CHAPTER 4 *Genetic Programming Methodology*

4.1 Introduction

Identification of approximation functions in the response surface methodology is fundamental. The function identification problem is to find a functional model in symbolic form that fits a set of experimental data.

In a conventional linear or nonlinear regression, the mathematical problem is reduced to finding the coefficients for a prespecified function. In contrast, if the search process works simultaneously on both the model specification problem (structure of the approximation) and the problem of fitting coefficients (tuning parameters), the technique is called symbolic regression (Koza, 1992).

To obtain the best quality approximation, the formulation of the symbolic regression problem should not specify the size or the structural complexity of the model in advance. Instead, these features of the problem should emerge during the problem-solving process, as part of the solution. With these premises, the search space is clearly too vast for a blind random search. We need to search it in some intelligent and adaptive way.

Evolutionary algorithms (EA) are search techniques based on computer implementations of some of the evolutionary mechanisms found in nature, such as selection, crossover and mutation, in order to solve a problem. Structures do not just happen, but rather evolve and simultaneously sample the search space. EAs are often referred to as global optimization methods because they can effectively explore very large solution spaces without being trapped by local minima. EAs are robust, global and may be applied without problem-specific heuristics. This makes EAs well suited to symbolic regression.

In structural optimization, Xie and Steven (1997) have developed a design method called Evolutionary Structural Optimization (ESO). However, despite the similarities of its name, this technique falls in a different category to EAs. The concept is to gradually remove inefficient material (lightly stressed) from a structure at the same time as it is being designed, so that the structure evolves to its optimum shape.

EAs maintain a population of structures that evolve according to the rules of natural selection and the sexual operators borrowed from natural genetics such as reproduction or crossover. Each individual in the population receives a measure of its fitness in the current environment, i.e. how good the individual is at competing with the rest of the population. At each generation, a new population is created by the process of selecting individuals according to their fitness and breeding them together using the genetic operators. Figure 4.1 shows the evolution system for each generation.

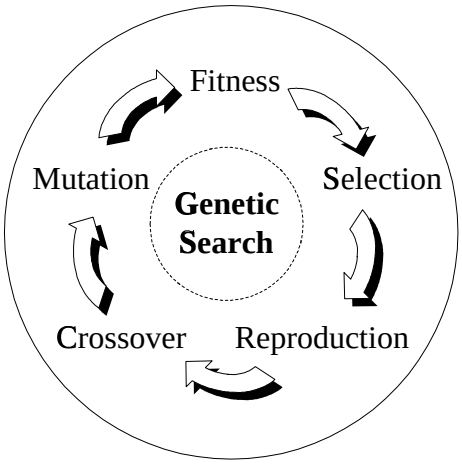


Figure 4.1 Genetic system using EAs

Two types of EAs are considered in this thesis, genetic algorithms and genetic programming. The former is used in parameter optimization, while the latter evolves the structure of the approximation model.

4.2 Genetic Algorithms

A genetic algorithm (Holland, 1975) is a machine learning technique modelled upon the natural process of evolution. It uses a stochastic, directed and highly parallel search based on principles of population genetics that artificially evolve solutions to a given problem.

Genetic algorithms differ from conventional optimization techniques in that they work on a whole population of individual objects of finite length, typically binary strings (chromosomes), that encode candidate solutions using a problem-specific representation scheme. These strings are decoded and evaluated for their fitness, which is a measure of how well each solution solves the problem objective.

GAs are problem-independent. To guide the search in highly nonlinear and multidimensional spaces, GAs do not have any knowledge about the problem domain, except the information provided by the fitness measure and the representation scheme. In practice, GAs are efficient in searching for the optimum solution.

The genetic algorithm attempts to find the best solution to the problem by genetically breeding the population of individuals over a number of generations. Following Darwin's principle of survival of the fittest, strings with higher fitness values have a higher probability of being selected for mating purposes to produce the next generation of candidate solutions.

Selected individuals are reproduced through the application of genetic operators. A string selected for mating is paired with another string and with a certain probability each pair of parents undergo crossover (sexual recombination) and mutation. The strings that result from this process, the children, become members of the next generation of candidate solutions.

In this thesis, a variant of the *generational* GAs is used in which almost the whole population is replaced in each generation, except the elite (see Section 4.2.7), as opposed to *steady-state* selection where only a few individuals are replaced in each generation, usually a small number of the least fit individuals.

This process is repeated for many generations in order to artificially evolve a population of strings that yield a very good solution to a given problem. Theoretical work and practical applications of genetic algorithms (Goldberg, 1989) reveal that

these algorithms are robust and capable of efficiently locating the regions of search spaces that yield highly fit solutions to a nonlinear and multidimensional problem.

One important aspect of GAs is the balance between exploration and exploitation. An efficient algorithm uses two techniques, exploration to investigate new and unknown areas in the search space, and exploitation to make use of the knowledge gained by exploration to reach better positions in the search space. Compared to classical search algorithms, random walk is good at exploration, but has no exploitation. Hill climbing is good at exploitation, but has little exploration.

The main factors that make GA different from traditional methods of search and optimization are:

1. GAs work with a coding of the design variables as opposed to the design variables themselves;
2. GAs work with a population of points as opposed to a single point, thus reducing the risk of getting stuck at local minima;
3. GAs require only the objective function value, not the derivatives. This aspect makes GAs application problem-independent;
4. GAs are a family of probabilistic search methods, not deterministic, making the search highly exploitative.

GAs have been widely applied in design optimization. Hajela (1992) and Hajela and Lin (1992) have implemented genetic search methods in multicriteria design optimization with a mix of continuous, integer and discrete design variables. Dhingra and Lee (1994) have studied single and multiobjective structural

optimization with discrete-continuous variables. The problem of parameter identification with GAs has been studied by Worden and Deacon (1996), Nair and Mujumdar (1996) and Wright (1991).

Other work can be found in the papers by Le Riche and Haftka (1993), Kosigo et al. (1994), Grierson (1995), Parmee (1998), Blachut (1997), Wright and Holden (1998), Keane and Brown (1996),, Mahfouz et al. (1998), Weldali and Saka (1999).

The next sections will describe the main elements of a GA mechanism.

4.2.1 The representation scheme

In most GAs, finite-length binary-coded strings of ones and zeros are used to describe the parameters for each solution. In a multiparameter optimization problem, individual parameter codings are usually concatenated into a complete string (Figure 4.2).

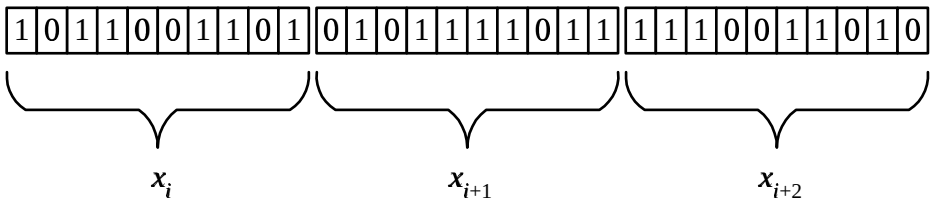


Figure 4.2 Binary representation of a design in a GA

To decode a string, substrings of specified length are extracted successively and mapped to the desired interval in the corresponding solution space.

Let us assume that each variable x_i, i=1...N is coded with a substring of length n and that each position in the substring is defined by q_{ij}, j=1...n, where $q_{ij} \in [0,1]$. A candidate solution to the problem is represented as a string of length $n*N$. To decode

a substring and map it to a particular interval in the solution space, the design variable x_i is defined as follows:

$$x_i = x_i^{min} + \frac{x_i^{max} - x_i^{min}}{2^n - 1} \sum_{j=1}^{n} q_{ij}\, 2^{j-1}, \quad i = 1 \ldots N \tag{4.1}$$

For the 3 design variables example in Figure 4.2 defined in the interval [-100,100] and represented by a 10-bit binary string, Table 4.1 shows the corresponding mapping:

Table 4.1 Mapping of design variables

	Binary string	**Real value**
1	1011001101	40.176
2	0101111011	-25.904
3	1110011010	80.254

Real coded GAs have also been proposed for continuous variable optimization problems (Golberg, 1990, Wright, 1991).

4.2.2 Fitness

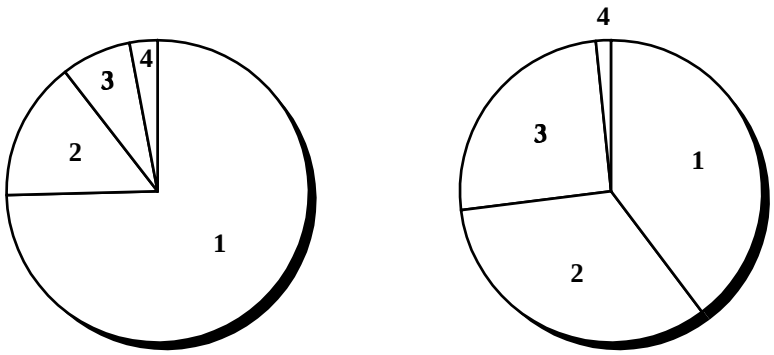
The evolutionary process is driven by the fitness measure. The fitness assigns a value to each fixed-length character string in the population. The nature of the fitness varies with the problem.

For unconstrained maximization problems, the objective function can be used for the formulation of the fitness function. The fitness function can be defined as the

inverse of the objective function or the difference between an upper limit value of the objective function and the objective value for each individual.

For constrained optimal design problems, an exterior penalty function can be adopted to transform a constrained optimization problem into an unconstrained one. Penalty functions can be applied in the exterior or in the interior of the feasible domain. With the exterior penalty function, constraints are applied only when they are violated. Generally, this penalty is proportional to the square of a violation and forces the design to move in the infeasible domain.

The choice of the fitness function is critical because this value is the basis for the selection strategy, discussed later in this chapter. If a few members of the population have a very high fitness in relation to the others, more fit individuals would quickly dominate and result in premature convergence. Figure 4.3 compares two fitness functions $F = 1/f$ and $F = f_u - f$, where f_u is a selected upper limit value for the fitness and f is a function to be minimised. Clearly, the latter example maintains diversity, while the former would direct the search toward a local optimum.



members of population	f_i	(a) $1 / f_i$	(b) $f_u - f_I$ ($f_u = f_{min} + f_{max}$)
1	0.2	5	5
2	1	1	4.2
3	2	0.5	3.2
4	5	0.2	0.2

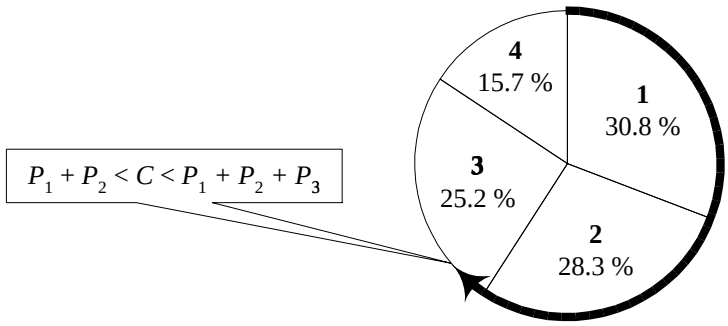
Figure 4.3 Definition of the fitness function for diversity

4.2.3 Selection scheme

The selection operator improves the average quality of the population by giving individuals with higher fitness a higher probability to undertake any genetic operation. An important feature of the selection mechanism is its independence of the representation scheme, as only the fitness is taken into account. The probabilistic feature allocates to every individual a chance of being selected, allowing individuals with poor fitness to be selected occasionally. This mechanism ensures that the

information carried out by unfit strings is not lost prematurely from the population. The GA is not merely a hill-climbing algorithm due to this non-local behaviour.

The most popular of the stochastic selection strategies is fitness proportionate selection, also called biased roulette wheel selection. It can be regarded as allocating pie slices on a roulette wheel, with each slice proportional to a string's fitness. Selection of a string to be a parent can then be viewed as a spin of the wheel, with the winning slice being the one where the spin ends up. Although this is a random procedure, the chance of a string to be selected is directly proportional to its fitness and the least fit individuals will gradually be driven out of the population. For example, if we generate a random number *C* between 0 and 1 and we get the value 0.61, string 3 in Figure 4.4 would be selected.



	F_i	$P_i = F_i / \sum F_i$
1	9.8	0.308
2	9	0.283
3	8	0.252
4	5	0.157
$C = 0.61$ ($0 \leq C < 1$ at random)		

Figure 4.4 Fitness proportionate method

A major drawback of fitness proportionate selection is that, for relatively small populations, early in the search a small number of strings are much fitter than the others and will quickly multiply. There is a high risk of premature convergence of the population characterized by a too high exploitation of highly fit strings at the expense of exploration of other regions of the search space.

A second selection strategy is called tournament selection (Goldberg and Deb, 1991). A subpopulation of individuals is chosen at random. The individual from this subpopulation with the highest fitness wins the tournament. Generally, tournaments are held between two individuals (binary tournament). However, this can be generalised to an arbitrary group whose size is called the tournament *size*. This algorithm can be implemented efficiently as no sorting of the population is required. More important, it guarantees diversity of the population. The most important feature of this selection scheme is that it does not use the value of the fitness function. It is only necessary to determine whether an individual is fitter than any other or not.

Other selection schemes and their comparative analysis have been reviewed by (Goldberg and Deb, 1991).

4.2.4 Crossover

The crossover operator is responsible for combining good information from two strings and for testing new points in the search space. The two offsprings are composed entirely of the genetic material from their two parents. By recombining randomly certain effective parts of a character string, there is a good chance of

obtaining an even more fit string and making progress towards solving the optimization problem.

Several ways of performing crossover can be used. The simplest but very effective is the one-point crossover (Goldberg, 1989). Two individual strings are selected at random from the population. Next, a crossover point is selected at random along the string length, and two new strings are generated by exchanging the substrings that come after the crossover point in both parents. The mechanism is illustrated in Figure 4.5.

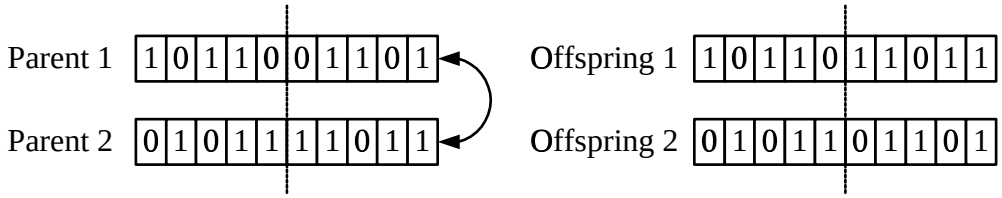


Figure 4.5 GA Crossover

A more general case is the multipoint crossover (De Jong, 1975) in which parts of the information from the two parents are swapped among more string segments. An example is the two-point crossover, where two crossover points are selected at random and the substrings lying in between the points are swapped.

Uniform crossover (Syswerda, 1991) is the method of choice in this thesis. Each bit of the offspring is created by copying the corresponding bit from one or the other parent selected at random with equal probability, as shown in Figure 4.6.

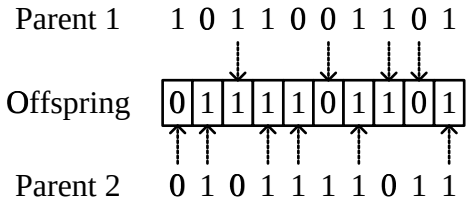


Figure 4.6 GA Uniform crossover

Uniform crossover has the advantage that the ordering of bits is entirely irrelevant because there is no linkage between adjacent bits. Multipoint crossover takes half of the material from each parent in alternation, while uniform crossover decides independently which parent to choose. When the population has largely converged, the exchange between two similar parents leads to a very similar offspring. This is less likely to happen with uniform crossover particularly with small population sizes, and so, gives more robust performance.

4.2.5 Mutation

Mutation prevents the population from premature convergence or from having multiple copies of the same string. This feature refers to the phenomenon in which the GA loses population diversity because an individual that does not represent the global optimum becomes dominant. In such cases the algorithm would be unable to explore the possibility of a better solution.

Mutation consists of the random alteration of a string with low probability. It is implemented by randomly selecting a string location and changing its value from 0 to 1 or vice versa, as shown in Figure 4.7.

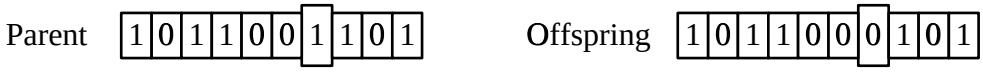


Figure 4.7 GA Mutation

4.2.6 Mathematical foundation

GA implicitly processes in parallel a large amount of useful information concerning schemata (Holland, 1975). A schema is a set of points from the search space with certain specified similarities. The schema is described by a string with a certain alphabet (0 and 1 if the alphabet is binary) and a "don't care" symbol denoted by an asterisk. For example, 1**0 represents the set of all 4-bit strings that begin with 1 and end with 0.

The GA creates individual strings in such a way that each schema can be expected to be represented in proportion to the ratio of its *schema fitness* to the *average population fitness* (Koza et al, 1999). The *schema fitness* is the average of the fitness of all the points from the search space contained in the population and contained in the schema. The *average population fitness* is the average of the fitness of all the points from the search space contained in the population. The *schema theorem* (Holland, 1975) explains that an individual's high fitness is due to the fact that it contains good schemata. The optimum way to explore the search space is to allocate *reproductive trials* to individuals in proportion to their fitness relative to the rest of the population. In this way, good schemata receive exponentially increasing number of trials in successive generations.

According to the *building block hypothesis* (Golberg, 1989), the power of GA is in its ability to find good *building blocks*. These are schemata of short defining lengths consisting of bits working well together that tend to lead to improved performance when incorporated into an individual.

4.2.7 Implementation of the GA

In this thesis, GAs are used to find an initial guess which serves as input to a gradient-based optimization algorithm (Madsen and Hegelund, 1991) in order to obtain the tuning parameters $\boldsymbol{a}$ in (3.2) or (3.3) of the approximate model, combined with a nonlinear regression algorithm. Generally, GAs work well even if the space to be searched is large, not smooth or not well understood, or if the fitness function is noisy and, in addition, when finding a good solution (not necessarily the exact global optimum) is sufficient.

Figure 4.8 shows a flowchart of the implementation of the GA used in this thesis. Assuming we have n tuning parameters encoded with l-bit strings, GA works as follows:

1) Start with a randomly generated population of individuals of length $n*l$-bits.
2) Iteratively perform the following steps on the population:
    a) calculate the fitness of each chromosome by least-squares,
    b) sort the population,
    c) create a new population:
        i) In the *reproduction* stage a strategy must be adopted as to which strings should die: either to kill the individuals with fitness below the average or, alternatively, to kill a small percentage of the individuals with the worst fitness. The second approach is preferred in this thesis as it provides more diversity.

ii) Calculate the *elite* (De Jong, 1975) according to input parameter P_e, which is an additional operator that transfers unchanged a relatively small number of the fittest individuals to the next generation. Such individuals can be lost if they are not selected to reproduce or if they are destroyed by crossover or mutation. In this thesis, *P*e=20% of the population has been used.

iii) Fill up the population with the surviving strings according to tournament selection of size 2.

iv) *S*elect a pair of individuals from the current population. The same string can be selected more than once to become a parent. Recombine substrings using the uniform *crossover*. Two new offsprings are inserted into the new population.

v) With the probability P_m taken as 0.01 in this thesis, *mutate* a randomly selected string at a randomly selected point.

3) Check the termination criterion. If not satisfied, perform the next iteration.

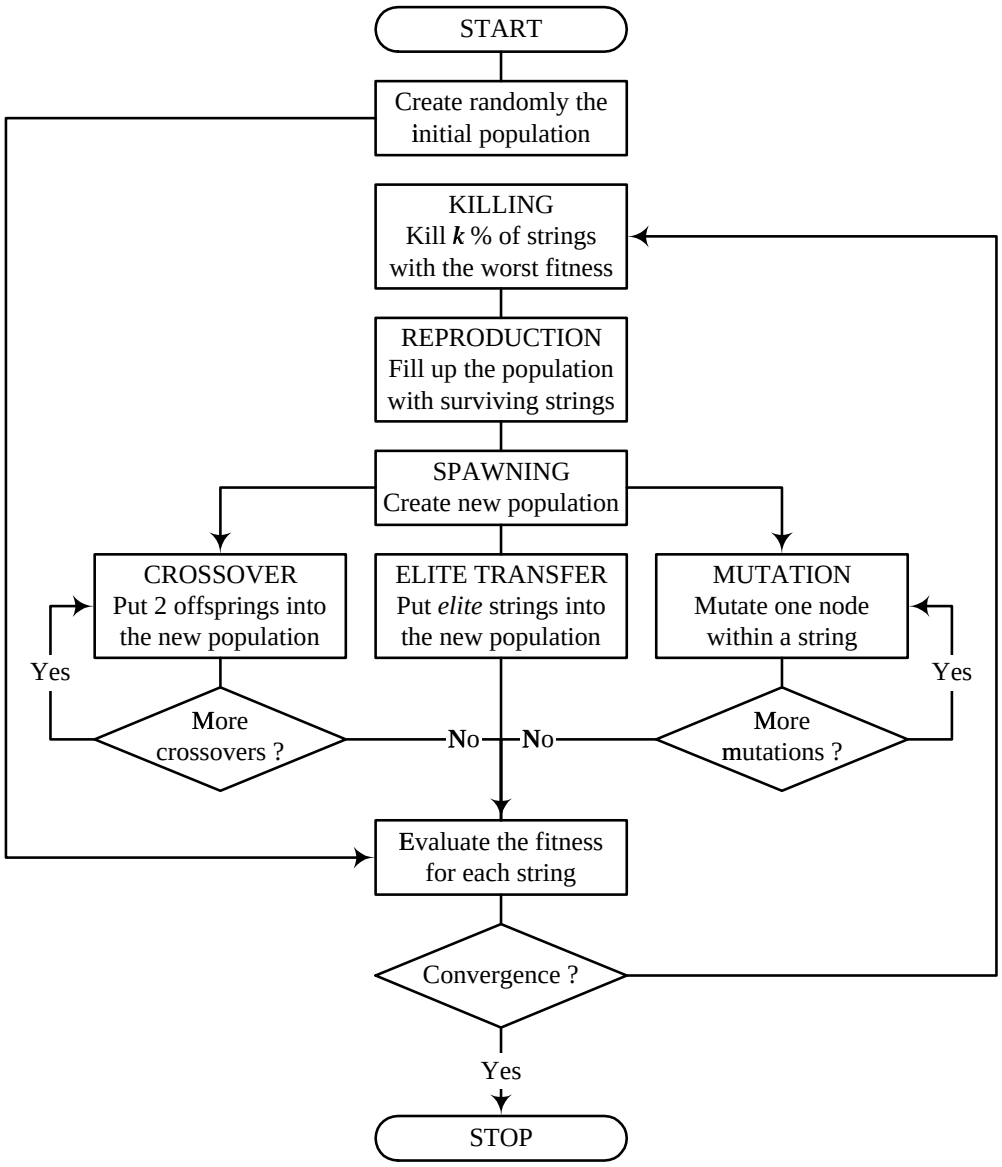


Figure 4.8 Flowchart of the GA

Each iteration of this process is called a *generation*. The entire set of generations is called a *run*. At the end of the run, there are one or more highly fit strings in the population. Generally, it is necessary to make multiple independent runs of a GA to obtain a result that can be considered successful for a given problem.

In this thesis, GA only performs 1 run with 30 generations due to computing time constraints and the fact that the solution is only used as a starting guess for the gradient-based optimization technique.

A limitation in the application of GAs is the fixed-length representation scheme and the need to encode the variables. These two aspects do not provide a convenient way of representing general computational structures like a symbolic regression model. In addition, GAs do not have dynamic variability as they require the string length to be defined in advance. To deal with this problem, Koza (1992) implemented an extension of the genetic model of GAs with parse trees called *genetic programming*.

4.3 Genetic Programming

Genetic Programming (GP) is a generalization and an extension of GAs. The same description of GA given in Section 4.2 is applicable to GP, so only new concepts and differences with respect to GAs will be discussed in this section.

GP combines a high-level symbolic representation with the search efficiency of the GA. Its basis is the same Darwinian concept of survival of the fittest. The innovation of the GP is the use of more complex structures. While a GA uses a string of numbers to represent the solution, the GP creates computer programs with a tree structure. In the case of design optimization, a program represents an empirical model to be used for approximation of response functions in the original optimization problem.

These randomly generated programs are general and hierarchical, varying in size and shape. GP's main goal is to solve a problem by searching highly fit computer programs in the space of all possible programs that solve the problem. This aspect is the key to finding near global solutions by keeping many solutions that may potentially be close to minima (local or global). The creation of the initial population is a blind random search of the space defined by the problem. In contrast to a GA, the output of the GP is a program, whereas the output of a GA is a quantity.

The main advantages of using GP for symbolic regression are that the size and shape of the approximation function do not need to be specified in advance and that the problem specific knowledge can be included in the search process through the use of the appropriate mathematical functions.

The term symbolic regression in genetic programming (Koza, 1992) stands for the process of discovering both the functional form of the approximation and all of its tuning parameters. Unfortunately, a weakness of GP is the difficulty of finding the numerical constants due to their representation as tree nodes and the fact that the genetic operators only affect the structure of the tree. Although GP can generate constants, dividing for example one variable by itself, the process becomes very inefficient (Evett and Fernandez, 1998). For this reason, in this thesis the tuning parameters are not modified by the evolutionary process but identified by a nonlinear least-squares surface fitting using an optimization method.

The evolutionary process in GP proceeds in a similar way to standard GA. GP starts with a population of randomly generated programs built from a library of available mathematical functions. These trees are assigned a fitness value and evolve

by means of the genetic operators of selection, crossover and mutation following the Darwinian principle of survival and reproduction of the fittest, similar to GAs.

GP has been applied to systems identification by Watson and Parmee (1996), McKay et al. (1996) and Gray et al. (1996) among others. Other applications can be in found in Kinnear (1994).

4.3.1 Representation scheme

The structures in GP are computer programs represented as expression trees. They are hierarchical and can dynamically change the size and shape during the evolution process. A typical program representing the expression $(x_1/x_2+x_3)^2$ is shown in Figure 4.9.

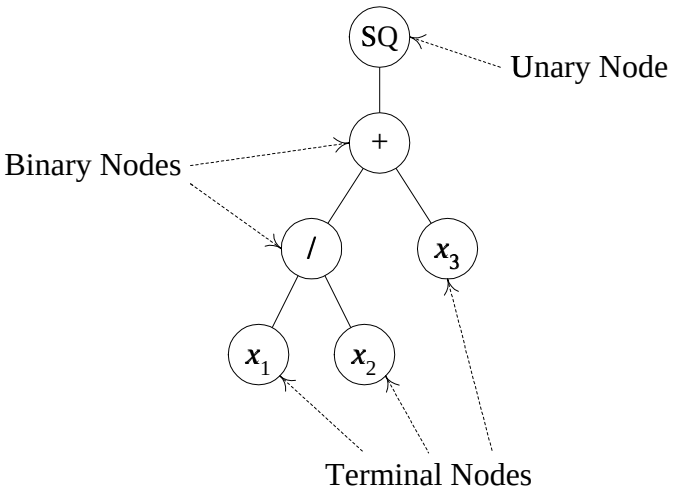


Figure 4.9 Typical tree structure for $\left(\frac{x_1}{x_2} + x_3\right)^2$

The programs are composed of nodes that are elements from a *terminal set* and a *functional set*, as described in Table 4.2.

Table 4.2. Definition of the terminal and functional set

Terminal Set	Design variables: x_1 , x_2 , ..., x_N
Functional Set	Mathematical operators that generate the regression model: { +, *, /, x^y, etc. }

The functional set can be subdivided into *binary nodes*, which take any two arguments (like addition), and *unary nodes*, which take one argument, e.g. a square root. The solution domain is created by the recursive composition of elements from the functional set for any internal node and from the terminal set for any external nodes (leaves).

All the functions and terminals must be compatible in order to faultlessly pass information between each other (*closure property*). The *sufficiency property* requires the identification of functions and terminals so that their combination can yield a valid approximation in the solution domain, e.g. including sufficient number of variables in the terminal set to describe the optimization problem.

An expression tree can evolve a large number of model structures using a relatively small functional set. As a starting point, basic operations like +, *, -, / are sufficient. However, the general idea is to take into account the mathematical knowledge of the engineering process and make the search more efficient. For example, although a sine function can be approximated by a power series involving only addition and multiplication operations, it is better to include sine in the functional set. Also, some functions may be added to the function set because they might facilitate a solution. This is the reason why in this thesis square and square

root functions are included in the functional set, even though the same result could be obtain with multiplication and power respectively at a more expensive computational cost.

Table 4.3 summarizes mathematical operators that are useful for a large range of problems. If the functional set contains irrelevant operators or if the terminal set contains more variables than necessary to define the problem, GP will usually be able to find a solution, although the performance of the search will be degraded.

Table 4.3 The functional set

Label	Description	Operation
+	Addition	$x_1 + x_2$
-	Subtraction	$x_1 - x_2$
*	Multiplication	$x_1 \times x_2$
/	Division	x_1 / x_2 if $x_2 = 0$ assign penalty
SQ	Square	x_1^2
SQRT	Square root	$\sqrt{x_1}$ if $x_1 < 0$ assign penalty
EXP	Exponential	e^{x_1}
SIN	Sine	$\sin(x_1)$
COS	Cosine	$\cos(x_1)$

An important aspect of the functional set is the handling of mathematical exceptions during fitness evaluation. Illegal mathematical operations like division by

zero or run-time overflow and underflow errors need to be removed in order to obtain valid expressions. In this thesis, infeasible expression trees are assigned the worst possible fitness in the population as a penalty.

The evolution of the programs is performed through the action of the genetic operators and the evaluation of the fitness function.

4.3.2 Genetic operators

Model structures evolve through the action of three basic genetic operators: reproduction, crossover and mutation.

In the *reproduction* stage, a strategy must be adopted as to which programs should die. In this implementation, a small percentage of trees with worst fitness are killed. The population is then filled with the surviving trees according to a binary tournament selection.

Crossover (Figure 4.10) is implemented as follows:

- select two trees from the whole population,
- within each of these trees, randomly select one node,
- swap the subtrees under the selected nodes, thus generating two offsprings belonging to the new population.

After crossover, a small number of random nodes are changed through *Mutation* (Figure 4.11):

- randomly select one node within a randomly selected tree,

- replace this node with another one from the same set (a function replaces a function and a terminal replaces a terminal) except by itself,

An additional operator, *elite transfer*, is used to allow a relatively small number of the fittest programs, called the elite, to be transferred unchanged to a next generation, in order to keep the best solutions found so far. As a result, a new population of trees of the same size as the original one is created, but it has a higher average fitness value.

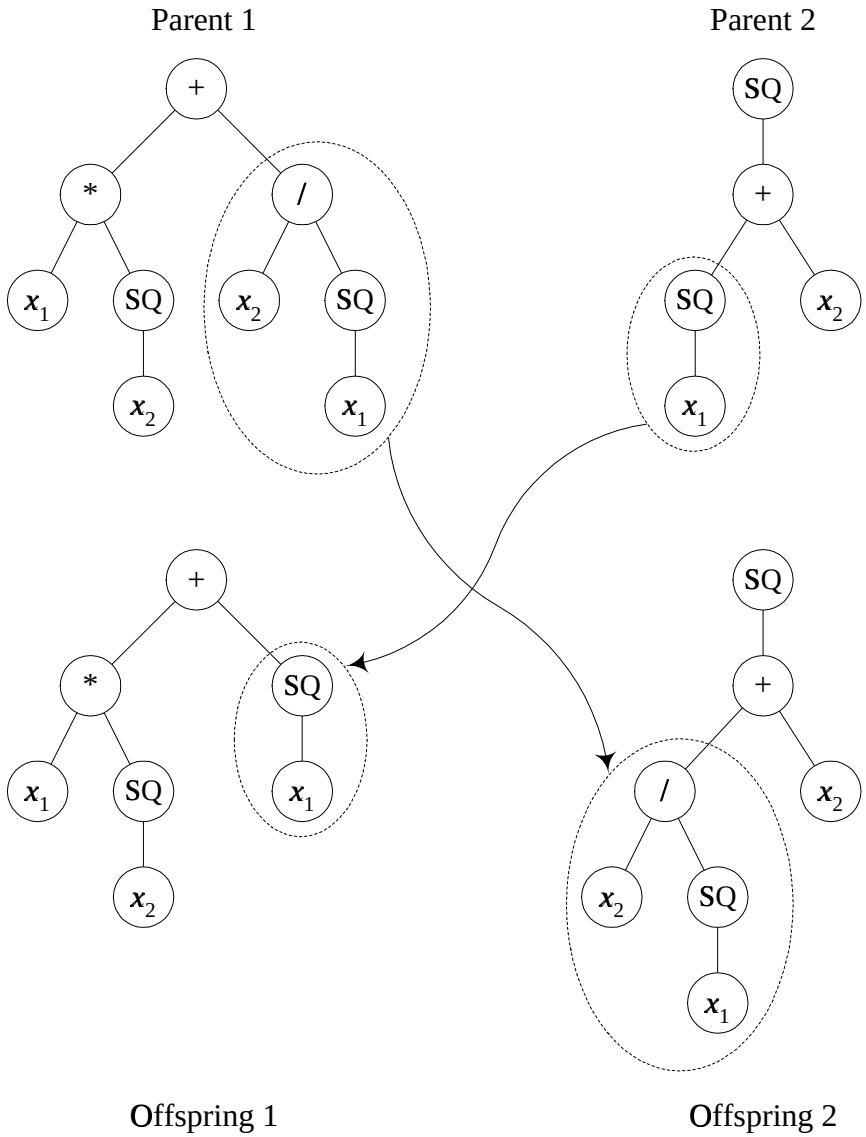


Figure 4.10 GP Crossover

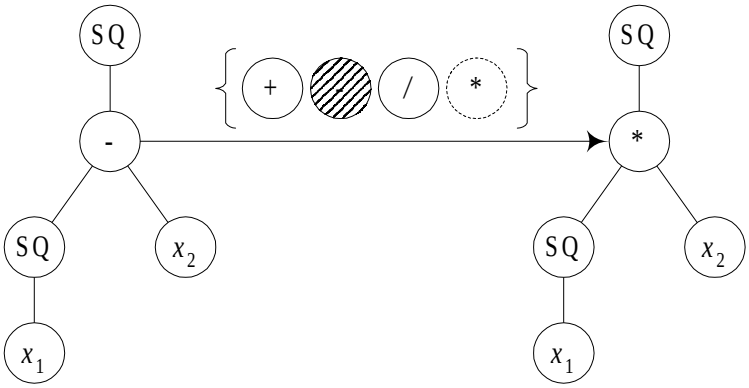


Figure 4.11 GP mutation

4.3.3 Fitness function

When selecting randomly a tree to perform any genetic operation, the tournament selection method is used here. This method specifies the probability of selection on the basis of the fitness of the solution.

The fitness of a solution shall reflect:

(*i*) The quality of approximation of the experimental data by a current expression represented by a tree.

(*ii*) The length of the tree in order to obtain more compact expressions.

In problems of empirical model building, the most obvious choice for the estimation of the quality of the model is the sum of squares of the difference between the simplified model output and the results of runs of the original model over some chosen plan (design) of experiments.

Generally, there can be two sources of error: incorrect structure and inaccurate tuning parameters. In order to separate these, the measure of quality $Q(S_i)$ is only calculated for the tuned approximation, as described in Section 4.3.5.

In a dimensionless form this measure of quality of the solution can be presented as follows:

$$Q(S_i) = \frac{\sum_{p=1}^{P} \left(F_p - \tilde{F}_p\right)^2}{\sum_{p=1}^{P} {F_p}^2} \tag{4.2}$$

or as (3.3) with equal weights when derivatives are used.

If $Q(S_i)$ is the measure of quality of the solution S_i, Q_u is an upper limit value of the quality for all N_t members of the population, ntp_i is the number of tuning parameters contained in the solution S_i and c is a coefficient penalizing the excessive length of the expression, the fitness function $\Phi(S_i)$ can be expressed in the following form:

$$\Phi(S_i) = Q_u - Q(S_i) - c * {ntp_i}^2 \quad \rightarrow \quad \max \tag{4.3}$$

Programs with greater fitness values $\Phi(S_i)$ have a greater chance of being selected in a subsequent genetic action. Highly fit programs live and reproduce, and less fit programs die.

In terms of computer implementation of the GP paradigm, it is more convenient and more efficient to make the best value of the fitness 0, i.e to solve a minimization problem. For this reason, the definition of the fitness used in the computer program developed in this thesis is the following:

$$\Phi(S_i) \;=\; Q(S_i) \;+\; c * ntp_i{}^2 \qquad \rightarrow \qquad \min \tag{4.4}$$

Another possible choice is the statistical concept of correlation, which determines and quantifies whether a relationship between two data sets exists. This definition was used for the identification of industrial processes (McKay et al. 1996).

To evaluate the goodness-of-fit, the standard root mean square (RMS) error will be used in this thesis according to the following expression:

$$\text{RMS} \;=\; \sqrt{\frac{\sum_{p=1}^{P} \left(F_p - \tilde{F}_p\right)^2}{P}} \tag{4.5}$$

4.3.4 Allocation of tuning parameters

Traditional implementations use GP to generate constants that are optimized by a nonlinear regression algorithm. In this thesis, the algorithm implements two different tasks. First, GP finds an appropriate symbolic model structure (without constant creation). Second, an automatic procedure allocates tuning parameters within the regression model in a symbolic form as shown in Figure 4.12, and optimizes the symbolic parameters with a gradient-based optimization method (Madsen and Hegelund, 1991).

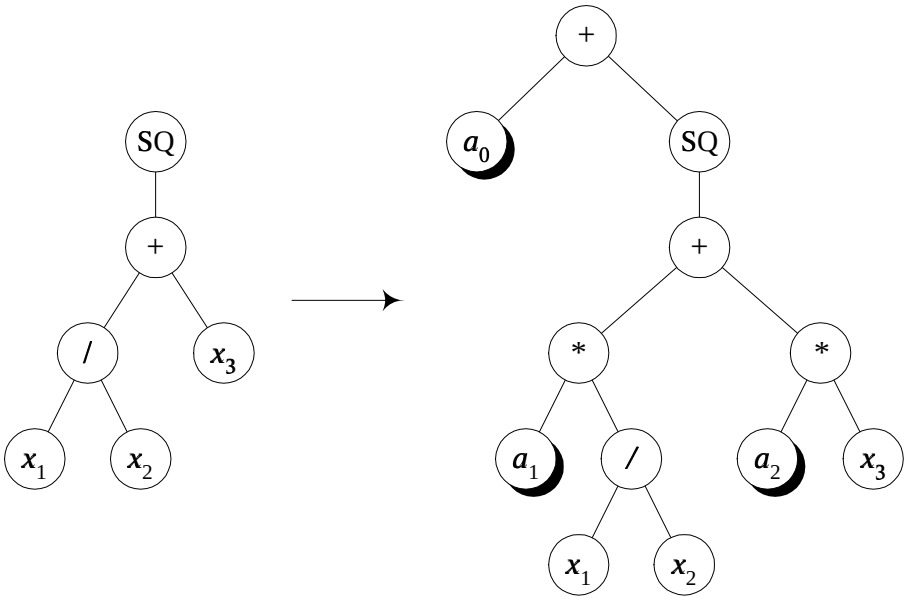


Figure 4.12 Symbolic allocation of parameters for $a_0 + \left(a_1 \frac{x_1}{x_2} + a_2 \; x_3 \right)^2$

This implementation has the advantages that the coefficients are optimized in the whole range of a prespecified interval, and subsequently, the complexity of the expression is reduced. In contrast, in Koza's implementation (1992), only a few constants to be used as coefficients were defined in the terminal set, leading to much bigger expressions than that of the minimal solution.

The allocation of tuning parameters ***a*** to an individual tree follows basic algebraic rules. Going through the tree downwards, tuning parameters are allocated to a subtree depending on the type of the current node and the structure of the subtree. The different cases are described as follows (according to Figure 4.13):

1. Current node is of type binary:

   - Multiplication and division operations only require one tuning parameter, e.g.

$$\tilde{F} = x_1 * x_2 \quad \Rightarrow \quad \tilde{F}(\boldsymbol{a}) = a_1 * x_1 * x_2$$

   - All other operations require two tuning parameters, e.g.

$$\tilde{F} = x_1 + x_2 \quad \Rightarrow \quad \tilde{F}(\boldsymbol{a}) = a_1 * x_1 + a_2 * x_2$$

$$\tilde{F} = x_1 \wedge x_2 \quad \Rightarrow \quad \tilde{F}(\boldsymbol{a}) = (a_1 * x_1) \wedge (a_2 * x_2)$$

   - When $\tilde{F}$ is a combination of the previous two approaches, tuning parameters are only applied to operations different from multiplication and division, e.g.

$$\tilde{F} = x_1 * (x_2 \,/\, x_3 + x_4) \quad \Rightarrow \quad \tilde{F}(\boldsymbol{a}) = x_1 * (a_1 * x_2 \,/\, x_3 + a_2 * x_4)$$

$$\tilde{F} = (x_1 + x_2) \wedge (x_3 * x_4) \quad \Rightarrow \quad \tilde{F}(\boldsymbol{a}) = (a_1 * x_1 + a_2 * x_2) \wedge (x_3 * x_4)$$

2. Current node is of type unary:

   - Ignore

3. Current node is of type variable (terminal node):

   - One tuning parameter is inserted, e.g.

$$\tilde{F} = (x_1)^2 \quad \Rightarrow \quad \tilde{F}(\boldsymbol{a}) = (a_1 * x_1)^2$$

4. Free parameter:

   - One free parameter is added to the expression, e.g.

$$\tilde{F}(\boldsymbol{a}) = a_1 * x_1 \quad \Rightarrow \quad \tilde{F}(\boldsymbol{a}) = a_1 * x_1 + a_0$$

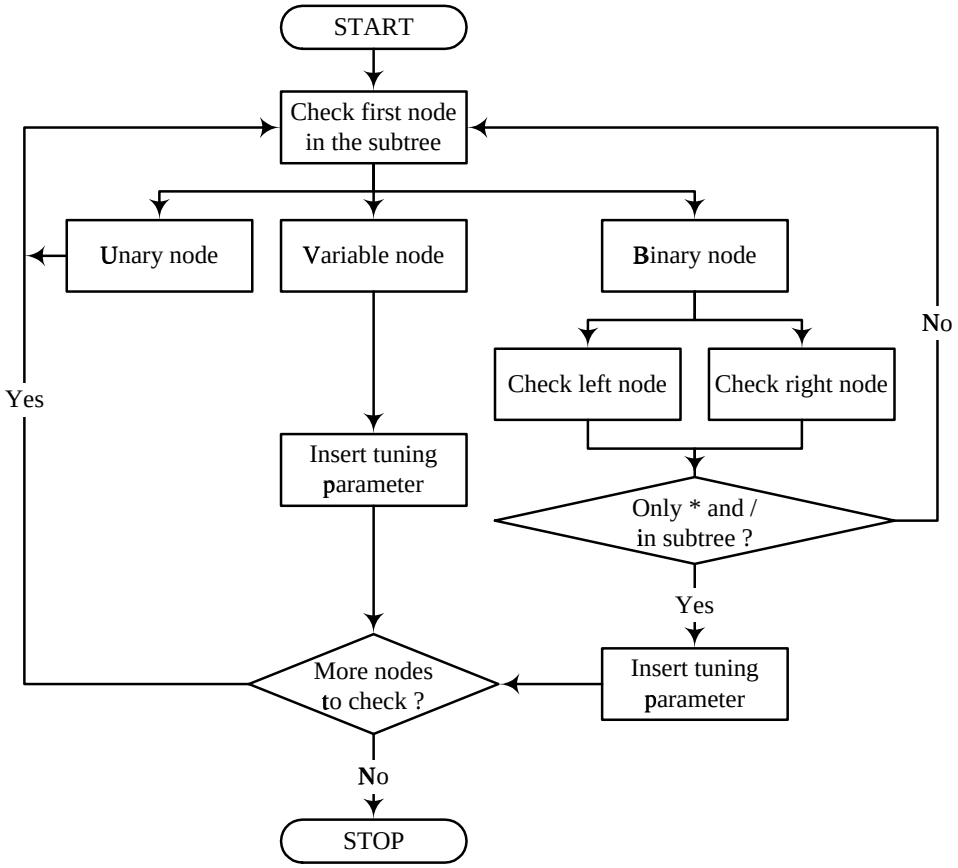


Figure 4.13 Flowchart for the symbolic allocation of tuning parameters

4.3.5 Tuning of an approximation function

The representation of the tuning parameters is a binary multiparameter coding mapped to the interval [-100, 100] with a 10-digit binary string, defining a precision of $100 - (-100) / (2^{10} - 1) = 0.196$ for each tuning parameter.

The objective function is defined here as the sum of squares of the difference between the simplified model output with the current guess, and the results of runs of the original model over some chosen plan of experiments, as defined in (3.2) with equal weights. If, in addition to the function values, the design sensitivity information is available, function (3.3) should be minimised instead.

The main parameters controlling the GA are the population size and the maximum number of generations to be run (termination criterion). The present algorithm works with a population size of 30 individuals and a number of generations of 30. These values are abnormally low as compared to recommendations in the literature (Mahfouz, 1999). Generally, the greater the number of populations and generations (hundreds, thousands or more) the higher the probability of finding the global optimum. The only limitations here are the execution time and the computing resources available. In the present case, GA is not the main mechanism for finding the tuning parameters, this is why the values are simply a compromise between low computing time and good quality of the initial guess for the further gradient-based optimization.

4.3.6 Implementation of GP

In this thesis, GP has been used to find the structure of the approximation model that will be used in the response surface methodology. The identification of the tuning parameters is achieved by a gradient-based optimization method in conjunction with the initial guess provided by the GA.

The termination criterion for the minimization problem (4.4) is that the fitness of the best individual found in the actual generation has a small value, typically of the order of 1.0E-19. In certain cases, if no individual in the population reaches a successful fitness, the run can terminate after a prespecified maximum number of generations. As usual no solution is 100% correct, there is a need for postprocessing the output in order to get a better understanding of the process. The purpose is to get

rid of those terms in the expression that give a null or tiny contribution, for example when the same value is added and subtracted. It is then suggested to run the problem several times in order to identify, by comparison, the most likely components.

The two major control parameters in GP are the population size and the maximum number of generations to be run when no individual reaches the termination criterion. These two parameters depend on the difficulty of the problem to be solved. Generally, populations of 500 or more trees give better chances of finding a global optimum. For a small number of design variables, a starting population of 100 has proven to be sufficient. The maximum number of generations has been chosen as 1000.

Figure 4.14 shows a flowchart of the GP methodology. The algorithm works as follows:

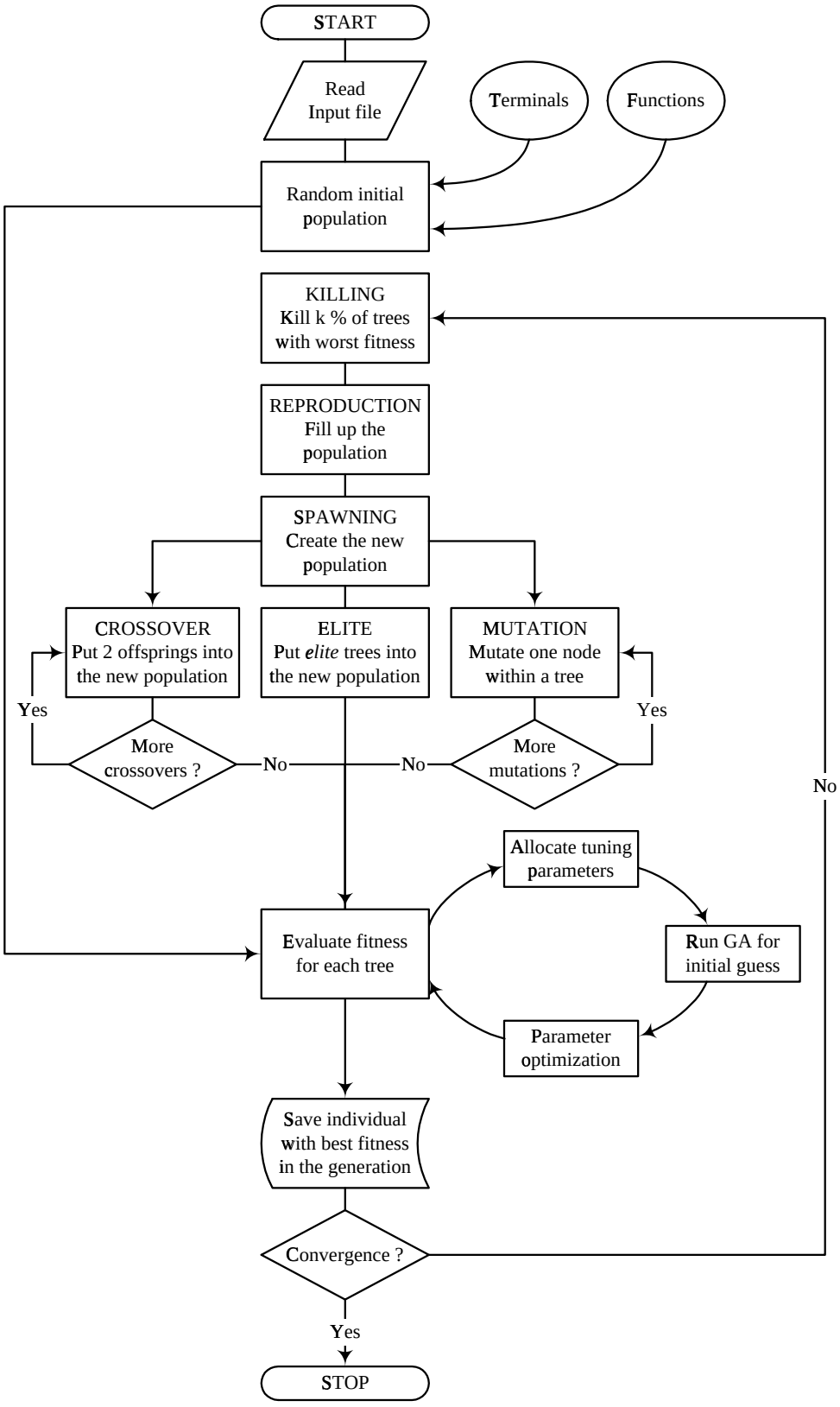


Figure 4.14 Flowchart of the GP methodology

1) Start with a randomly generated population of trees composed of elements from the functional set and the terminal set. The root node of every tree must be restricted to a function. If a terminal is chosen, that node is an endpoint of the tree. To limit the complexity of the initial trees, an input parameter defines the maximum depth of the tree. In subsequent generations, the length of the tree is limited by the maximum allowed number of tuning parameters allocated in the tree.

2) Iteratively perform the following steps on the population until the termination criterion has been satisfied:

   a) Calculate the fitness of each tree according to (4.4). Prior to fitness evaluation, tuning parameters are allocated in the tree as described in Section 4.3.4. A GA finds the initial guess for the parameters that are then optimized by a gradient-based algorithm (Madsen and Hegelund, 1991).

   b) Sort the population according to the fitness.

   c) Create a new population

      i) In the *reproduction* stage kill a small percentage of the individuals with the worst fitness.

      ii) Calculate the *elite* according to input parameter P_e taken as 20%.

      iii) Fill up the population with the surviving trees according to binary tournament selection.

      iv) *S*elect a pair of individuals from the current population. The same tree can be selected more than once to become a parent. Recombine subtrees

using the *crossover* operation. Two new offsprings are inserted into the new population. Crossover takes place starting from the second node, not the root, to avoid duplication of trees.

v) With probability P_m taken as 0.01 in this thesis, *mutate* a randomly selected tree at a randomly selected node.

3) Check the termination criterion. If not satisfied, perform the next iteration.

4.4 Conclusion

The theory behind GAs and GP has been reviewed. They are a relatively new form of artificial intelligence based on the ideas of Darwinian evolution and genetics. They use a stochastic, directed and parallel search technique that makes them well suited for global optimization.

GP is a generalization of a GA with high-level symbolic representation. A common drawback of GP is the difficulty to handle constants. Therefore, in this thesis, the structure of the approximation function is evolved by the GP, while the tuning parameters are optimized using a combination of a GA and a gradient-based optimization method.

The definition of the fitness function has been modified from the standard least-squares to accommodate derivatives, if available.

Applications of this methodology are described in Chapters 5 and 6.

Interim results of this section have been reported in Toropov and Alvarez (1998a, 1998e, 1998f).