working variables, organized in a structure according to its role in the algorithm. This structure will be referred to as vars throughout this manual. It is composed of four fields, params, state, pop, data. Saving vars to a file stores all the information GPLAB uses, produces, and will ever need to continue a previously started run.

- params stores all the variables that determine different ways of running the different parts of the algorithm. These are settings that are not supposed to vary during the course of a run, although the user can continue a GPLAB run with a different set of parameters from how it started. Chapter 3 is dedicated to the different running aspects of GPLAB each subsection refers to one or more parameters related to that aspect.
- state stores all the variables that represent the current state of the algorithm. These settings are constantly updated during the run, and should not be modified by the user. Chapter 4 is dedicated to describing the meaning of the various state variables.
- pop stores the current population. This variable is constantly updated as the population evolves. It can be considered a state variable and, accordingly, its description can be found in Chap. 4.
- data is the data set(s) used by the algorithm to guide the evolutionary process and, optionally, perform cross-validation, imported from files in the beginning of each run. Because it is stored along with the other algorithm's variables, continuing a previously started run does not require the user to provide the data files again.

2.3 Usage

The large amount of available control parameters may lead to the wrong conclusion that it will take a long time before one can start using the toolbox comfortably, and that only expert users will ever be able to use it properly. On the contrary, GPLAB is very easy to use and suits even the unknowledgeable users, due to the automatic parametrization of most parameters. Here is a summary of three different profiles of usage that may be given by different types of users: the layman, the regular user, and the advanced researcher.

2.3.1 The layman

This user wants to try a genetic programming algorithm to achieve a solution to a standard problem, without having to learn about available parameters, or how to set them. The available functions are

```
[vars,b]=gplab(g,n);
[vars,b]=gplab(g,vars);
```

where g is the maximum number of generations to run the algorithm and n is the population size.

The first function initializes all the parameters of the algorithm with the default values and runs it for g generations with n individuals. The user will be asked about the location of the data files to use (see Sect. 3.8). It returns vars, all the variables of the algorithm, and b, the best individual found, which is the

same as vars.state.bestsofar. The second function continues a previously started run for another g generations, and also needs vars as an input argument. These two functions correspond to the operation modules GEN POP and GENERATION shown in Fig. 2.1.

GPLAB also provides some demonstration functions to illustrate its usage in different types of problems (see Chap. 6 for a complete list of functions):

- demo runs a symbolic regression problem (the quartic polynomial) with 50 individuals for 25 generations, with automatic adaptation of operator probabilities, and performing cross-validation in a different data set (the exponential). It draws all the available plots in runtime (see Sect. 6.19), and finishes with several additional output plots (see Sect. 5), including the pareto front and the drawing of the best individual found.
- demoparity runs the parity-3 problem with 50 individuals for 20 generations, with fixed operator probabilities, drawing some of the available runtime plots, and finishing by drawing the best individual found.
- demoant runs the artificial ant problem in the Santa Fe food trail with 20 individuals for 10 generations, drawing half of the available plots in runtime, and finishing by drawing the best individual found.

2.3.2 The regular user

This is the type of user who knows what the parameters mean and wants to test different sets of values besides the defaults. To set the parameters the available functions are

```
params=resetparams;
params=setparams(params,'param1=value1,param2=value2,etc');
[vars,b]=gplab(g,n,params);
```

where param1, param2 are the names of parameters, and value1, value2 the values pretended.

The first function initializes and returns the parameters structured variable with the default values, and the second alters some of the parameters according to the list given as argument. The third acts like the first function described for the layman, except that it uses the parameter values previously set instead of initializing them with the default values. The parameter setting functions correspond to the module SET VARS in Fig. 2.1. resetparams is appropriate for symbolic regression problems. For different types of problems, one should see the parameter settings used on the demo functions demoparity and demoant.

Please see Chap. 6 for a complete list of functions. There are also functions dedicated to setting some specific parameters, like the genetic operators, and the functions and terminals used to build the trees (see Sects. 3.4 and 3.3 for details).

2.3.3 The advanced researcher

Here is the user who wants to build and test new sampling methods, new genetic operators, in short, new user functions as shown in Fig. 2.1, without having to construct a new toolbox from the beginning. GPLAB allows this with a minimum amount of effort, thanks to its plug and play operational structure. As an example, the user who wants to test a new genetic operator only has to build a new function that implements it, using the tree manipulation functions provided. This function should use the same input and output arguments as the other genetic operators (a template for building new genetic operators is provided in Sect. 3.4). To tell the algorithm about the new genetic operator the available function is

```
params=addoperators(params, 'newoperator', nparents, nchildren);
```

where newoperator is the name of the new function, nparents is the number of parents the new operator needs, and nchildren is the number of offspring it produces. Details on how to build new plug and play user functions can be found in Chap. 3 (please search for the particular subsection that applies) and the way to integrate them into GPLAB is described in Sect. 2.4.

2.4 Plug and play

Figure 2.1 shows that most modules of the GPLAB operational structure are based on a set of user functions that act as plug and play devices. There are three important aspects related to these functions: how to build them, how to use them, and how to integrate them in GPLAB.

2.4.1 Building plug and play functions

Building a new plug and play function is like building any other MATLAB function while following the rules pertaining input and output arguments. Each module defines its own set of input and output arguments, so the interested user should refer to the appropriate section in Chap. 3.

2.4.2 Using new plug and play functions

To use a newly built plug and play function, the user must declare its existence in the algorithm's parameters. Once again, each module is associated to different parameter variables, and the user should refer to the appropriate section in Chap. 3, but the general form of doing this is

```
vars.params.<specificvariable>='name_new_func';
```

where **<specificvariable>** is the parameter that refers to the module adopting the new function. This may look equivalent to doing

```
params=setparams(params,'<specificvariable>=name_new_func');
```

but this form of setting parameters will be refused for the new plug and play function until it is fully integrated as part of GPLAB.

2.4.3 Integrating new plug and play functions in GPLAB

Integrating a new function in GPLAB is done by editing the toolbox file availableparams. This file contains the declarations of the fields that constitute the structure variable params, as well as their possible and default values - where the possible values may be the names of the plug and play functions. This file is divided in three parts: the first specifies which variables form the structure params; the second specifies the possible values for each variable; the third specifies the default values for each variable. As an example, to integrate a new plug and play function called 'newfitness' that implements a new way of measuring fitness, a new line should be added:

```
myparams.calcfitness={'regfitness', 'antfitness', 'newfitness'};
```

where 'regfitness' and 'antfitness' are the standard procedures for calculating fitness already provided by GPLAB. This line tells GPLAB that all three procedures can be used for calculating fitness. When the algorithm begins, 'regfitness' is still the default fitness procedure, but the user can change it before starting the run. Because 'newfitness' is already declared as a standard GPLAB function, this change can be made with the setparams function:

```
params=setparams(params,'calcfitness=newfitness');
```

To make 'newfitness' the default procedure without the need to change the setting before running the algorithm, the line

```
defaults.calcfitness=''', 'regfitness''';
```

in the availableparams file should be replaced with

```
defaults.calcfitness='', 'newfitness'';
```

Names of functions have to be accompanied by the triple "',", but numeric settings can be made like in this example:

```
defaults.hits='[100 0; 90 10]';
```

The exceptions to the description above are all the cases when the new plug and play function is to be used along with other plug and play functions, like the genetic operators and the functions and terminals. Please see file availableparams for examples.

Similarly, the file availablestates may also be edited to include new fields in the structure variable state. This may have to be done if a new plug and play function intends to use state variables other than the ones available. This is an advanced action that should not be attempted without proper care.

Chapter 3

Parameters

The next sections describe aspects related to the parameters used by GPLAB—what are the parameters involved in each part of the algorithm, and how their modification affects its behavior. Each subsection concerns one or more parameter variables, and each parameters may appear in more than one subsection. Table 3.1 indicates the location of each parameter in this manual, and Table 3.2 specifies their possible and default values. When setting parameters, using the function setparams will ensure minimum range checking, whereas setting the fields of the variable vars.params directly will not. Some parameter settings are automatically corrected to allowed values (with a warning to the user) in case they are set incorrectly. Others are automatically set when left empty. Generally speaking, the only parameters that must be set by the user are the maximum number of generations, the population size, and the names of the files that contain the data set (see Sect. 2.3).

Table 3.1: Location of parameters in this manual

Parameter	Section	Page
adaptinterval	3.12	31
${\tt adaptwindowsize}$	3.12	31
autovars	3.3	19
calccomplexity	3.9	29
calcdiversity	3.9	29
calcfitness	3.8	27
datafilex	3.8	27
datafiley	3.8	27
depthnodes	3.1, 3.2, 3.5	17,18,24
dynamiclevel	3.2, 3.5	18,24
expected	3.7	26
files2data	3.8	27
filters	3.5	24

continued on next page

Table $3.1:\ continued$

Parameter	Section	Page
fixedlevel	3.2, 3.5	18,24
functions	3.3	19
gengap	3.10	29
graphics	3.17	34
hits	3.14	32
inicdynlevel	3.2	18
inicmaxlevel	3.1	17
initialfixedprobs	3.13	32
initialprobstype	3.13	32
initialvarprobs	3.13	32
initpoptype	3.1	17
keepevalssize	3.8	27
lowerisbetter	3.8	27
minprob	3.12	31
numbackgen	3.12	31
numvars	3.3	19
operatornames	3.4	22
operatornchildren	3.4	22
operatornparents	3.4	22
operatorprobstype	3.12	31
output	3.16	33
percentback	3.12	31
percentchange	3.12	31
precision	3.8	27
realmaxlevel	3.2	18
reproduction	3.4	22
sampling	3.6	25
savedir	3.15	33
savetofile	3.15	33
smalldifference	3.13	32
survival	3.11	30
terminals	3.3	19
testdatafilex	3.8	27
testdatafiley	3.8	27
tournamentsize	3.6	25
usetestdata	3.8	27

Table 3.2: Possible and default values of the parameters

Parameter	Possible values	Default value	
adaptinterval	integer > 0	[], see Sect. 6.18	
adaptwindowsize	$\frac{\text{integer } \leq 0}{\text{integer } \geq 0}$	[], see Sect. 6.18	
autovars	'0','1'	'1'	
calccomplexity	'0'.'1'	'0'	
carccomplexity	(list of diversity measures,	·	
calcdiversity	see Sect. 3.9)	{ }	
calcfitness	'regfitness', 'antfitness'	'regfitness'	
datafilex	(name of a valid input file)	(user provided, see Sect. 3.8)	
datafiley	(name of a valid input file)	(user provided, see Sect. 3.8)	
depthnodes	'1','2'	'1'	
dynamiclevel	'0','1','2'	'1'	
expected	'absolute','rank85','rank89'	'rank85'	
files2data	'xy2inout','anttrail'	'xy2inout'	
TITESZUATA	(list of filter functions,		
filters	see Sect. 3.5)	{ }	
fixedlevel	'0','1'	'1'	
Tixedievel	0,1	'plus','minus','times',	
functions	(see Sect. 3.3)	'sin', 'cos', 'mylog'	
manman	integer> 0	[], see Sect. 3.10	
gengap	(list of plot names,	*	
graphics	see Sect. 3.17)	{ }	
	(list of stop conditions,		
hits	see Sect. 3.14)	[100, 0]	
	see Sect. 3.14)	6 if depthnodes='1'	
inicdynlevel	integer > 0	28 if depthnodes='2'	
		6 if depthnodes='1'	
inicmaxlevel	integer > 0	28 if depthnodes='2'	
initialfixedprobs	(list of probability values)	[], see Sect. 3.13	
initialprobstype	'fixed','variable'	'fixed'	
initialvarprobs	(list of probability values)	[], see Sect. 3.13	
initpoptype	'fullinit','growinit','rampedinit'	'rampedinit'	
keepevalssize	$\frac{\text{integer} \geq 0}{one of the support of the sup$	[], see Sect. 3.8	
lowerisbetter	0,1	1	
minprob	> 0 and ≤ 1	0.1	
numbackgen	integer> 0	3	
numvars	[] or integer ≥ 0	[], see Sect. 3.3	
Hullivals	(list of operator names,	·	
operatornames	see Sect. 3.4)	$\{$ 'crossover','mutation' $\}$	
operatornchildren	(list of number of children produced)	[2,1]	
operatornparents	(list of number of parents needed)	[2,1]	
<u> </u>	'fixed','variable'	'fixed'	
operatorprobstype output	'silent','normal','verbose'	'normal'	
percentback	> 0 and < 1	0.25	
percentchange	≥ 0 and ≤ 1 > 0 and ≤ 1	0.25	
	0 integer > 0	12	
precision	mreger > 0		
realmaxlevel	integer > 0	17 if depthnodes='1' 512 if depthnodes='2'	
reproduction	≥ 0 and < 1	0.1	
1 chi oducciion	'roulette','sus',	0.1	
sampling	'tournament','lexictour'	'lexictour'	
savedir	(name for a new directory)	(user provided, see Sect. 3.15)	
	(name for a new directory)	continued on next nage	

continued on next page

Table 3.2: continued

Parameter	Possible values	Default value	
savetofile	'never','firstlast', 'every10','every100','always'	'never'	
smalldifference	> 0 and ≤ 1	[], see Sect. 3.13	
survival	'replace','keepbest', 'halfelitism','totalelitism'	'replace'	
terminals	(see Sect. 3.3)	{ }	
testdatafilex	(name of a valid input file)	(user provided, see Sect. 3.8)	
testdatafiley	(name of a valid input file)	(user provided, see Sect. 3.8)	
tournamentsize	[] or > 0 (integer if ≥ 1)	[], see Sect. 3.6	
usetestdata	0,1	0	

3.1 Tree initialization

inicmaxlevel, depthnodes, initpoptype

The initial population of trees, created in runtime in the beginning of a GPLAB run, is done by choosing random functions and terminals from the respective sets (Sect. 3.3). The initial maximum depth/size of the new trees, determined by the parameter inicmaxlevel, must not be violated, but besides this rule there is still room for different options that may influence the structure of the initial trees. These options constitute what is called the generative method, specified by the parameter initpoptype. There are three different methods available in GPLAB, used in the plug and play fashion described in Sect. 2.4, and each of them uses either the standard procedure based on depth [8], or the new variation based on size, *i.e.*, number of nodes [12], depending on the parameter depthnodes ('1' for depth, '2' for size, see Sect. 3.2):

- 'fullinit' this is the Full method. In the standard procedure, the new tree receives non terminal (internal) nodes until the initial tree depth (inicmaxlevel parameter) is reached the last depth level is limited to terminal nodes. As a result, trees initialized with this method will be perfectly balanced with all the branches of the same length. If size is used instead of depth, internal nodes are chosen until the size of the new tree is close to the specified size (inicmaxlevel), and only then terminals are chosen. Unlike the standard procedure, the size variation may not be able to create trees with the exact size specified, but only close (never exceeding).
- 'growinit' this is the Grow method. In the standard procedure, each new node is randomly chosen between terminals and non terminals, except nodes at the initial tree depth level, which must be terminals. Trees created with this method may be very unbalanced, with some branches much longer than others, and their depth may be anywhere from 1 to the value of the inicmaxlevel parameter.

If using the size variation, nodes are also chosen randomly, but prior to reaching the size specified in <code>inicmaxlevel</code>, care is taken on the choice on the internal nodes, based on their arity, so as to guarantee the <code>inicmaxlevel</code> will not be exceeded by the respective arguments (which now have to be terminals).

• 'rampedinit' - this is the Ramped Half-and-Half method. In the standard procedure, an equal number of individuals are initialized for each depth between 2 and the initial tree depth value. For each depth level considered, half of the individuals are initialized using the Full method, and the other half using the Grow method. The population of trees resulting from this initialization method is very diverse, with balanced and unbalanced trees of several different depths.

In the size variation, an equal number of individuals are initialized with sizes ranging from 2 to inicmaxlevel. As in the standard procedure, for each size, half of the trees are initialized with the Full method, and the other half with the Grow method.

3.2 Tree depth and size limits

fixedlevel, realmaxlevel, dynamiclevel, inicdynlevel, depthnodes

Trees in GPLAB may be subject to a set of restrictions on depth or size (number of nodes), by setting appropriate parameters. These restrictions are meant to avoid bloat, a phenomenon consisting of an excessive code growth without the corresponding improvement in fitness. The standard way of avoiding bloat is by setting a maximum depth on trees being evolved - whenever a genetic operator produces a tree that breaks this limit, one of its parents enters the new population instead [8].

GPLAB implements this strict limit on depth, as well as a dynamic limit, similar to the first, but with two important differences: it is initially set with a low value; it is increased when needed to accommodate an individual that is deeper than the dynamic limit but is better than any other individual found during the run. Both limits can be used in conjunction. For each new individual produced by a genetic operator there are three possible scenarios:

- The individual does not exceed the dynamic maximum depth it can be used freely because no constraints have been violated.
- The individual is deeper than the dynamic maximum depth, but does not exceed the strict maximum depth stored in realmaxlevel its fitness is measured. If the individual proves to be better than the best individual found so far, the dynamic maximum depth is increased and the new individual is allowed into the population; otherwise, the new individual is rejected and one of its parents enters the population instead.

The individual is deeper than the strict maximum depth stored in real-maxlevel - it is rejected and one of its parents enters the population instead.

The dynamic maximum tree depth technique is a recent technique that has shown to effectively control bloat in two different types of problems (see [11] for details). The parameter dynamiclevel can be used to turn it on (dynamiclevel='1', the default) or off (dynamiclevel='0'). When on, its initial value is determined by the parameter inicdynlevel. This should not be confounded with the maximum depth of the initial random trees, inicmaxlevel (see Sect. 3.1). The strict depth limit can also be turned on (fixedlevel='1') or off (fixedlevel='0'). When on, the strict maximum depth of trees is determined by the parameter realmaxlevel.

Even more recently, two variations on the dynamic limit technique have been introduced: a heavy dynamic limit (dynamiclevel='2'), where the dynamic limit can (unlike the original one) fall back to a lower value in case the new best individual allows it, and the dynamic limit on size (number of nodes), regardless of depth (see [12] for details). The parameter depthnodes is used to switch between depth (depthnodes='1') and size (depthnodes='2') restrictions. Any combination of fixedlevel, dynamiclevel and depthnodes can be used. The default initial values for realmaxlevel and inicdynlevel depend on the setting of depthnodes (see Table 3.2).

The dynamic limits are turned on in the demo functions of the toolbox, and the (original) dynamic limit on depth is even used as default, along with the strict limit, because this combination seems to be very effective in controlling bloat. Nevertheless, the user should keep in mind that they are still experimental techniques.

3.3 Functions and terminals

functions, terminals, numvars, autovars

As any genetic programming algorithm, GPLAB needs functions and terminals to create the population, in this case the parse trees that represent individuals.

Functions GPLAB can use any MATLAB function that verifies closure, plus some protected and logical functions and the if-then-else statement, also available as part of the toolbox. The user indicates which functions the algorithm should use by setting the parameter variable functions. Table 3.3 contains information on the available toolbox functions.

All the functions described in Table 3.3 are used in the plug and play fashion described in Sect. 2.4. The advanced users who want to build and use their own functions only have to implement them as MATLAB functions (and make sure the input arguments can be either scalars or vectors – see MATLAB user's manual) and declare them using one of the toolbox functions (use "help setfunctions" and "help addfunctions" in the MATLAB prompt for usage):

```
params=setfunctions(params,'func1',2,'func2',1);
params=addfunctions(params,'func1',2,'func2',1);
```

setfunctions defines the set of available functions as containing functions 'func1' and 'func2', replacing any other functions previously declared. 'func1' has arity 2 - it needs two input arguments; 'func2' has arity 1. Any number of functions can be declared at one time, by adding more arguments to setfunctions. addfunctions accepts the same arguments but adds the declared functions to the already defined set, keeping the previously declared functions untouched. setfunctions and addfunctions are friendly substitutes to directly setting the parameter variable functions. The declaration of genetic operators is done similarly (see Sect. 3.4).

Some examples of MATLAB functions that verify closure, fit for use with GPLAB:

- plus, minus, times
- sin, cos
- and, or, not, xor
- ceil, floor
- min, max
- eq (equal), gt (greater than), le (less than or equal)

GPLAB also includes some functions for artificial ant problems, namely antif, antprogn2, antprogn3, arities 2, 2, 3 respectively.

Terminals GPLAB can use any constant as a terminal, plus a random number between 0 and 1, generated in runtime, as the function 'rand' with null arity. The declaration of terminals is done similarly to the declaration of functions, by using friendly substitutes to directly setting the parameter variable terminals. For example, to declare the constant '1' and the random number generator as members of the set of terminals (use "help setterminals" in the MATLAB prompt for usage):

```
params=setterminals(params,'rand','1');
```

Unlike in **setfunctions**, there is no need to indicate the arity, which is always null. To add a new terminal to an already declared set of terminals (use "help addterminals" in the MATLAB prompt for usage):

```
params=addterminals(params,'new_terminal');
```

Any number of terminals can be declared or added at one time, by adding more input arguments. The terminals available for artificial ant problems are antright, antleft, antmove.

Table 3.3: Protected and logical functions for use with GPLAB

Protected function	MATLAB function	Input arguments	Output argument ¹
Division	mydivide	a, b	a (if b = 0) $a/b (otherwise)$
Square root	mysqrt	a	$0 \text{ (if } a \le 0)$ sqrt(a) (otherwise)
Power	mypower	a, b	a^b (if a^b is a valid non-complex number) 0 (otherwise)
Natural logarithm	mylog	a	0 (if a = 0) log(abs(a)) (otherwise)
Base 2 logarithm	mylog2	a	0 (if a = 0) log2(abs(a)) (otherwise)
Base 10 logarithm	mylog10	a	0 (if a = 0) log10(abs(a)) (otherwise)
If-then-else statement	myif	a,b,c	eval(c) (if $eval(a) = 0$) eval(b) (otherwise)
Negation of AND	nand	a, b	$\mathtt{not}(\mathtt{and}(a,b))$
Negation of OR	nor	a, b	$\mathtt{not}(\mathtt{or}(a,b))$

 $^{^1{\}rm sqrt,log,log2,log10,abs,eval,not,and,or}$ are MATLAB functions. eval(x) returns the result of evaluating the expression x.

Variables needed to evaluate the fitness cases are also part of the set of available terminals for the algorithm to work with, and these can only be generated (automatically) in the beginning of the run, according to the settings of the parameters numvars and autovars:

- numvars=[] and autovars='0' the parameter numvars is automatically filled with 0 and no variables are generated. This setting is appropriate for artificial ant problems.
- numvars=[] and autovars='1' the parameter numvars is automatically filled with the number of columns of the input data set and these many variables are generated. This setting is appropriate for symbolic regression and parity problems.
- numvars=x customized setting, where x is the number of variables generated, corresponding to the x first columns of the input data set.

3.4 Genetic operators

reproduction, operatornames, operatornparents, operatornchildren

GPLAB may use any number of genetic operators to create new individuals. A proportion of individuals, specified in parameter **reproduction**, may also be copied into the next generation without suffering the action of the operators.

Tree crossover and tree mutation are the genetic operators provided by GPLAB, implemented as follows:

Crossover In tree crossover, random nodes are chosen from both parent trees, and the respective branches are swapped creating two offspring. There is no bias towards choosing internal or terminal nodes as the crossing sites.

Mutation In tree mutation, a random node is chosen from the parent tree and substituted by a new random tree created with the terminals and functions available. This new random tree is created with the Grow initialization method and obeys the size/depth restrictions imposed on the trees created for the initial generation (see Sect. 3.1).

Although these are the only genetic operators provided, the addition of others is straightforward, thanks to the modular structure shown in Fig. 2.1. A new genetic operator is simply a MATLAB function used as a plug and play device to module OPERATOR, and the declaration of its existence to the algorithm is made similarly to the setting of functions and terminals (see Sect. 3.3), with one of the toolbox functions (use "help setoperators" and "help addoperators" in the MATLAB prompt for usage):

```
params=setoperators(params,'operator1',2,2,'operator2',2,1);
params=addoperators(params,'operator1',2,2,'operator2',2,1);
```

The first function defines the set of genetic operators as containing operators 'operator1' and 'operator2', replacing any operator previously declared. 'operator1' needs two parents and produces two children; 'operator2' also needs two parents but produces only one child. Any number of genetic operators can be declared at one time, by adding more arguments to the function. The second function accepts the same arguments but adds the declared operators to the already defined set, keeping the previously declared operators untouched. These functions have the same effect as directly setting the parameter variables operatornames, operatornparents, operatornchildren.

'operator1' and 'operator2' are the names of the new MATLAB functions that implement the new operators. The only rules these functions must follow concern their input and output arguments. Please see functions crossover and mutation for examples on how to correctly build genetic operators. A set of tree manipulation functions is available (use "help <function_name>" in the MATLAB prompt for usage):

- maketree(level, functions, arities, exactlevel, depthnodes) this function returns a new random tree no deeper/bigger than level, using the functions with respective arities. If exactlevel is true, the new tree will be initialized using the Full method; otherwise, it will be initialized using the Grow method (see Sect. 3.1). depthnodes indicates whether restrictions are to be applied in tree depth or tree size (number of nodes)
- tree2str(tree) returns the string that tree represents
- findnode(tree,x) returns the subtree of tree with root on node number x. The nodes are numbered depth-first
- swapnode(tree,x,node) returns the result of swapping node number x in tree for node
- tree2str(tree) returns the translation of tree into a string
- treelevel(tree) returns the depth of tree
- nodes(tree) returns the number of nodes of tree
- intronnodes(tree,params,data,state) returns the number of introns of tree. Needs the variables params, data and state.

Unlike in previous versions of GPLAB, the genetic operators do not need to return offspring that conform to the tree depth/size restrictiona being applied (see Sect. 3.2) - this is now performed afterwards by applying validation (also called filter) functions (see Sect. 3.5).

Of all the fields an individual contains, only origin, parents, tree and str must be filled. id should be left empty ([]) to be filled by the validation functions mentioned above. All the other fields (xsites, fitness, result, testfitness, nodes, introns, level) can also be left empty if not needed by the genetic

operator, because they will be calculated and stored as needed by other procedures. xsites is the exception - as a merely informative field, that may contain information concerning the nodes where the parent trees were split to create the child tree, if left empty it will remain so, as no other other function in the current version of GPLAB uses it.

3.5 Validating new individuals

filters, fixedlevel, dynamiclevel, depthnodes

After a new individual is produced by any of the genetic operators, it must be validated in terms of depth/size before being considered as a candidate for the new population. Several validation functions, or filters, are provided in GPLAB, and others may be built and integrated as plug and play functions (see Sect. 2.4). The filters parameter is simply a list of those functions, by the order in which they should be applied. It should not, however, be set by the user, but instead be automatically set, in the beginning of the run, depending on the parameters fixedlevel, dynamiclevel and depthnodes. Bellow is a list of available filter functions along with the description of their purpose (see Sect. 3.2 for more details):

- 'strictdepth' this filter rejects an individual that is deeper than the strict maximum allowed depth; does nothing otherwise.
- 'strictnodes' this filter rejects an individual that is bigger (contains more nodes) than the strict maximum allowed size; does nothing otherwise.
- 'dyndepth' this filter measures the fitness of an individual that is deeper than the dynamic maximum allowed depth: if the individual is better than the best so far, the dynamic depth is increased and the new individual is accepted; otherwise it is rejected. The filter does nothing if the individual is no deeper than the limit.
- 'dynnodes' the same as the previous one, but considering size (number of nodes) instead of depth.
- 'heavydyndepth' this filter measures the fitness of an individual and checks its depth. If it is deeper than the dynamic maximum allowed depth: if the individual is better than the best so far, or if it is no deeper than the deepest of its parents, the filter increases the dynamic depth if needed and accepts the individual, otherwise rejects it. If the individual is less deep than the dynamic maximum allowed depth: if it is the better than the best so far, the filter accepts it and lowers the dynamic depth, and does nothing otherwise.
- 'heavydynnodes' the same as the previous one, but considering size (number of nodes) instead of depth.

Table 3.4: List of filters for each combination of parameters

Filters list	fixedlevel	dynamiclevel	depthnodes
{ }	0	0	-
$\{$ 'dyndepth' $\}$	0	1	1
$\{$ 'dynnodes' $\}$	0	1	2
$\{ exttt{'heavydyndepth'} \}$	0	2	1
$\{ exttt{'heavydynnodes'} \}$	0	2	2
$\{ ext{'strictdepth'} \}$	1	0	1
$\{$ 'strictnodes' $\}$	1	0	2
$\{$ 'strictdepth','dyndepth' $\}$	1	1	1
<pre>{'strictnodes','dynnodes'}</pre>	1	1	2
<pre>{'strictdepth','heavydyndepth'}</pre>	1	2	1
<pre>{'strictnodes','heavydynnodes'}</pre>	1	2	2

The above filters may reject an individual, accept an individual, or do neither. After passing through all the filters, the individuals that still haven't been rejected or accepted will finally be accepted as candidates for the new population.

Table 3.4 lists the appropriate list of filters for each combination of the 3 depth/size related parameters (fixedlevel, dynamiclevel, depthnodes). Once again, the list of filters is chosen automatically by GPLAB in the beginning of the run.

3.6 Selection for reproduction

sampling, tournamentsize

As shown in Fig. 2.1, genetic operators need parent individuals to produce their children. In GPLAB these parents are selected according to one of four sampling methods, as indicated in the parameter variable sampling:

- 'roulette' this method acts as if a roulette with random pointers is spun, and each individual owns a portion of the roulette that corresponds to its expected number of children (see Sect. 3.7).
- 'sus' this method also relies on the roulette, but the pointers are equally spaced [3].
- 'tournament' this method chooses each parent by randomly drawing a number of individuals from the population and selecting only the best of them.

• 'lexictour' - this method implements lexicographic parsimony pressure [9]. Like in 'tournament', a random number of individuals are chosen from the population and the best of them is chosen. The main difference is, if two individuals are equally fit, the shortest one (the tree with less nodes) is chosen as the best. This technique has shown to effectively control bloat in different types of problems (see [9] for details).

When either of the tournament methods is chosen, the number of individuals participating in each tournament is determined by the parameter variable tournamentsize. Like gengap (see Sect. 3.10), the value of this parameter can represent either the absolute number of individuals (tournamentsize>=1), or a proportion of the population size (otherwise). When the tournament method is chosen and tournamentsize is left blank (tournamentsize=[]), GPLAB sets it with the default value (10% of the population size or 2, which one is larger) in the beginning of the run. If tournamentsize equals 1, the selection of parents is random; if tournamentsize equals the population size, only the best individual in the population is chosen to produce all the offspring. The tournament method does not need to know the expected number of children of each individual, unlike the other two methods.

Alternative sampling methods may be built and easily used in GPLAB, as plug and play devices to module SAMPLING (see Fig. 2.1). All the user has to do is build a new function that implements the sampling method, respecting the input and output arguments, and set the parameter variable sampling with the name of the new function:

params.sampling='new_sampling_method';

The new function must accept as input arguments the current population, parameters and state (vars.pop, vars.params, vars.state), the number of individuals to draw, and a list of identifiers of individuals that must not be drawn. This last input argument is not being used in the current version of GPLAB, but the available sampling procedures contemplate this possibility. The function must output the identifiers of the parents chosen, their indices in the current population, the expected number of children of all individuals in the population, and the normalized fitness of all individuals in the population. The last two output arguments may be left blank ([]) if the sampling procedure does not calculate them. Please see functions roulette, sus and tournament for a prototype.

3.7 Expected number of children

expected

As described in Sect. 3.6, some sampling procedures choose the parents based on their expected number of children, while others only need to know which are better than which. Likewise, the calculation of the expected number of children may use the actual fitness values, or simply their rank in the population. The

parameter variable expected determines with method is used for calculating the expected number of children for each individual. This calculation is performed only if the selection for reproduction so requires. Three different methods are available in GPLAB:

- 'absolute' the expected number of children for each individual is proportional to its absolute fitness value (it is equal to its normalized, or relative, fitness) [7].
- 'rank85' the expected number of children for each individual is based on its rank in the population [2].
- 'rank89' the expected number of children for each individual is based on its rank in the population and on the state of the algorithm (how far it is from the maximum allowed generation). The differentiation between individuals increases in later generations [10].

Alternative methods for calculating the expected number of children may be built and used as plug and play devices to module EXPECTED (see Fig. 2.1), by simply implementing the new method in a MATLAB function and declaring it in the parameter variable expected:

```
params.expected='new_expected_number_of_children_method';
```

The new function must accept as input arguments the current population and state (vars.pop, vars.state), and output the expected number of children of all individuals in the population, and the normalized fitness of all individuals in the population. The last output argument may be left blank ([]) if its calculation is not needed. Please see functions absolute, rank85 and rank89 for a prototype.

3.8 Measuring fitness

files2data,datafilex,datafiley,testdatafilex,testdatafiley usetestdata,calcfitness,precision,lowerisbetter,keepevalssize

When starting a GPLAB run the user is required to indicate the names of the files where the fitness cases are stored. The files should be in a format readily importable to MATLAB, like Tab delimited text. For symbolic regression and parity problems, the first file should contain the input values, and the second the expected - or desired - output value, one row for each fitness case. For artificial ant problems, the first file should contain the food trail, in the form of a binary matrix, and the second file should contain the number of food pellets in it. After importing the data stored in these files to the algorithm's variables, according to the procedure specified in the parameter files2data, GPLAB saves its names with complete path in the parameter variables datafilex and datafiley.

The parameter usetestdata may be used to indicate whether the best individual found so far should have its fitness measured in a different data set (usetestdata=1) or not (usetestdata=0). If yes, this extra measurement will be done in every generation, and the user must provide the names of the two (input and desired output) extra data files, to be stored in testdatafilex and testdatafiley. When restarting a run, the user does not have to provide any file names again.

Two different methods for importing the text files into the algorithm's variables are available in GPLAB (not shown in Fig. 2.1):

- 'xy2inout' for symbolic regression and parity problems.
- 'anttrail' for artificial ant problems.

Accordingly, there are also two methods for calculating fitness in GPLAB, implemented as plug and play functions (see Fig. 2.1):

- 'regfitness' calculates, for each individual, the sum of the absolute difference between the expected output value and the value returned by the individual on all fitness cases. The best individuals are the ones that return values less different than the expected values the ones with a lower fitness. This function should be used with the parameter lowerisbetter set to '1'.
- 'antfitness' calculates, for each individual, the number of food pellets eaten in the artificial ant food trail during 400 time steps the best individuals are the ones who eat more pellets, meaning they have higher fitness. This function should be used with the parameter lowerisbetter set to '0'.

When regfitness is used, all the fitness values stored in the algorithm's variables are rounded to a certain number of decimal places, given by the parameter precision. This is meant to avoid rounding errors that affect the comparison of two different individuals who have the same fitness. For example, in symbolic regression problems, it is common to see individuals with fitness values like 5.9674e-016 and 1.0131e-015. Without using the precision parameter, the first individual would be chosen as the best, even when the second one is smaller, because these two values are not the same - just because of the rounding error, since they are in fact both null. By default, precision is set to 12, but the user can give it any integer number higher that 0.

To use an alternative method for calculating fitness, all the user has to do is build a new function, respecting the input and output arguments, and set the parameter variable calcfitness with the name of the new function:

params.calcfitness='new_calcfitness_method';

The new function must accept as input arguments the string expression of the individual to measure (vars.pop(i).str), the parameters (vars.params), the data variable (vars.data), the terminals (vars.state.terminals) and the varsvals string (see Sect. 4.5) containing all the fitness cases in a format ready for assignment; it must output the fitness value of the individual, the vector

of values returned by the individual on each fitness case, and if necessary the updated state variable. Please see functions regfitness and antfitness for prototypes. The parameter lowerisbetter should be set accordingly.

Calculating fitness may be a time consuming task, and during the evolutionary process the same tree is certainly evaluated more than once. To avoid this, the parameter keepevalssize specifies how many evaluations are kept in memory for future use, in case their results are needed again. Evaluations used less often are the first to be discarded when making room for new ones. If left empty ([]), keepevalssize will be automatically set to the population size. The ideal balance between CPU time and memory is not easy to find, and one must not forget that searching the memory for the results of previous evaluations may also be a time consuming task. Nevertheless, it is almost essential to use this option in runs where the user chooses to measure the amount of introns of the generated trees (see Sect. 3.9), particularly in problems like the artificial ant, where every tree branch is repeated many times throughout the population, and takes the same amount of time steps to evaluate.

3.9 Measuring complexity and diversity

calccomplexity, calcdiversity

During the run it may be useful to gather more information about the evolutionary process, namely the structure, complexity and diversity of the population. When the parameter calccomplexity is turned on (calccomplexity='1'), GPLAB stores information regarding the number of nodes and intron nodes of the trees, depth level and balancing between branches (tree fill rate, see [12]). Obtaining some of this information is extremely time consuming, particularly the number of introns, so it must not be used unless absolutely necessary.

GPLAB may also store information regarding the population diversity. Two different diversity measures are provided ('uniquegen' and 'hamming', use "help uniquegen" and "help hamming" in the MATLAB prompt for details), and the user can add more as plug and play functions (see Sect. 2.4). Several diversity measures may be calculated at the same time, and calcdiversity contains the list of measures to be used (it is a list like the one for graphics, Sect. 6.19). Measuring diversity may be more or less time consuming, depending on the measure(s) chosen.

3.10 Generation gap

gengap

The number of new individuals necessary to create a new GPLAB generation is determined by the parameter variable gengap. Like tournamentsize (see Sect. 3.6), the value of this parameter can represent either the absolute number of individuals (gengap>=1), or a proportion of the population size (otherwise).

When gengap is left blank (gengap=[]) GPLAB sets it with the default value in the beginning of the run.

The default value is the population size, which corresponds to using the algorithm in the generational mode of operation. If gengap is set to a very low value, like 2, it clearly corresponds to a steady-state mode of operation, but there is no frontier between both modes in GPLAB. In fact, gengap may even be set to a value higher than the population size, which corresponds to what may be called a batch mode of operation: many more individuals are produced than the ones needed for the new population, but the SURVIVAL module (see Fig. 2.1) discards the worst of them (independently from the elitism level chosen - see Sect. 3.11).

3.11 Survival

survival

After producing gengap new individuals for the new population (see Sect. 3.10), GPLAB enters the SURVIVAL module (see Fig. 2.1) where, from the current population plus all the new children, a number of individuals is chosen to form the new population. One of four elitism levels may be used, indicated in the parameter variable survival:

- 'replace' the children replace the parent population completely, even if they are worse individuals than their parents. This option is not elitist at all.
- 'keepbest' the best individual from both parents and children is kept for the new population, independently of being a parent or a child. The remaining places in the new population are occupied by children only. If not all children produced can be used in the new population, due to size constraints, the worst are discarded.
- 'halfelitism' half of the new population will be occupied by the best individuals chosen from both parents and children. The remaining places will be occupied by the best children still available.
- 'totalelitism' the best individuals from both parents and children are chosen to fill the new population.

The survival module is in fact elitist, even when the non elitism option is chosen. If GPLAB is operating in batch mode (see Sect. 3.10), the best children are always chosen, and the worst discarded.

3.12 Operator probabilities in runtime

operatorprobstype,adaptwindowsize,numbackgen percentback,adaptinterval,percentchange,minprob

GPLAB implements an automatic adaptation procedure for the genetic operator probabilities of occurrence, based on [5]. This procedure can be turned on by setting the parameter variable operatorprobstype to 'variable', and turned off by setting the same variable with 'fixed'. What follows is a brief description of this procedure, along with the parameters that affect its behavior.

The algorithm keeps track of some information regarding each child produced, like which operator was used and which individuals were the parents. The first children to enter this information repository are also the first to leave it, so only the younger children are tracked. This repository of information is like a moving window on the individuals created, and its capacity, or length, is controlled by the parameter variable adaptwindowsize. Another information stored in this repository for each child is how good its fitness is when compared to the best and worst fitness values of the population preceding it. Each child receives a credit value based on this information, and a percentage of this credit is attributed to its ancestors. The number of back generations receiving credit is indicated in the parameter variable numbackgen, and the percentage of credit that is passed from each generation back to its ancestors is indicated by percentback.

Every adaptinterval individuals, the performance for each genetic operator is calculated by summing the credits of all individuals (currently inside the moving window) created by that operator, and dividing the sum by the number of individuals (currently inside the moving window) created by that operator. Each operator probability value is then adapted to reflect its performance. A percentage of the probability value, percentchange, is replaced by a value proportional to the operator's performance. Operators that have been performing well see their probability values increased; operators that have been producing individuals worse than the population from which they were born see their probability values decreased. Operators that haven't been able to produce any children since the last adaptation will receive a substantial increase of probability, as if their performance was twice as good as the performance of the best operator. This will provide them with a chance to produce children again. The parameter variable minprob can be used to impose a lower limit on each operator's probability of occurrence. The default minprob value is 0.01 divided by the number of genetic operators used.

All the parameter variables described here can be set by the user, but when left blank ([]) automatic parameterization will occur. The adaptation interval, adaptinterval, is set to every generation as defined by the generation gap (see Sect. 3.10); the length of the moving window, adaptwindowsize, is set with numbackgen times the population size, or numbackgen times the generation gap, which one is larger. The remaining default values are the ones indicated in the availableparams file, and can also be consulted in Table 3.2.

3.13 Initial operator probabilities

initialprobstype, initialfixed probs, initial varprobs, small difference

Regardless of the operator probabilities in runtime being variable or fixed, their initial values in the beginning of a run can be set either by the user or subject to an initial adaptation procedure closely related to the one previously described.

To specify the desired initial operator probabilities, one should set the parameter variable initialprobstype to 'fixed' and initialfixedprobs to a list of probability values (following the same order as operatornames - see Sect. 3.4). If initialfixedprobs is left blank ([]) all the probabilities will be set to equal values. To allow the initial adaptation procedure to run one should set initialprobstype to 'variable'. Additionally, and because the initial adaptation procedure also needs initial probability values to start the adaptation, one can set initialvarprobs with a list of probability values. If left blank all the probabilities will be set to equal values.

The initial adaptation procedure creates an initial random population of individuals and runs the algorithm until adaptinterval new individuals have been created. It then adapts the operator probabilities as described in Sect. 3.12, repeats the process (including the creation of a random population) and averages both sets of adapted operator probabilities. With the new operator probabilities set to the average values, the whole process is repeated until the difference between old and new probabilities is no larger than smalldifference. This parameter is initially set with the the maximum change of the operator with minimum probability (percentchange times minprob, divided by the number of genetic operators). It is increased 10% in each iteration of the process, to avoid an excessive wait time for the stabilization of the initial operator probabilities.

3.14 Stop conditions

hits

GPLAB will run until the maximum generation indicated by the user is reached (see Sect. 2.3), or until a stop condition is reached. Stop conditions are defined by setting the parameter variable hits.

One hit is a tuple [f d] where f is the percentage of fitness cases that must obey the stop condition and d is the definition of the stop condition itself, meaning that the result obtained by the best individual in the population must be no lower than the expected result minus d% (of the expected result) and no higher that the expected result plus d%. The default value of hits is [100 0], which means "stop if the best individual produces exact results in all fitness cases". [50 10] would mean "stop if the best individual produces results within minus or plus 10% of the expected results, in at least 50% of the fitness cases".

Several stop conditions can be used, by adding rows to the hits variable. If the two previous stop conditions were to be used concurrently, hits should be set

to [100 0; 50 10]. GPLAB tests each stop condition, starting with the first row, until one is satisfied or all have been tested. It is possible not to use any stop condition (hits=[]), in which case GPLAB will only stop when reaching the maximum number of generations allowed.

3.15 Saving results to file

savetofile, savedir

During a run, GPLAB can save all of the algorithm's variables (vars, see Sect. 2.2) to file periodically, according to the parameter variable savetofile:

- 'never' this setting never saves the results to file.
- 'firstlast' this setting causes the variables of the algorithm to be saved after the initial generation has been created, and after a stop condition, or the maximum generation indicated by the user, is reached.
- 'every10' this setting causes the variables to be saved to file in the first and last generations, as in 'firstlast', plus every 10 generations.
- 'every100' this setting behaves like 'every10', but saves the results every 100 generations, instead of every 10.
- 'always' this setting causes the variables to be saved to file after every new generation created. Disk space may become a problem if this option is often used.

Except for the 'never' option, all the settings will cause GPLAB to request from the user the name of the directory where to save the variables, before the algorithm begins, unless it was already stored in the parameter variable savedir. The new directory is created inside GPLAB's working directory and its complete path stored in savedir. If a directory with the same name already exists, the algorithm will refuse the name given by the user, to avoid the overwriting of files from a previous run. Each file will be named after the current generation.

3.16 Runtime textual output

output

During the run, GPLAB may output more or less textual information concerning the state of the algorithm. The amount is determined by setting the parameter variable output:

• 'silent' - this setting produces the minimum amount of textual output during the run. Only what are considered important messages will be displayed, like the beginning and ending of the algorithm, automatic setting of some parameters, and overriding of settings made by the user.

- 'normal' this setting produces textual additional output during the run of the algorithm, like the identification, fitness, depth and size of the best individual found so far. If the usetestdata parameter is true (see Sect. 3.8), it also shows the test fitness (cross validation in a different data set) of the best individual found so far.
- 'verbose' this setting will produce the same output as 'normal' plus the parameter and state variables lists in the beginning of the run.

3.17 Runtime graphical output

graphics

GPLAB can represent some of the algorithm's state variables graphically, as plots that are updated in runtime, every generation. Additionally, some specialized functions are available for offline use (Sect. 5).

The graphics parameter indicates which of the four different possible plots will be shown in runtime. It is a list of plot names - it can be empty (graphics=), in which case there will be no runtime graphical output, or it can contain either or all of the plots described below. The order of the plot names inside the graphics list is respected when positioning the figures on the screen, beginning on the top right corner of the screen, followed by the bottom right corner, the top left corner, and finally the bottom left corner (the idea is to also keep the textual output visible for as long as possible). Each plot may contain more or less information, depending on other parameter settings:

- {'plotfitness'} Figure 3.1. This plot shows the evolution of the maximum (best of current generation), median, average, and average±std.dev. values of fitness. In bold, it also shows the fitness of the best individual found so far; if the usetestdata parameter is true (see Sect. 3.8), it will also show the evolution of the test fitness (cross validation in a different data set) of the best individual found so far. When the survival parameter is set to other than 'replace' (see Sect. 3.11) the maximum and best so far fitness values are always the same.
- {'plotdiversity'} Figure 3.2. This plot shows the evolution of the population diversity measures indicated in the parameter calcdiversity (see Sect. 3.9). Showing more than one diversity measure at the same time may not be very practical due to differences in the range of possible values.
- {'plotcomplexity'} Figure 3.3. This plot shows the evolution of tree depth and size, and the percentage of introns, during the run. If the calccomplexity parameter is on (see Sect. 3.9), the plot will show the values concerning the best individual found so far and the population average; otherwise, only the values concerning the best so far will be shown. The bold line shows the (dynamic) limit on depth or size, depending on

the parameter depthnodes (see Sect. 3.2). If calcomplexity is on, the mean tree fill rate (see [12]) will also be shown.

• {'plotoperators'} - Figure 3.4. This plots shows the evolution of the operators probabilities (in bold) and (cumulative) frequencies of occurrence. Both the plots and the legends showing the current values are updated every generation, even if the operators probabilities of occurrence are updated more or less often. Also shown are the number of reproductions (see Sect. 3.4) and clonings resulting from failed genetic operators (see Sect. 3.2), of the current generation.

Other examples of possible graphics settings:

- {'plotfitness', 'plotcomplexity'} this setting draws both fitness and complexity plots, on the top right corner and bottom right corner of the screen, respectively.
- {'plotfitness', 'plotdiversity', 'plotoperators'} this draws the fitness, diversity and operators plots, leaving only the bottom left corner of the screen empty.

Every generation the plots are updated with the values of the current generation. The legends of the plots show the last values plotted - they may indicate absolute instead of relative values, whatever seemed to be more useful. When a previously stopped algorithm is run for some additional generations, all the previous history values are drawn, and the plots continued, as if the algorithm was never interrupted.

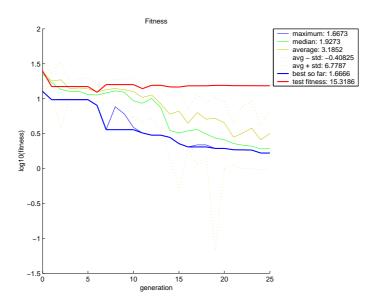


Figure 3.1: Graphical output produced by the 'plotfitness' option in the graphics parameter

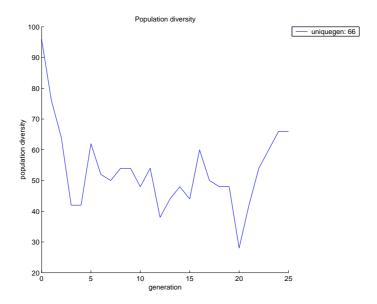


Figure 3.2: Graphical output produced by the 'plotdiversity' option in the $\mathsf{graphics}$ parameter

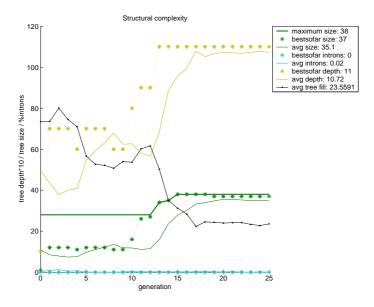


Figure 3.3: Graphical output produced by the 'plotcomplexity' option in the graphics parameter

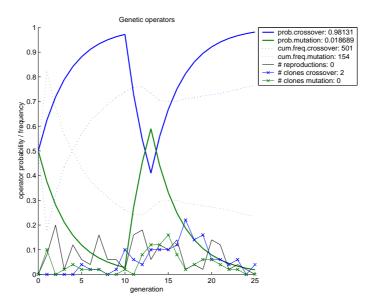


Figure 3.4: Graphical output produced by the 'plotoperators' option in the graphics parameter

Chapter 4

State

The next sections describe aspects related to the state variables used by GPLAB. These variables store information that reflect the current running conditions of the algorithm, as well as the last batch of results produced. Some variables also store historic information concerning the results produced, useful for a posterior analysis (including visualization - see Sect. 5) of the complete run. Although not part of the state structure, the current population of individuals (pop) will also be described as a state variable (see Sect. 2.2). Each subsection concerns one or more state variables. Table 4.1 indicates the location of each state variable in this manual.

Table 4.1: Location of state variables in this manual

State variable	Section	Page
adaptwindow	4.4	41
arity	4.3	41
avgfitness	4.6	42
avgintronshistory	4.9	43
avglevelhistory	4.9	43
avgnodeshistory	4.9	43
${\tt avgtreefillhistory}$	4.9	43
bestfithistory	4.7	42
bestintronshistory	4.7	42
bestlevelhistory	4.7	42
bestnodeshistory	4.7	42
bestsofar	4.7	42
bestsofarhistory	4.7	42
cloninghistory	4.4	41
clonings	4.4	41
depthnodes	4.2	40
diversityhistory	4.9	43

continued on next page

Table 4.1: continued

C+-+:-1-1-	C4:	D
State variable	Section	Page
fithistory	4.6	42
functions	4.3	41
generation	4.8	43
iniclevel	4.2	40
keepevals	4.5	41
lastadaptation	4.4	41
lastid	4.1	39
levelhistory	4.2	40
maxfitness	4.6	42
maxgen	4.8	43
maxlevel	4.2	40
medianfitness	4.6	42
minfitness	4.6	42
operatorfreqs	4.4	41
operatorprobs	4.4	41
opfreqhistory	4.4	41
ophistory	4.4	41
рор	4.1	39
popexpected	4.5	41
popfitness	4.5	41
popnormfitness	4.5	41
popranking	4.5	41
popsize	4.1	39
reproductionhistory	4.4	41
reproductions	4.4	41
stdfitness	4.6	42
terminals	4.3	41
varsvals	4.5	41

4.1 Population

pop,popsize,maxlevel,levelhistory,lastid

The variable that holds the information concerning the current population the algorithm is using in each moment is pop, a one-dimensional array of individuals. Each individual is a structure with fields:

• id - a unique identifier. If an individual survives from one generation to the next, its identifier will not be changed. If two individuals are identical but were generated independently, their identifiers will be different.

- origin the name of the operator that generated this individual, or 'random' if it was randomly generated for the initial population.
- tree the parse tree.
- str the translation of the parse tree into a valid MATLAB expression.
- parents the list of identifiers of the parents that produced this individual, or the empty list ([]) if the individual has a random origin.
- xsites the numbers of the nodes where the genetic operator split the parent trees. This field is merely informative.
- nodes the number of nodes that constitute the parse tree. This field remains empty until needed.
- introns the number of nodes on the parse tree that are considered introns. This field remains empty until needed.
- level the depth of the parse tree. This field remains empty until needed.
- fitness the fitness of the individual in the current data set, data (see Sect. 2.2).
- result the results obtained by the individual in each fitness case of the current data set.
- testfitness the fitness of the individual in a different data set, for cross validation.

The state variable popsize indicates how many individuals are in pop, and lastid contains the last unique identifier generated (and used in the last individual created).

4.2 Tree depth/size

depthnodes, iniclevel, maxlevel, level history

The state variable depthnodes is the same as the parameter with the same name, determining whether restrictions on the shape of the trees allowed into the population are related to depth or size (number of nodes). iniclevel specifies the initial maximum depth/size allowed for the randomly created trees on the initial generation (see Sect. 3.1), and maxlevel indicates the current (updated every generation) maximum depth/size allowed for any parse tree (this is the dynamic depth/size - see Sect. 3.2). levelhistory stores all the past settings of maxlevel, one row per generation.

4.3 Functions and terminals

functions, terminals, arity

The state variables functions and terminals are similar to the parameter variables with the same names (see Sect. 3.3), but they present some important differences. terminals includes not only the constants or null arity functions specified in the parameters, but also all the variables needed to evaluate the individuals in the current data set, generated automatically before the run starts (see Sect. 3.3). functions includes not only the functions specified in the parameters, but also all the terminals included in the state variable terminals. arity contains the second column of the state variable functions, *i.e.*, the number of input arguments of all the functions and terminals used. This seemingly redundant organization of variables increases the efficiency of the algorithm when creating new parse trees.

4.4 Operator probabilities and frequencies

 $operator probs, ophistory, operator freqs, opfreqhistory\\ reproductions, reproduction history, clonings, cloning history\\ adapt window, last adaptation$

The state variable operatorprobs contains the current operator probabilities, one value for each operator, and ophistory contains the past settings of operatorprobs, one row per generation and one column per operator. The cumulative absolute frequency of occurrence of each operator is stored in operatorfreqs, and opfreqhistory stores the past settings of operatorfreqs, one row per generation and one column per operator.

Also stored are the current number of reproductions (see reproduction parameter in Sect. 3.4) and its past settings, reproductionhistory. The current number of clonings resulting from failed genetic operators (see Sect. 3.2) is also stored, one column per operator, as well as its past settings, in cloning-history, one row per generation and one column per operator.

When the operator probabilities are automatically adapted, adaptwindow is the moving window that stores the information about past produced children (see Sect. 3.12) and lastadaptation stores the last identifier generated when the last adaptation occurred.

4.5 Population fitness

 $\verb|popfitness,popnormfitness,popex|| popranking, keepevals, varsvals||$

Although each individual in pop stores its own fitness value, the state variable popfitness also stores a list of the fitness values of all individuals. Depending on the sampling procedure used (see Sect. 3.6), the normalized fitness, expected

number of children, and ranking may also need to be calculated. These are stored in the state variables popnormfitness, popexpected, and popranking.

Evaluating an individual for its fitness may be a time consuming task, so previous evaluations may be stored in memory in case they are needed again (see Sect. 3.8), in the state variable keepevals, with the following fields:

- inds the string of the individual.
- fits the fitness of the individual.
- ress the result of the evaluation in each fitness case.
- used how many times this evaluation has been used.

The memory used by this variable is cleared when the run ends.

Because a great part of the time consumed in the evaluation of individuals consists on the assignment of the fitness cases to the variables (particularly when in presence of several inputs), a string containing all the inputs, ready for assignment, is also kept as the varsvals state variable. This string is constructed every time the fitness cases change (*i.e.*, only once in the beginning of the evolutionary process, in this version of the toolbox).

4.6 Fitness statistics

maxfitness, minfitness, avgfitness, stdfitness, medianfitness, fithistory

Every time a new generation is completed, the maximum, minimum, average, std.dev. and median fitness found in the population are stored in the state variables maxfitness, minfitness, avgfitness, medianfitness, and stdfitness. Additionally, every time these variables are updated, a new row is added to the variable fithistory, which contains five columns, one for each fitness measure, and as many rows as generations completed so far.

4.7 Best individual

bestsofar, bestsofarhistory, bestfithistory bestnodeshistory, bestintronshistory, bestlevelhistory

Ultimately, the result of a genetic programming algorithm is one individual - the best individual found during the whole run. bestsofar is a structure like each individual in pop, and stores the individual with better fitness found since the beginning of the run. bestsofarhistory stores a list of all the individuals that have once been considered the best so far. Each time a new individual updates the variable bestsofar, the same individual is added to bestsofarhistory. bestfithistory, bestnodeshistory, bestintronshistory and bestlevelhistory contain, respectively, the fitness, number of nodes, number of introns, and depth of the parse trees of all the individuals in

bestsofarhistory. bestfithistory may also contain the test fitness (cross validation in a different data set) of the best individual, in a separate column, in case the usetestdata parameter was on (see Sect. 3.8).

4.8 Control

generation, maxgen

GPLAB runs until either a stop condition (Sect. 3.14) or the maximum generation indicated by the user (see Sect. 2.3) is reached. The state variable generation indicates which generation is currently running, and maxgen indicates the maximum number of generations allowed.

4.9 Complexity and diversity statistics/history

 $\label{lem:avgnodeshistory,avgintronshistory,avglevelhistory,} avgtreefill history, diversity history$

When complexity and diversity is measured during the run (see Sect. 3.9), the results are stored in state variables. The average number of tree nodes and intron nodes per generation are kept in the variables avgnodeshistory and avgintronshistory. The average tree depth and fill rate (unbalanced trees have lower fill rates than balanced trees) per generation are kept in the variables avglevelhistory and avgtreefillhistory. Diversity measures per generation are kept in the variable diversityhistory, one column per measure used (see Sect. 3.9).

Chapter 5

Offline graphical output

After completing a run, the user has some specialized functions available for visualization of different aspects of the evolution and results obtained by the algorithm. Some of them provide arguments to define the size of the plot and whether it should be drawn in color or black and white.

5.1 Accuracy versus Complexity

This plot is drawn by the function accuracy_complexity (use "help accuracy_complexity" in the MATLAB prompt for usage). It draws lines representing the evolution of the fitness, the depth, and the number of nodes of all the best individuals found during the run (Fig. 5.1).

5.2 Pareto front

This plot is drawn by the function plotpareto (use "help plotpareto" in the MATLAB prompt for usage). It shows the best fitness found for each tree size, the pareto front (*i.e.*, the set of solutions for which no other solution was found which both has a smaller tree and better fitness), and the sizes and fitnesses of the current population (vars.pop). This plot can easily be coupled as a runtime plot updated in every generation, as it does not request a new figure to be drawn upon. Use the command "figure" before calling this function to see the plot in a different window, if necessary.

5.3 Desired versus Obtained

This plot is drawn by the function desired_obtained (use "help desired_obtained" in the MATLAB prompt for usage). It draws lines representing the

function the algorithm was trying to approximate and several approximations obtained in different generations (Fig. 5.3). Appropriate for symbolic regression problems only.

5.4 Operator Evolution

This plot is drawn by the function operator_evolution (use "help operator_evolution" in the MATLAB prompt for usage). It draws lines representing the evolution of the operator's probabilities during the run (Fig. 5.4). It is not as detailed as the plotoperators drawn in runtime (see Sect. 6.19).

5.5 Tree visualization

This plot is drawn by the function drawtree (use "help drawtree" in the MAT-LAB prompt for usage). It draws a GPLAB tree with the respective node labels. Enlarge the figure if labels are overlapped.

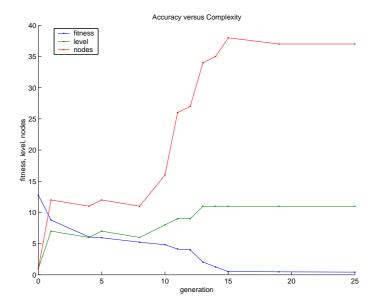


Figure 5.1: Graphical output produced by the function accuracy_complexity

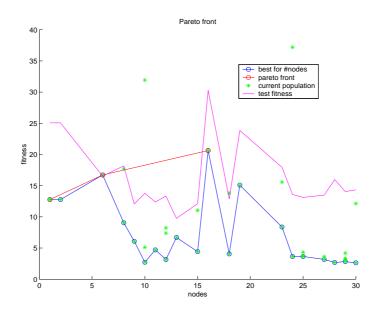


Figure 5.2: Graphical output produced by the function plotpareto

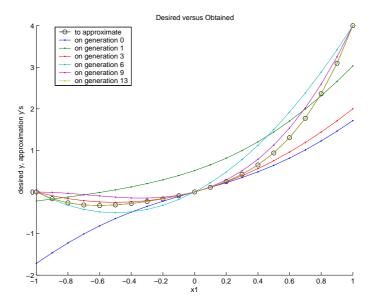


Figure 5.3: Graphical output produced by the function desired_obtained

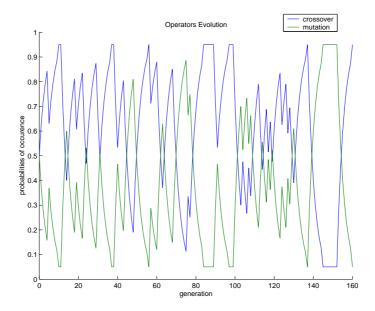


Figure 5.4: Graphical output produced by the function ${\tt operator_evolution}$

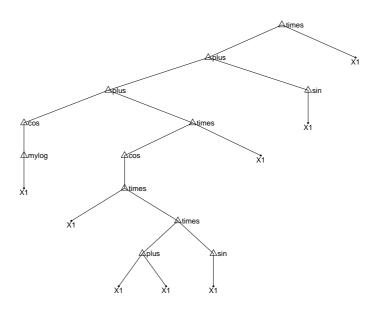


Figure 5.5: Graphical output produced by the function drawtree

Chapter 6

Summary of toolbox functions

The more than one hundred functions provided in the toolbox GPLAB can be divided into different functional groups. What follows is a list of the functions included in each group. The same function may be listed in more than one group. For help on a particular function, use "help <function_name>" in the MATLAB prompt.

6.1 Demonstration functions

- demo
- demoparity
- demoant

6.2 Running the algorithm and testing result

- gplab
- testind

6.3 Parameter and state setting

- setparams
- resetparams
- resetstate
- setoperators

- addoperators
- setfunctions
- addfunctions
- setterminals
- addterminals

6.4 Automatic variable checking

These are called by gplab and should not be called by the user:

- checkvarsparams
- checkvarsstate
- checkvarsdata

6.5 Description of parameter and state variables

- availableparams
- availablestate

6.6 Creation of new generations

- genpop
- generation
- pickoperator
- applyoperator
- pickparents
- applysurvival
- updatestate
- stopcondition

6.7 Creation of new individuals

- initpop
- fullinit
- growinit
- rampedinit
- newind
- maketree

6.8 Filtering of new individuals

- validateinds
- strictdepth
- strictnodes
- dyndepth
- dynnodes
- heavydyndepth
- heavydynnodes

6.9 Protected and logical functions

- mydivide
- mylog
- mylog2
- mylog10
- mysqrt
- mypower
- myif
- kozadivide
- kozasqrt
- nand
- nor

6.10 Artificial ant functions

- demoant
- antmove
- antleft
- antright
- antprogn2
- antprogn3
- \bullet antif
- antfoodahead
- antfitness
- anttrail

6.11 Tree manipulation

- maketree
- treelevel
- nodes
- intronnodes
- tree2str
- findnode
- swapnode

6.12 Data manipulation

- xy2inout
- anttrail
- saveall

6.13 Expected number of children

- absolute
- rank85
- rank89
- calcpopexpected

6.14 Sampling

- roulette
- sus
- tournament
- lexictour
- sampling

6.15 Genetic operators

- crossover
- mutation

6.16 Fitness

- calcfitness
- regfitness
- antfitness
- calcoopfitness

6.17 Diversity measures

- uniquegen
- hamming

6.18 Automatic operator probability adaptation

- isoperator
- setinitialprobs
- automaticoperatorprobs
- moveadaptwindow
- addcredit
- updateoperatorprobs

6.19 Runtime graphical output

These are called by gplab and should not be called by the user:

- graphicsinit
- graphicsstart
- graphicscontinue
- graphicsgenerations

6.20 Offline graphical output

- desired_obtained
- accuracy_complexity
- plotpareto
- operator_evolution
- drawtree

6.21 Utilitarian functions

- explode
- implode
- scale
- normalize
- shuffle
- orderby

- intrand
- countfind
- findfirstindex
- isvalid
- ranking
- fixdec
- uniquenosort

6.22 Text input files

These are used in pairs. $\exp_*.txt$ (exponential) and $\operatorname{quartic}_*.txt$ (quartic polynomial $x^4+x^3+x^2+x$) contain 21 equidistant points in the interval -1 to +1. $\operatorname{parity*bit}_*.txt$ contain all cases. $\operatorname{santafetrail.txt}$ and $\operatorname{santafepellets.txt}$ contain, respectively, the Santa Fe artificial ant trail and the number of food pellets in it.

- exp_x.txt and exp_y.txt
- quartic_x.txt and quartic_y.txt
- parity3bit_x.txt and parity3bit_y.txt
- parity5bit_x.txt and parity5bit_y.txt
- santafetrail.txt and santafepellets.txt

6.23 License file

• license.txt

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